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Quasiparticle interactions in the infinite-U Anderson lattice: Effects of crystal electric fields of cubic symmetry

Trees, Bradley Russell, Ph.D.
The Ohio State University, 1993
Quasiparticle Interactions in the Infinite-U Anderson Lattice: Effects of Crystal Electric Fields of Cubic Symmetry

DISSERTATION

Presented in Partial Fulfillment of the Requirements for the Degree of Doctor of Philosophy in the Graduate School of the Ohio State University

by

Brad R. Trees, B.A., M.S.

The Ohio State University
1993

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Approved by
Advisor
Department of Physics
To My Family
ACKNOWLEDGEMENTS

Wenn man fast am Ziel ist, soll man nicht aufgeben.

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CHAPTER I

A Review of Heavy Fermion Systems (mostly CeCu$_2$Si$_2$):
Experiment and Theory

1.1 Introduction

This thesis is concerned with the effects of crystal electric fields on quasiparticle interactions in the Ce based heavy Fermion compounds. In general, the heavy Fermion materials are excellent examples of systems exhibiting strong correlations among the constituent particles [1] [2], [3], [4], [5], [6]. Generally, the compounds are comprised of intermetallics and rare-earth or actinide atoms (such as uranium or cerium) with a strong on-site Coulomb repulsion. This large electrostatic energy arises from the extremely localized nature of the 4f or 5f wavefunctions in the solid and markedly influences the electron occupation at these "rare-earth" sites. When hybridization between a rare-earth electron and a conduction electron is allowed, the physics of this strong interaction is communicated to the solid at large, giving rise to a metal of strongly correlated, interacting electrons. In such a system one might expect to find a ground stated manifesting collective properties of the coupled rare-earth and conduction elec-
Table 1.1:

Examples of Heavy Fermion Systems. $T_N$ represents the Neel temperature of an antiferromagnetic transition, and $T_c$ represents the temperature of a superconducting transition. A dash means no such transition has been seen.

<table>
<thead>
<tr>
<th>Compound</th>
<th>$T_c$ (K)</th>
<th>$T_N$ (K)</th>
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<tr>
<td>CeCu$_2$Si$_2$ (tetragonal)</td>
<td>0.7 [1]</td>
<td>–</td>
</tr>
<tr>
<td>UBe$_{13}$ (cubic)</td>
<td>0.87 [1]</td>
<td>–</td>
</tr>
<tr>
<td>UPt$_3$ (hexagonal)</td>
<td>0.48 [1]</td>
<td>5.0</td>
</tr>
<tr>
<td>URu$_2$Si$_2$ (hexagonal)</td>
<td>1.20 [1]</td>
<td>17.0</td>
</tr>
<tr>
<td>UNi$_2$Al$_3$ (hexagonal)</td>
<td>1.0 [8]</td>
<td>4.6</td>
</tr>
<tr>
<td>UPd$_2$Al$_3$ (hexagonal)</td>
<td>2.0 [9]</td>
<td>14.0</td>
</tr>
<tr>
<td>CeAl$_3$</td>
<td>–</td>
<td>1.6 [1]</td>
</tr>
<tr>
<td>U$<em>2$Zn$</em>{17}$</td>
<td>–</td>
<td>9.5 [1]</td>
</tr>
<tr>
<td>CeCu$_6$</td>
<td>–</td>
<td>–[1]</td>
</tr>
</tbody>
</table>

trons, e. g. superconductivity or magnetism. Indeed such ground states are seen. There are also heavy Fermion systems that apparently retain a metallic state down to zero temperature. See Table 1.1 for a partial listing of some more thoroughly studied compounds. Note that there are to-date six known heavy Fermion superconductors, all based on either cerium or uranium.

For this thesis, the material of greatest interest will be the superconductor CeCu$_2$Si$_2$, which undergoes the phase transition from a so-called normal metal to a superconductor at a critical temperature of about 0.6K ($T_c \approx 0.6$K) [7]. There
are a couple of reasons for this restriction to one compound: the local physics at
the Ce sites (which have a nominal 4f\textsuperscript{1} configuration above the closed shells of
Xe structure) are more easily studied than that of the U based materials (indeed,
for UBe\textsubscript{13} there is still strong debate as to whether the configuration is 5f\textsuperscript{3} or
5f\textsuperscript{2} on the U sites); and there are simply too many details and anomalies to
warrant a broad, sweeping theoretical attack on the heavy Fermion problem as
a whole. The author feels it is wiser at this stage to focus on a single system
and to model it as realistically as we are able. For these reasons we have focused
on CeCu\textsubscript{2}Si\textsubscript{2}, with its tetragonal unit cell. For completeness, let a represent
the in-plane dimension of the unit cell, and let c represent the out of plane
dimension. This thesis reports on our attempts to calculate effective electron
(or quasiparticle, more precisely) interactions in the presence of the crystalline
symmetry of CeCu\textsubscript{2}Si\textsubscript{2}. Such details have been neglected in earlier work. In
this manner, within the structure of a given model, we can attempt to quantify
the effects of the lattice symmetry on the particle interactions and perhaps also
gain insight into the microscopic cause of the superconductivity.

The vast amount of work, both theoretical and experimental performed in
the last fifteen years prevents us from discussing many interesting properties of
these compounds. We refer the reader to the referenced review articles [1],[2],[3],
[4],[5], [6] for a wealth of information. We shall attempt to narrow our vision as
much as possible to discuss some of the experimental properties of CeCu\textsubscript{2}Si\textsubscript{2} in
both the normal and superconducting states. As no true consensus exists among
the physicists working in this field about the microscopic cause of the pairing
in heavy Fermions, such data should guide us in determining which theory(ies)
have a chance of being correct. We thus begin by studying experimental results
in the normal state.

1.2 Experimental Behavior of CeCu$_2$Si$_2$.

The specific heat, $C_n$, of CeCu$_2$Si$_2$ in the normal state has proved an informative tool for studying the average low temperature electron interactions. For a small temperature range of $T_c < T < 1$ K one sees an approximate linear dependence of $C_n$ on $T$\cite{7}. From the inset of Figure 1.1, which is a plot of $C/T'$ vs. $T$, we see a flat region just above the superconducting transition. Within a simple Sommerfeld picture for the electron gas the coefficient of this linear term, $\gamma$, is about $1$ J/mole K$^2$ \cite{1},\cite{10},\cite{7}. (See Figure 1.1.) For copper, the linear coefficient of specific heat is $\gamma_{Cu} \approx 0.7 \times 10^{-3}$ J/mole K$^2$. As long as a Fermi liquid picture is valid, we know that $\gamma$ is proportional to an effective, or dressed, density of states $\hat{N}(E)$, which is in turn proportional to an effective mass, $m^*$, for the interacting quasiparticles. Within this interpretation, we can see that the effective quasiparticle mass in CeCu$_2$Si$_2$ is probably about two orders of magnitude larger than that of a typical metal. The name heavy Fermion now seems appropriate.

The low temperature static susceptibility, $\chi_o$, is also indicative of a Fermi liquid made of heavy Fermions, although there is some subtlety in the interpretation of the data\cite{11}. Apparently, there is often some type of magnetic dirt present in the samples but which is not quenched at low temperatures. Lieke and co-workers claim this dirt gives a Curie-Weiss contribution to the temperature dependence of the dc-susceptibility,

$$\chi(T) = \chi(0) + \frac{C_{dirt}}{T + \theta_{dirt}},$$

which contains all of the temperature dependence of $\chi_{dc}$ for temperatures $T \leq 6$ K. The value of the zero-temperature intercept, $\chi(0)$, is deduced by saturating
Figure 1.1:
Molar specific heat of CeCu$_2$Si$_2$ as a function of temperature T. The arrow marks the transition temperature $T_c = 0.51 \pm 0.04$ K. Inset shows in a $C/T$ vs. T plot the specific heat jump of two other samples. (from reference [7])
Figure 1.2:

dc-susceptibility of CeCu$_{2.2}$Si$_2$ polycrystals. The black triangles represent the raw data, and the open triangles represent the data after the subtraction of the impurity contribution. The inset is the temperature dependence of the Wilson ratio for CeCu$_{2.2}$Si$_2$ in zero-field (open triangle), and in B=4 T (open, inverted triangle); the full black circles are for CeCu$_2$Si$_2$. (Taken from reference [58].)

the magnetic dirt in a very strong external field and measuring the slope of the magnetization versus field plot. Then $\chi(0)$ is assumed to represent the constant Pauli susceptibility of a Fermi liquid. Lieke et al. claim that

$$\chi_{Pauli} = 0.08 \text{ emu/mole}$$ \hspace{1cm} (1.2)

is valid for $T_c \leq T \leq 6K$. Figure 1.2 shows the susceptibility for CeCu$_{2.2}$Si$_2$ as a function of temperature[70]. The open triangles represent the data with the contribution from the magnetic dirt subtracted off. Apparently, for CeCu$_{2.2}$Si$_2$, the Pauli susceptibility is temperature independent up to about 15 K.

In Fermi liquid theory we would predict that $\chi_o$ is proportional to the renormalized density of states evaluated at the Fermi energy, $N(0)$. Thus we are not surprised that the measured susceptibility is very large compared to that of a typical metal (for example, in copper $\chi_{oCu} \approx 10^{-6} \text{ emu/mole}$ [12]). This
Figure 1.3:

Susceptibility data for CeCu$_2$Si$_2$ (squares) and CeCu$_{1.9}$Si$_2$ (circles) polycrystals. Main part shows $\chi T$ vs $T$. Insert shows $\chi^{-1}$ vs $T$ to demonstrate the Curie-Weiss behavior. Hypothetical curves for free Ce$^{3+}$ ions are shown as dashed lines (Taken from reference [27]).

is consistent with the low temperature specific heat data and a strongly renormalized liquid of interacting electrons (quasiparticles). For temperatures greater than about 100 K, the susceptibility exhibits Curie-Weiss behavior as expected for free magnetic moments on the Ce sites. The effective magnetic moment is $\mu_{\text{eff}} \approx 2.62 \mu_B$ for Ce ions in free space[13], where $\mu_B$ is a fundamental unit of magnetic moment, the Bohr magneton. As is seen in Figure 1.3, the susceptibility is reduced significantly at low temperatures. Clearly, excitations of the Ce spins could be of importance in this material, and one has a motivation to look at neutron scattering studies.

In the language of the famous Kondo problem [15], which is widely believed to be applicable to heavy Fermions, CeCu$_2$Si$_2$ will have low energy spin excitations available as possible excited states. In the case of a single magnetic Ce ion in
a metal, the Ce spin and a conduction electron form a spin singlet. The energy difference between the spin singlet ground state and the excited triplet states defines the Kondo temperature, $T_K$. We assume there is an analogous excitation energy (called the lattice Kondo temperature, $T_o$) for the concentrated system. This spin fluctuation energy for the lattice will be quite small and will manifest itself as a broadening in the quasi-elastic peak measured by neutron scattering experiments. The linewidth, $\Gamma(T)$, of the quasi-elastic peak has been measured in CeCu$_2$Si$_2$ using low energy incident neutrons (The incident energy was about 3.5 meV.), and the corresponding spin fluctuation, or Kondo lattice, temperature is $T_o=\Gamma(T\to0)/2k_B \approx 10$ K [14], where $k_B$ is Boltzmann's constant. Finally, we remark that inelastic neutron scattering will see magnetic excitations of around 5 meV and higher. Such experiments have also been done for CeCu$_2$Si$_2$ [14] and have yielded important information about the crystal field splitting of the cerium 4f multiplet structure. We shall discuss these results in detail in Chapter 3.

The electrical resistivity also reveals something about the normal state of CeCu$_2$Si$_2$. It is a basic result of the Kondo effect that magnetic dirt in a metal, through spin flip scattering with the conduction electrons, raises the resistivity over that of the nominally pure metal [15]. Unlike the case for magnetic dirt, however, we know that a pure concentrated system would have zero resistivity in the limit of zero temperature. This is just Bloch's theorem [16] and is a manifestation of the (discrete) translational symmetry. At finite but low temperatures (low here means $T<<T_F$, the degeneracy temperature for the conduction electrons) it is well known that electron-electron interactions give rise to a $T^2$ contribution to the resistivity, with a coefficient, $A$, that depends on the effective mass $m^*$. Thus, the observance (See Figure 1.4.) of resistivity data in CeCu$_2$Si$_2$
Figure 1.4:
Resistivity $\rho(T)$ for a polycrystalline sample of CeCu$_2$Si$_2$. Dashed line is the extrapolation to $T=0$ assuming that $\rho_{\text{normal}}(T<1 \text{ K})=\rho_{\text{res}}+(10 \ \mu\Omega\text{cm}/\text{K}^2) \ T^2$, where $\rho_{\text{res}}$ is the low temperature, residual resistivity due to defects (Taken from reference [33].)

which can be fit by

$$\rho = \rho_{\text{res}} + AT^2$$

(1.3)

is further evidence for the validity of a Fermi liquid picture just above the superconducting transition [33]. The above equation is valid in the temperature range $T_c < T < 4 \ \text{K}$; $\rho_{\text{res}}$ is the left over resistivity due to temperature independent defect scattering, and $A \approx 10 \ \mu\Omega\text{cm}/\text{K}^2$. For a typical metal like Pd, the $T^2$ coefficient is $A_{\text{Pd}} \approx 2.5 \times 10^{-2} \mu\Omega\text{cm}/\text{K}^2$ [33]. This is yet another demonstration that the Fermi liquid is composed of heavy Fermions.

The last normal state measurement we shall discuss is that of the quasiparticle effective mass via de Haas-van Alphen (dHvA) techniques [18]. Sensitivity to the orientation of an applied magnetic field relative to the Fermi surface gives rise to oscillations in the magnetization, which can then be Fourier analyzed to yield information about: (i) the Fermi surface; (ii) electron effective masses; (iii) Fermi velocities; (iv) scattering rates; (v) and g factors [19]. Calculations
by Wasserman et al. [20] find the amplitude, $K$, of the measured dHvA signal should depend on the quasiparticle effective mass as

$$K \approx \left( \sinh \left[ a \left( \frac{m^*}{m} \right) \right] \right)^{-1},$$

(1.4) where

$$a = \frac{2\pi r^2 k_B T}{\hbar \omega_c}.$$  

(1.5)

In the above equation, $r$ is the radius of the orbit, and $\omega_c = eB/m_B$ is the cyclotron frequency, which depends on the applied field ($B$) and inversely on the mass of the band electrons. From equation 1.4, we see that the heavier the electron the weaker the corresponding dHvA oscillations and the more difficult the experiment becomes. The measurements of Hunt et al. [21] show effective masses of only about four or five times that of a free electron. Admittedly, this is not very compelling evidence for heavy electrons, but the authors believe it is a sign of truly heavy electrons. They claim, also, that there are not a large number of light electrons (with masses, $m^* \approx m_e$) at the Fermi surface, because these light electrons would produce a much larger signal than the "heavy" ones and would be impossible to miss. They attribute the lack of signs of effective masses like $m^* \approx 50 m_e$ to sample imperfections and the fact that heavy electrons, from equation 1.4, produce weak signals. The amplitude of the signal also depends inversely on the size of the external magnetic field. As Table 1.2 shows, very large fields were used; thus one might expect weak signals. It should be noted, however, that effective masses of the size of 90 times a free electron mass have been seen in UPt$_3$[69].

There was also not a significant variation in $m^*$ for the magnetic field along the a- or c-axis of the tetragonal unit cell. (See Table 1.2) Said differently, the effective mass appears to have near cubic symmetry. The tentative conclusions
Table 1.2:
Measured quasiparticle masses in CeCu$_2$Si$_2$ using the de Haas-van Alphen technique. Both frequencies and masses are averaged over the field range indicated. a and c refer to the tetragonal unit cell directions. (Taken from reference [21])

<table>
<thead>
<tr>
<th>Orientation</th>
<th>Field (T)</th>
<th>Frequency (T)</th>
<th>$m^*/m_e$</th>
</tr>
</thead>
<tbody>
<tr>
<td>a-axis</td>
<td>4.8-5.8</td>
<td>171 ± 2</td>
<td>4.62 ± 0.07</td>
</tr>
<tr>
<td></td>
<td>7.5-11.5</td>
<td>162 ± 2</td>
<td>5.15 ± 0.10</td>
</tr>
<tr>
<td>c-axis</td>
<td>9.5-11.5</td>
<td>295 ± 5</td>
<td>5.81 ± 10.05</td>
</tr>
</tbody>
</table>

from the dHvA data are thus: (i) there are heavy electrons in CeCu$_2$Si$_2$; (ii) the effective mass $m^*$ have approximate cubic symmetry; (iii) and there are no "light" electrons at the Fermi surface.

We now proceed to a study of experimental properties of the superconducting state.

1.2.1 Superconducting State ($T < T_c$)

The first heavy Fermion superconductor, CeCu$_2$Si$_2$, was discovered in the late 1970s [7]. The news was received, at first, with skepticism, most likely because of the confusion over the materials problems inherent to this compound [2],[22]. For example, stoichiometric single crystals do not superconduct at ambient pressure but will superconduct under a relatively small amount of pressure ($p > 1$ kbar) [23]. For polycrystalline CeCu$_2$Si$_2$, there is a spread in transition temperatures; samples with copper excess (e.g. CeCu$_{2.2}$Si$_2$) have the highest $T_c$, while even a small copper deficient effectively hinders pairing (e.g. CeCu$_{1.8}$Si$_2$ does not superconduct) [24],[25],[27]. Certainly copper stoichiometry plays an important role in the pairing, but exactly how is not understood. To be honest, it is not
clear how such effects can be included in our “standard model” for heavy Fermion systems, the Anderson model[26]; apparently, little thought has been given by theorists to such materials aspects. We shall also not be directly concerned with stoichiometry, but it was perhaps useful to remind the reader that such effects are present.

As first seen by Steglich and co-workers [7], the specific heat jump at $T_c$ is of the size of the corresponding normal state specific heat, $C_n(T_c)$ (See Figure 1.5.). Since $C_n(T_c)$ is large due to the heavy quasiparticles, this is a clear indication that the heavy quasiparticles take part in the pairing. The ratio of the specific heat jump to the normal state value at $T_c$ is of the order of unity, i.e. $\Delta C/C_n(T_c) \approx 1$. Note that the value predicted by the standard Bardeen, Cooper, Schrieffer (BCS) [28] theory of superconductivity is 1.43. It might indeed be coincidental that $\text{CeCu}_2\text{Si}_2$ has a relative specific jump of approximately the BCS value, for we will soon see that this material is decidedly unBCS-like in many of its properties. For example, at low temperatures ($T << T_c$), the BCS theory would predict an activated specific heat

$$C_s \approx e^{-\Delta/k_BT}, \quad (1.6)$$

where $\Delta$ is the famous isotropic energy gap [28]. The data in Figures 1.5 and 1.6 show no evidence of exponential behavior. Although both taken by the Steglich group, the data in these two figures are not the same. Figure 1.6 is plotted so as to extract an apparent $T^{2.8}$ temperature dependence well below $T_c$. They also claim that there is component of the data there is linear in $T$ below $T_c$, such that the best fit to the data follows the expression

$$C_s \approx \gamma_s T + \beta_s T^{2.8}[1]. \quad (1.7)$$
Figure 1.5:

a.) $C/T$ vs. $T$ for CeCu$_2$Si$_2$ showing the jump $\Delta C/T_c$ is approximately equal to $\gamma \approx 1.0$ J/mole K$^2$.  
b.) Upper critical field, $H_{c2}$ vs. $T$ for CeCu$_2$Si$_2$, showing the very steep slope at $T_c$. (Taken from reference [1])
Figure 1.6:
Plot of low-temperature specific heat: $C / T^{2.8}$ vs. $T$ for CeCu$_2$Si$_2$ and CeCu$_{2.2}$Si$_2$. The zero temperature intercept would give the coefficient of the $T^{2.8}$ term (Taken from reference [1]).

A cursory study of Figure 1.5 shows that $C_s \approx T^2$ below $T_c$, so we shall not put too much weight on the claimed $T^{2.8}$ dependence of the data.

It is well known that power law behavior in the specific heat (and other quantities) can result when the energy gap is an anisotropic function in momentum space, $\Delta(\vec{k})$. Besides depending on the nature of the quasiparticle interactions, the symmetry of the gap function also depends on the symmetry of the underlying crystal, as can be demonstrated by general group theoretic arguments. Thus, for a given lattice, one can calculate the possible gap functions and then the temperature dependence of such quantities as the specific heat, thermal conductivity, ultrasound attenuation, nuclear spin-lattice relaxation rate, and the Knight shift. The allowed gap symmetries for the various heavy Fermion superconductors have been calculated, under the realization that parity (P) and
time-reversal (T) are the only good quantum numbers in the presence of spin-orbit coupling [29], which on general grounds should be strong in such heavy materials. For odd parity ("triplet") pairing, the gap function can vanish only at distinct points on the Fermi surface; for even-parity ("singlet") pairing, $\Delta(\vec{k})$ can vanish at points and also along lines at the Fermi surface. Thus the momentum dependences of the various allowed gap functions, through the resulting power law behavior of measurable quantities, would leave tell-tale signs of their presence at low temperatures. In principle, it should be possible to deduce the symmetry of the gap function from the experimental data. Unfortunately, life is not so simple in the case of the heavy Fermions. For the specific heat, we expect a $T^3$ behavior for a gap function with point nodes and a $T^2$ behavior for a gap with line nodes on the Fermi surface (see Table 1.2). CeCu$_2$Si$_2$, however, exhibits neither power law behavior definitively.

It is possible that strong pair breaking could be the culprit here. It is well known that magnetic dirt in an isotropic superconductor will break the Cooper pairs and can lead, in the gapless regime, to a linear specific heat at low temperatures [30]. At present it is unclear what we can deduce from these data. Let us look to other experiments for guidance.

The upper critical field, $H_{c2}$, is the highest field, at a given temperature, in which a superconducting region can nucleate in a given material. Figure 1.5(b) plots $H_{c2}$ as a function of temperature. Of interest, at first, is the steep slope near $T_c$, where we define

$$H'_{c2}(T_c) = -\left(\frac{dH_{c2}}{dT}\right)_{T_c}.$$  \hspace{1cm} (1.8)

In CeCu$_2$Si$_2$ experiments give $H'_{c2} \approx 23$ T/K [24],[31], for magnetic fields along the a and c axes of a single crystal. For comparison, in the A15 superconductor
Table 1.3:
Possible power law behaviors in the superconducting state based on an anisotropic gap function, \( \Delta(\vec{k}) \) that has either point or line nodes. Also given is the actual experimental results for CeCu_2Si_2.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>point-node</th>
<th>line-node</th>
<th>CeCu_2Si_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specific heat, C</td>
<td>( T^3 )</td>
<td>( T^2 )</td>
<td>( \gamma_s T + \alpha_s T^{2.8} ) [1]</td>
</tr>
<tr>
<td>Thermal cond., ( \kappa )</td>
<td>( T^3 )</td>
<td>( T^2 )</td>
<td>( \lambda_s T + \beta_s T^2 ) [1]</td>
</tr>
<tr>
<td>( 1/T_1 )</td>
<td>( T^3 )</td>
<td>( T^2 )</td>
<td>( \approx T^3 ) [1]</td>
</tr>
<tr>
<td>Knight Shift, K</td>
<td>( T )</td>
<td>not clear</td>
<td>[39]</td>
</tr>
</tbody>
</table>

\( \text{Nb}_3\text{Sn} \ H'_{c2} \approx 0.2 \, \text{T/K} \) [34], which is considerably smaller. From the linearized Ginzburg-Landau equations near \( T_c \), we know that the upper critical field depends on the correlation length, \( \xi \) (which is basically the real-space size of a Cooper pair) as:

\[
H_{c2} = \frac{\Phi_0}{2\pi \xi^2(T)},
\]

where \( \Phi_0 = \hbar c/2e \) is the flux quantum [32]. Thus \( H'_{c2} \) will also depend inversely on the correlation length. We can think generally of the correlation length as being inversely proportional to an effective mass, \( m^* \), which then gives \( H'_{c2} \approx m^* \). So we expect an abnormally large value for \( H'_{c2} \) in CeCu_2Si_2 if the heavy quasiparticles are indeed participating in the pairing. This appears to be the case, and so the result is at least qualitatively consistent with the existence of a large specific heat jump at \( T_c \).

Rauchschwalbe and colleagues have interpreted the slope of the upper critical field [33] in CeCu_2Si_2 in terms of BCS theory renormalized to include strong electron-phonon coupling. Their analysis is built upon earlier work, done in the
late 70s, by Orland et al. in a study of A15 compounds [34]. Rauchschwalbe claims this fit to an extended BCS theory (in the clean limit) is consistent with other measured quantities in CeCu$_2$Si$_2$ such as: effective mass, Fermi velocity, BCS coherence length, and London penetration depth. It is, however, uncertain how much weight should be placed upon the shoulders of BCS. We remark here that phonon-based pairing is suspect, at least intuitively, because the effective electronic degeneracy temperature ($T_\theta$, the Kondo lattice temperature $\approx 10$ K) is much smaller than the Debye temperature, which is of the order of 200 K. We can, however, still take the large value of $H'_{c2}(T_c)$ as further evidence of heavy electron pairing in CeCu$_2$Si$_2$. Next, we turn to the low temperature behavior of the upper critical field.

The study of $H_{c2}(T)$ at low temperatures was initiated by Steglich's group in Germany [27],[35],[33]. They were the first to suggest the existence of strong Pauli limiting in CeCu$_2$Si$_2$, which we shall now discuss. The coupling of strong magnetic fields to the electron spins can have a detrimental effect on superconductivity. Such an influence was first suggested by Clogston [36] and separately by Chandrasekhar [37]. At a simple level, the physics is as follows. As long as the total energy of the superconducting state is lower than the total energy of the normal state at the same temperature, the superconductivity will win out. Thus the energy difference between the two states is crucial. We know that in the presence of an external magnetic field there will be an energy due to the coupling of the field with the electron spins. Let us define an energy difference

$$E_{\text{spin}} = \frac{1}{2} \left( \chi_n^{\text{spin}} - \chi_s^{\text{spin}} \right) H^2,$$

(1.10)

where $\chi_n^{\text{spin}}$ are the spin susceptibilities in the normal and superconducting states respectively, and where $H$ is the magnitude of the applied magnetic field. This
number quantifies how differently the spins behave in the normal and superconducting states in the presence of the field.

In a BCS singlet superconductor two conduction electrons of opposite spin bind energetically into pairs, leading to an exponentially small spin susceptibility at low temperatures \( T \to 0 \). In this case, \( E_{\text{spin}} = \frac{1}{2} \chi_{n}^{\text{spin}} H^2 \), and if \( H \) becomes large enough such that \( E_{\text{spin}} \) equals the superconducting condensate energy, then the system has to return to the normal state. That is, when

\[
\frac{1}{2} \chi_{n}^{\text{spin}} H^2 = \frac{1}{2} N(0) \Delta^2(0),
\]

the superconductor is driven normal \( (N(0) \) is the density of states at the Fermi level and \( \Delta(0) \) is the BCS energy gap for \( T \to 0 \)). For a typical normal metal \( \chi_{n}^{\text{spin}} \) is just the Pauli susceptibility and equals \( 2\mu_B^2 N(0) \). Thus we have an effective upper limit for the applied field at low temperatures, or said differently, we have a limit for the upper critical field:

\[
H_{c2}^{\text{max}}(T \to 0) = \frac{\Delta(0)}{\sqrt{2}\mu_B} = \left( 1.84 \frac{T}{K} \right) T_c
\]

for a BCS superconductor. This is the physics of Pauli limiting.

Next consider a simple triplet superconductor, in which electrons are paired so as to have a net spin 1. It would certainly be possible to spin polarize such pairs in an external magnetic field. Thus at temperatures well below \( T_c \) we expect to find a finite spin susceptibility. At the simplest level, we assume that the spin susceptibilities are the same in the superconducting and normal states \( (\chi_{n}^{\text{spin}} = \chi_{s}^{\text{spin}}) \), in which case \( E_{\text{spin}} = 0 \) and there is no Pauli limiting at all. More generally, it should at least be true that \( \chi_{s}^{\text{spin}}(\text{singlet}) < \chi_{s}^{\text{spin}}(\text{triplet}) \), implying that Pauli limiting will play a more important role in singlet than in triplet superconductors.
Steglich et al. [27], [35] have attempted to fit their low temperature CeCu$_2$Si$_2$ data for $H_{c2}(T)$ in two different ways: with and without Pauli limiting (See Figure 1.7.). They used seven different pairing states, the first six of which did not include the effects of Pauli limiting. The seventh state, which appears to fit the data acceptably, is based on an s-wave pairing state with Pauli limiting and spin-orbit scattering. We do not take this as evidence that simple s-wave pairing occurs in CeCu$_2$Si$_2$, but the striking difference between the first six curves and the seventh of Figure 1.7 certainly implies the existence of strong Pauli limiting in this material. Furthermore, from our simplistic discussion of Pauli limiting, this could also be evidence for singlet as opposed to triplet pairing.

The previous statement is not hard and fast. In the presence of spin-orbit coupling, it is possible to have a triplet state exhibit some Pauli limiting [29]. Thus we can only say that the clear difference between curves one through six and curve seven in figure 1.7 is strongly suggestive of singlet (or even-parity, more precisely) pairing in CeCu$_2$Si$_2$. It is worth noting here that the heavy Fermion superconductor UPt$_3$ behaves markedly differently from CeCu$_2$Si$_2$ in this regard. One can fit the low temperature $H_{c2}$ data in UPt$_3$ with a dirty, p-wave (triplet) state that requires very little Pauli limiting [33]! Clearly, not all heavy Fermion superconductors act alike.

There is one more aspect of the upper critical field data that is useful to discuss. Surprisingly, for CeCu$_2$Si$_2$, which has a tetragonal unit cell, there is very little anisotropy in the upper critical field slope at $T_c$ [33]. That is,

$$\frac{H'_{c2}(\vec{H} \parallel \hat{c})}{H'_{c2}(\vec{H} \perp \hat{c})} \leq 0.05. \tag{1.13}$$

It was shown by Tilly and co-workers [38] that any anisotropy in $H'_{c2}$ due to an
Figure 1.7:
The scaled upper critical field vs. $T/T_c$ for CeCu$_{2.6}$Si$_2$. The first six curves are for the following pairing states: (1) a triplet superconductor (in the so-called polar state) (2) a conventional, clean superconductor with no Pauli limiting (3) a triplet superconductor (in the so-called SK state) (4) a conventional, dirty superconductor with no Pauli limiting (5) a triplet superconductor (in the ABM state) (6) a polar state with strong pair-breaking (7) a conventional s-wave state with strong Pauli limiting. They used a Wilson ratio of 0.8, which is accurate for CeCu$_2$Si$_2$ (Taken from reference [35]).
anisotropic Fermi surface should obey the relation:

\[
\frac{H'_{c2}(\vec{H} \parallel \hat{c})}{H'_{c2}(\vec{H} \perp \hat{c})} = \sqrt{\frac{m^*(\vec{H} \parallel \hat{c})}{m^*(\vec{H} \perp \hat{c})}}.
\] (1.14)

The effective mass in CeCu\textsubscript{2}Si\textsubscript{2} thus has cubic symmetry, which leads us to conjecture that the Fermi surface should also be approximately of cubic symmetry. We shall discuss this point again in the next chapter as we set up the calculations performed in this thesis work. Certainly, the upper critical field has proved a useful tool for studying the superconducting state.

Let us turn now to the thermal conductivity of CeCu\textsubscript{2}Si\textsubscript{2} (See figure 1.8.). Again, there is no clear dominating power law behavior below T\textsubscript{c}. There is, for T < 0.2 K, a combination of a linear and a quadratic term

\[
\kappa_s = \lambda_s T + \beta_s T^2,
\] (1.15)

where the existence of the linear term is inferred from the non-zero intercept in the plot of \(\kappa/T\) versus T. Steglich et al. [27] interpret the linear term as a remnant of the normal state, coming from light quasiparticles that have not undergone pairing. It is not clear, however, that this is corroborated by the dHvA measurements [21], which find no signs of light electrons at the Fermi surface. Thus we have another example where power law behavior does not lead to a simple interpretation of the nature of the pairing.

Next, we shall discuss the nuclear spin-lattice relaxation rate (1/T\textsubscript{1}) of the \textsuperscript{63}Cu nuclei in CeCu\textsubscript{2}Si\textsubscript{2} below T\textsubscript{c} (See figure 1.9.) [39]. First, notice the absence of the famous Hebel-Slichter peak [40] just below T\textsubscript{c}. This peak is due to the piling up of the density of states as the superconducting state is formed, and there are two well known cases when no such peak is expected: when there is strong pair-breaking in the presence of s-wave pairing, or an anisotropic gap
Figure 1.8:
Plot of thermal conductivity, $\kappa$, vs. $T$ for CeCu$_2$Si$_2$. The straight line shows the region of $T^2$ behavior, and the intercept, approximately 0.3 mW/cmK$^2$, gives the coefficient of a term linear in temperature (Taken from reference [1]).
Figure 1.9:

$^{63}$Cu nuclear spin-lattice relaxation rate, $1/T_1$, vs. $T$ for CeCu$_2$Si$_2$ in an external magnetic field of 0.572 Tesla. Note the absence of a Hebel-Slichter peak just below $T_c$ a region of $T^3$ dependence (Taken from reference [1]).

The Knight shift has also been measured for the $^{29}$Si and $^{63}$Cu nuclei in CeCu$_2$Si$_2$ [39] (See figure 1.10.). In general, the Knight shift measures the static spin susceptibility at a given nucleus. It can be written $K = A_{hf} \chi^{spin}$, where $A_{hf}$ is a so-called hyperfine coupling constant. The relatively rapid decline of the spin susceptibility below $T_c$ is further evidence for even-parity pairing. That

\[ \Delta(\vec{k}) \text{ that vanishes at special points or lines on the Fermi surface. The data show a } T^3 \text{ dependence to } 1/T_1 \text{ for about one decade of temperature below } T_c. \text{ This is consistent with an anisotropic gap function that vanishes along a line on the Fermi surface, and it is also consistent with even-parity ("singlet") pairing.} \]
Figure 1.10:

$^{29}\text{Si}$ and $^{63}\text{Cu}$ Knight shifts for a magnetic field perpendicular to the $\hat{c}$ direction in CeCu$_2$Si$_2$. Note the drop-off as the temperature is lowered below $T_c$ (Taken from reference [39]).

is, because of the antiparallel spin pairing, $\chi^{\text{spin}}$ is expected to have a stronger temperature dependence in an even-parity state than in an odd-parity state. This data is also consistent with the guess of even-parity pairing as deduced from the presence of strong Pauli limiting in the upper critical field.

One could search for power law behavior in the Knight shift, but it is not clear from figure 1.10 that such behavior exists. It is, however, worthwhile noting that a linear temperature dependence to the Knight shift would be consistent with the $T^3$ data measured in $1/T_1$. 
1.2.2 Conclusions for Experimental Section

In the normal state CeCu$_2$Si$_2$ behaves as a Fermi liquid with heavy quasiparticles as evidenced by:

1.) an approximate linear temperature dependence of the specific heat ($C=\gamma T$) with a huge coefficient $\gamma \approx 1$ J/mole K$^2$, implying a quasiparticle effective mass $m^*$ at least two orders of magnitude larger than that of a free electron.

2.) a nearly temperature independent (Pauli) susceptibility that is also abnormally large and proportional to the conduction electron effective mass.

3.) a $T^2$ contribution to the resistivity with a coefficient that is also related to $m^*$.

4.) dHvA measurements of effective mass at the Fermi surface see heavy quasiparticles; apparently, there is no evidence of more typical, “light” quasiparticles.

In the superconducting state it is more difficult to piece together a unified picture from the many experimental results. We know that the heavy quasiparticles participate in the pairing because:

1.) the specific heat jump at $T_c$ is comparable to the normal state value.

2.) the slope of the upper critical field is very large $H'_{c2} \approx 23$ T/K.

It is impossible to make draw detailed conclusions about the nature of the superconductivity based on the various power law dependences measured. We can say that:

1.) there is no simple activated (BCS-like) behavior for $T << T_c$.

2.) The nuclear spin-lattice relaxation rate shows the clearest evidence for an anisotropic gap function, $\Delta(\vec{k})$, that vanishes along a line at the Fermi surface. There also is evidence that CeCu$_2$Si$_2$ is an even-parity superconductor:
1.) the strong Pauli limiting as seen in the low temperature dependence of \( H_{c2} \).

2.) the relatively strong temperature dependence of the Knight shift below \( T_c \). Finally, the apparent (near) isotropy of the upper critical field slope at \( T_c \) points to an effective mass tensor for the heavy quasiparticles that has cubic as opposed to tetragonal symmetry. This is corroborated by dHvA measurements in the normal state.

It is helpful to retain these facts as we turn now to the review of theoretical work, of which there has been a staggering amount, in this field. It seems prudent to keep the above conclusions handy, to serve as a guide as we work through this thesis.

1.3 Theoretical Studies of Superconductivity in Heavy Fermion Systems

1.3.1 Introduction

It is a tall order for theorists to explain at a microscopic level the cause and nature of the superconductivity in heavy Fermion materials. As we have seen, the experimental data do not offer concrete help but rather only give useful hints as to what the leading interactions are. That these systems are superconducting at all is surprising, and we are lead to the following observations:

1.) The coexistence of magnetism and superconductivity must be understood at a basic level. The same 4f electrons in CeCu_2Si_2 that behave as independent local moments at high temperatures, are screened by the conduction electrons at about 10 K and finally undergo some form of Cooper pairing at about 0.6 K. It is incumbent upon us to explain how magnetism and superconductivity, conventionally viewed as antagonistic to each other, can be so closely connected and arise from the same electronic reservoir.
2.) In a similar vein, we know that Ce impurities in an otherwise pristine superconductor are strongly pair-breaking. How is it that a lattice of Ce ions in CeCu$_2$Si$_2$ becomes the foundation for the pairing (e.g. LaCu$_2$Si$_2$ is not a superconductor)?

3.) The electronic degeneracy temperature for heavy Fermions is basically set by the lattice version of the Kondo temperature ($T_o$) as taken, for example, from the linewidth of the quasi-elastic neutron scattering peak. Conventional phonon-mediated pairing seems unlikely simply because the Debye temperature (typically about 200 K) is much larger than the Kondo temperature.

4.) Power laws in measurable quantities, although not completely consistent with each other, point to the likelihood of some sort of anisotropic pairing with a gap function $\Delta(\vec{k})$ that has zeroes on the Fermi surface.

Although the major portion of these observations remain unexplained, they led us to postulate at a broad level the existence of non-phononic, anisotropic superconductivity in the heavy Fermions. Many theorists have, of course, contributed to this body of knowledge since the late 1970s, when CeCu$_2$Si$_2$ was discovered [7]. We cannot hope to study in depth all the previous work in this field. The remainder of this chapter, therefore, will be limited to reviewing briefly some ideas that have been put forward as possible sources of pairing.

1.3.2 Phonon-based pairing

This is not the conventional phonon mediated pairing we are accustomed to thinking about in the case of aluminum. Intuitively, as we just discussed, the low Kondo temperature should render the lattice vibrations too weak to assist in pairing. There is a proposal, however, that it is still possible to have a
superconducting glue with the deformation of the lattice that is strong enough to do the job. Such an idea rests heavily on the so-called Kondo volume collapse.

Allen and Martin studied the physics of the Kondo volume collapse for their description of the $\gamma \rightarrow \alpha$ structural phase transition in cerium metal [41]. They began with the well known dependence of the Kondo temperature on the unit cell volume [42] and the knowledge that the unit cell shrinks by roughly 15% during the phase transition. They could calculate a phase diagram for Ce with the Anderson model as a starting point that gave good agreement between calculated and measured unit cell volumes in the two phases. The physics of the Kondo effect seemed to be driving the transition.

Razafimandimby, Fulde, and Keller (RFK) [43] were the first to suggest this physics as giving rise to superconductivity. They worked within a phenomenological Fermi liquid picture based on phase shifts of the conduction electrons due to scattering off of a Ce impurity (as first discussed by Nozieres [44]). For energies, $\epsilon$, near the Fermi surface this phase shift is

$$\delta(\epsilon) \approx \frac{\pi}{2} + \frac{1}{T_K} (\epsilon - \mu),$$

(1.16)

where $\mu$ is the chemical potential and $T_K$ is the Kondo temperature.

RFK, thinking specifically of CeCu$_2$Si$_2$, then performed a KKR band structure calculation [45], in which the phase shifts for conduction electron scattering off of Ce electrons were forced to have the form given by equation 1.16. Next they introduced a type of electron-phonon coupling whose source lies in the fact that the hybridization between conduction and Ce 4f electrons can couple to the so-called unit cell “breathing mode” (i. e. the physics of the Kondo volume collapse). The strength of this coupling depends on $dT_K/d\Omega$, where $\Omega$ is the unit cell volume. The value of this derivative is roughly known for CeCu$_2$Si$_2$.
and so RFK find

\[ \frac{dT_K}{d\Omega} \approx -\frac{T_K}{\Omega}, \]  

(1.17)

with \( \eta \approx 80 \). Clearly it is the large value of this parameter \( \eta \) that saves this model from oblivion, otherwise the coupling strength would be very small (i.e. \( \approx T_K \)). RFK then have an s-wave pairing instability.

Others have pushed harder on this particular problem. Both Grewe [46] and Jichu and co-workers [47] thought to put this idea on a firmer microscopic foundation. Grewe used a perturbative scheme for the Anderson lattice, which is an extension of the single-impurity Anderson model to a lattice of "impurities". This scheme assumes an infinite Coulomb repulsion for two electrons an an impurity site. Grewe's results did not appear to differ in a substantial way from those of RFK.

Jichu et al [47] also started with the Anderson lattice, but they retained a finite Coulomb repulsion for two electrons on the same impurity. For the full details of the calculation, the interested reader is referred to the paper. Briefly, they calculated the electron-electron scattering amplitude (See figure 1.11.) \( \Gamma_{ij} \) for one electron at site \( i \) and the other at site \( j \) by summing ladder diagrams built out of the single site scattering amplitude \( \Gamma_i \). Including the phonon mediated electronic interaction, they find an effective coupling between electrons at sites \( i \) and \( j \)

\[ V_{ij} \approx -\frac{\eta^2}{T_F} (\epsilon - \mu)^2, \]  

(1.18)

where they used \( \eta^2 \approx 10^3 \) and \( T_F \approx 10^4 \) K. Notice that \( V_{ij} \) vanishes quadratically as the energy approaches the Fermi surface. This was not seen by RFK or Grewe and says the interaction must by dynamical to lead to pairing. As \( \epsilon \) gets arbitrarily close to the Fermi surface, the coupling becomes arbitrarily weak.
This could represent a limitation for the model, although it is not clear at present how it can be utterly ruled out.

Phonon-mediated pairing would probably require strong pair-breaking to have a chance at explaining heavy Fermion superconductivity. The work we have just discussed would yield isotropic s-wave pairing, which does not agree with experiment. With the addition of pair-breaking, however, the theory can not be utterly dismissed. Recall that the microscopic underpinning of this theory is that of the Anderson lattice plus an electron-phonon coupling added by hand that arises from the dependence of the Kondo temperature on the unit cell volume. It is perhaps more theoretically pleasing to study in detail just the Anderson lattice itself before adding other interactions to complicate the problem. Just such a philosophy underlies this thesis, as shall be seen in the next chapter.
1.3.3 Non-phonon mediated pairing

A great deal of theory has been done in an attempt to attribute heavy Fermion superconductivity to the exchange of spin fluctuations. Most of this work, however, has focused on UPt$_3$ because of the following experimental facts:

1.) Neutron scattering has measured antiferromagnetic correlations with energy around 5 meV ($\approx 50$ K) between adjacent planes of uranium atoms. These correlations become measurable at the temperature at which the bulk magnetic susceptibility has a maximum [48].

2.) There is a contribution to the normal state specific heat that goes as $T^3\ln T$, which is consistent with the presence of spin fluctuations in a Fermi liquid near a magnetic instability [49],[50].

Our discussion here shall not pick out UPt$_3$ specifically but will try to focus on general physical principles that could be useful throughout this thesis. We have discussed, in the previous section, why phonon-mediated pairing seems, on energetic grounds, unlikely in these systems. Interest in forms of electron-mediated pairing, however, has been high.

Anderson[51], Valls and Tešanović[58], and Varma[57] were among the first to argue for an analogy between heavy Fermions and liquid $^3$He. These ideas build upon the earlier work of Berk and Schrieffer[59], in which we learn that strong local Coulomb interactions between two electrons, giving rise to ferromagnetic correlations, can suppress even-parity (s-wave) pairing. Anderson and Brinkman[60] later showed that the same physics favored odd-parity (p-wave) pairing. This is not surprising, since odd-parity pair wavefunctions must have a node at the origin and thereby avoid the strong Coulomb repulsion. Anderson and Brinkman were thinking specifically of superfluid $^3$He, which shows signs of
Figure 1.12:

(a) Contributions to the particle-hole t matrix from a localized Coulomb interaction. The solid lines represent quasiparticle propagators, and the dashed line is the momentum-independent Coulomb repulsion, $U$. (b) Same as part (a) but with the dashed Coulomb interaction shrunk to a point. This reveals the susceptibility nature of the internal quasiparticle lines.

having an enhanced ferromagnetic spin correlations[68], and thus was a prime candidate for a $p$-wave superconductor.

Berk and Schrieffer[59] showed how to include the strong Coulomb interaction between quasiparticles of opposite spins. One must calculate the diagram shown in Figure 1.12, in which a solid line represents a quasiparticle of a specified momentum, and the dashed line represents the momentum-independent Coulomb repulsion. There is no such contribution between quasiparticles of the same spin, since the Pauli principle forbids them from being on the same lattice site. In systems with a large susceptibility and a large electron-phonon interaction, such as Pd[59], evidently there is a competition in the spin-singlet channel between the attractive electron-phonon interaction and the repulsive spin-induced interaction. The general belief is that, whichever of the two effects is more pronounced,
In $^3$He, and also in heavy Fermion systems, we do not worry about the electron-phonon coupling. For heavy Fermions, we thus need to ask: what are the important quasiparticle interactions, and what are the important diagrams to sum to get a superconducting instability? In terms of the language of Feynman diagrams, we put the question as follows: what is the appropriate quasiparticle scattering amplitude, $\Gamma(\vec{k}, \vec{k}')$, to describe the quasiparticle interactions? (See Figure 1.13(a).) Given $\Gamma(\vec{k}, \vec{k}')$ in the spin-singlet or spin-triplet channels, we can then construct the dressed scattering amplitude, $\overline{\Gamma}(\vec{k}, \vec{k}')$ (See Figure 1.13(b).) and ask if $\overline{\Gamma}$ diverges as a function of model parameters. Such a divergence would signal a superconducting instability.
Miyake, Schmitt-Rink, and Varma[61], MSV, shed some light on the subject by studying a phenomenological exchange interaction of the form
\[ H_{ex} = \frac{1}{2} \sum_{k,k',q} J(\tilde{k} - \tilde{k}') (\sigma_{\alpha\beta} \cdot \sigma_{\gamma\delta}) c_{k+\frac{q}{2},\gamma}^\dagger c_{-\tilde{k}+\frac{q}{2},\gamma}^\dagger c_{-\tilde{k}+\frac{q}{2},\alpha} c_{k+\frac{q}{2},\beta}, \quad (1.19) \]

where \( c_{k,\alpha} \) destroys a quasiparticle of momentum \( \tilde{k} \) and spin \( \alpha \). \( \sigma_{\alpha\beta} \) is a vector composed of Pauli matrices. MSV considered both ferromagnetic and antiferromagnetic spin correlations. In the case of ferromagnetic correlations, the exchange strength, \( J \), is peaked at zero momentum, while for antiferromagnetic correlations, \( J \) is peaked at a finite momentum, say \( \tilde{Q}_{AFM} \). In the approximation of weak-coupling, in which the superconducting transition temperature, \( T_c \), is much smaller than the quasiparticle degeneracy temperature, \( T_F \), MSV averaged the exchange interaction over a spherical Fermi surface. They also projected the interaction onto states of spherical symmetry, in this case Legendre polynomials, \( P_l(x) \), where \( x = \cos\theta \) (\( \theta \) is the polar angle of spherical coordinates.). The averaged interaction in the \( l^{th} \) channel is
\[ \Gamma_l = \left( \frac{3}{-2} \right) 2 \int_0^1 dx x P_l(1 - 2x^2) [-J(2k_F x)], \quad (1.20) \]

where the momentum dependence of the exchange interaction is presented in Figure 1.14, and where the "3" corresponds to even-parity (spin-singlet) pairing, and the "-1" corresponds to odd-parity (spin-triplet) pairing. An s-wave pairing instability requires \( \Gamma_{l=0} \) be negative, for only in that case can the dressed scattering amplitude, \( \Gamma_{l=0} \), diverge as a finite temperature, \( T_c \). The case of \( l = 1 \) corresponds to a p-wave instability, and \( l = 2 \) to a d-wave instability. With this phenomenological form for the exchange, MSV were able to show the following:

(1) In the case of ferromagnetic exchange, \( \Gamma_0 > 0 \) and \( \Gamma_1 < 0 \); that is, s-wave
Figure 1.14:
An effective exchange interaction $J(q)$ as a function of $q$ for ferromagnetic (1) and antiferromagnetic (2) spin fluctuations. Taken from reference [61].

Pairing is suppressed, and $p$-wave pairing is favored. This is in agreement with the results of Berk and Schrieffer[59] and Anderson and Brinkman[60]. (2) In the case of antiferromagnetic exchange, both $\Gamma_0 > 0$ and $\Gamma_1 > 0$. Both $s$- and $p$-wave pairing is suppressed. The values of $\Gamma_1$ for $l \geq 2$, depend on the specific functional form of $J(\vec{k}' - \vec{k})$, but if $\Gamma_2 < 0$, than a $d$-wave pairing instability would be possible. It is clear, in general, that ferromagnetic and antiferromagnetic spin correlations behave differently when it comes to mediating interactions between two quasiparticles in a state of odd parity. Since we have argued in this chapter that experimental evidence in CeCu$_2$Si$_2$ points to pairing states of even pairing, we would not expect antiferromagnetic spin correlations to yield odd-parity pairing. Similar general conclusions were attained by Matsuura et al.[62], by Béal-Monod, Bourbonnais, and Emery[63], and by Hirsch[64].

All this work does not, of course, prove that spin fluctuations are the true source of superconductivity in heavy Fermions. That is a much more fundamen-
tal and important question. For the remainder of this chapter, we shall discuss some of the calculations done in an attempt to understand the microscopic source of the pairing.

We can characterize the different calculations we wish to discuss by their bare scattering amplitudes, $\Gamma(\vec{k}, \vec{k}')$. For example, Scalapino, Loh, and Hirsch[55], [56], SLH, studied spin fluctuations due to a strong, local Coulomb repulsion between the quasiparticles of opposite spin. (See Figure 1.15.) Their work is based upon that of Berk and Schrieffer[59] and Anderson and Brinkman[60], but their contribution was to include the dependence of $\Gamma$ on the chemical potential, $\mu$, in a three-dimensional, cubic tight-binding band, $\epsilon_\mathbf{k} = -2t(cosk_x + cosk_y + cosk_z) - \mu$. In the dispersion relation, $t$ is the average kinetic energy of the quasiparticles.

Note that in the spin singlet channel, there are two possible diagrams. The first diagram in Figure 1.15 is just Coulomb scattering between two quasiparticles of opposite spin and represents a contribution to the particle-hole $t$ matrix. The third diagram in Figure 1.15 represents a screening of the Coulomb interaction through particle-hole excitations. In the triplet channel, the only possible diagram is that due to screening, since there can be no direct Coulomb scattering between quasiparticles of the same spin.

SLH discover that for $-0.8eV \leq \mu < 0$ eV, which is small compared to the bandwidth of 12 eV, there is a strong superconducting instability of $d_{x^2-y^2}$ symmetry. They also found that pairing states of $(d_{xy}, d_{xz}, d_{yz})$ and p-wave symmetries are suppressed. Note also that the small chemical potential is close to the value $\mu=0$, which corresponds to a perfectly nested Fermi surface and an antiferromagnet instability of wavevector $\vec{Q}_{AFM} = (\pi/a, \pi/a, \pi/a)$. Thus, near
Figure 1.15:

Quasiparticle scattering amplitude in both the spin singlet and spin triplet channels. All interactions are due to a momentum-independent Coulomb repulsion, \( U \), between quasiparticles of opposite spin. Note that in the triplet channel, the only possibility is to have particle-hole excitations screen the Coulomb interaction. There can not be a direct Coulomb scattering between quasiparticles of the same spin.
an antiferromagnetic instability, they predict anisotropic d-wave pairing.

Finally, we consider a series of related calculations. The first of these is due to Lavagna, Millis, and (Patrick) Lee[65], LML. They calculated the bare scattering amplitude depicted in Figure 1.16(a). As usual, the solid lines represent quasiparticle Green functions, but the wavy line is an exchanged Boson that causes the quasiparticles to scatter. The basic physics behind this exchanged Boson is as follows. Unlike the calculation of Scalapino, Loh, and Hirsch, Lavagna, Millis, and Lee used a microscopic model with (effectively) two species of electrons: a set of delocalized (or conduction) electrons, and a lattice of strongly correlated, localized electrons that experience a large Coulomb repulsion when there are two electrons on the same site. When these two systems are allowed to mix, the resultant quasiparticles are a linear combination, or hybrid, of the two species. The Boson exchanged in Figure 1.16 represents a density fluctuation of these hybrid particles in the presence of the strong Coulomb repulsion. There is no spin nature to this exchanged Boson, since it behaves identically in the spin-singlet and spin-triplet cases (unlike the Coulomb repulsion in the SHL calculation). The symbol $\gamma$ in the figure, represents an isotropic function describing the strength of the coupling of the Boson to the quasiparticles.

One may ask why only the diagram in Figure 1.16(a) was included in the calculation. As we shall see in the next chapters, the Boson propagator in this formalism are generally quite small in magnitude. Thus diagram 1.16(b), with two exchanged Bosons, will on average have a small contribution to $\Gamma(\vec{k}, \vec{k}')$ than diagram (a). In fact, for CeCu$_2$Si$_2$, diagram (b) should contribute about 1/6 as much as diagram (a). So, as a first pass, LML included only the contribution from diagram (a). They discovered that such a model has a d-wave, spin-singlet
(a) Quasiparticle scattering amplitude for quasiparticles of opposite spin. The wavy line is an exchanged Boson, carrying momentum $k' - k$ and representing a density fluctuation of the coupled electron systems that comprise the quasiparticles. $\gamma$—note the lower case here—is an isotropic vertex representing the coupling strength between Bosons and quasiparticles. (b) Second order (in the exchanged Boson) contribution to the bare scattering amplitude. This diagram was not included by LML since it is generally smaller than the contribution from the diagram in part (a). For CeCu$_2$Si$_2$, (b) is 1/6 the size of (a). This diagram was included in the by Houghton, Read, and Won [67].
Figure 1.17:
F. C. Zhang’s and T. K. Lee’s bare scattering amplitude, with anisotropic vertices, $\gamma(\vec{k}, \vec{k'})$, for quasiparticles of opposite spin.

Next, F. C. Zhang and T. K. Lee[66] included spin-orbit coupling in the mixed electron systems of the model. Since heavy Fermions in general are composed of such big atoms as cerium or uranium, the inclusion of spin-orbit coupling is laudatory. They also allowed for an anisotropic coupling between the quasiparticles and Bosons, $\gamma(\vec{k}, \vec{k'})$. This is also more realistic than the isotropic vertex assumed by LML, as we shall see in the next chapter. These changes gives rise to a bare scattering amplitude depicted in Figure 1.17. This new anisotropy in the presence of spin-orbit coupling is sufficient to kill off all spin-singlet, even-parity instabilities. That is, the d-wave instability reported by LML in the isotropic limit, disappears in the presence of an anisotropic vertex, $\gamma(\vec{k}, \vec{k'})$.

Houghton, Read, and Won[67], HIRW, included the higher order exchange diagram represented in Figure 1.16(b). This diagram, topologically the same as the first diagram in Figure 1.15, represents spin fluctuation contributions to
the quasiparticle interactions. *HRW* also included the frequency dependence of the two exchanged Bosons in Figure (b). They discovered both a p-wave (spin-triplet) and d-wave (spin singlet) instability. Even so, to be able to include this higher order diagram, *HRW* assumed, as did *LML*, that the Boson-quasiparticle coupling was isotropic. They also neglected spin-orbit coupling. Thus one may worry slightly about the relevancy of their results to heavy Fermion systems.

This brings us to a few words before we close this chapter. We iterate, once more, that just because superconducting instabilities have been found for various models believed to be appropriate to heavy Fermions, does not tell us what the true microscopic source of the pairing is. This could only be accomplished by detailed calculation of all measurable quantities and agreement with experimental results. We believe that the assumption of isotropic Boson-quasiparticle vertices, made by *LML* and *HRW* are not accurate reflections of real heavy Fermion systems. This thesis enters the picture at this juncture. Our goal, in part, has been to include anisotropies appropriate to the heavy Fermion superconductor CeCu$_2$Si$_2$. This includes the influence of crystal electric fields upon the system of localized, strongly correlated electrons. Further specifics of this process will be discussed in detail in the following chapters. In Chapter 2, we use experimental data to construct our model for CeCu$_2$Si$_2$. This is built upon the famous Anderson lattice model. In Chapter 3, we solve the model at mean field level, which describes the nature of the quasiparticle states. In Chapter 4, we allow the exchanged Bosons (similar to those of *LML*) to fluctuate spatially away from the mean field values.
In Chapter 5, we show how these Bosons give rise to quasiparticle interactions by calculating the bare quasiparticle scattering amplitude. Our results of possible superconducting instabilities will be given at the end of Chapter 5.
Chapter I REFERENCES


16. see, e. g., ref [12], p. 133.


18. see, e. g., ref [12], p. 264.


2.1 Basic Physics Behind the Model

2.1.1 Introduction

This chapter marks the beginning of the formal portion of this thesis, in which we shall study the Anderson lattice in depth. Ubiquitous in the field of strongly correlated systems, the Anderson lattice is actually an extension of Anderson’s original Hamiltonian [2], which describes the mixing of conduction states in a metal with the localized states of a magnetic impurity.

For the sake of concreteness, let us discuss at the outset the basic physical ingredients of this problem. We will start with the Anderson model for a single magnetic impurity before proceeding to the lattice problem, since much of the basic physics can be understood without resorting immediately to an array of magnetic moments. Much of the introductory material in this chapter is based on a pedagogical review article by Newns and Read[1].
We start with a popular picture used to describe the properties of a Ce ion embedded in a metal. The ground state energy $E(n_f)$ of the system can be schematically plotted as a function of the occupancy of the 4$f$ state ($n_f$) of the Ce impurity. (See Figure 2.1.) If we measure the zero of energy from $E(0)$, the 4$f^0$ configuration, then, for a cerium impurity, $E(1) \equiv E_m$ is typically at about -2 eV. The Coulomb energy, $U$, for double occupation of the 4$f$ site is defined by the expression $E(2) = E_m + U$. Calculations of $U$ for Ce impurities gives $U \approx 5 - 6 \text{eV}[4]$. Thus, we expect the 4$f^2$ configuration to be considerably less important than the 4$f^1$ and 4$f^0$ configurations.

That the previous statement is appropriate for CeCu$_2$Si$_2$, with a lattice of Ce ions, can be understood from the discussion by Kang et al.[3] of the electron
spectroscopic data available as of 1990. They analyze their own data of the Ce 3d x-ray photoelectron spectrum (XPS) and 4f bremsstrahlung isochromat spectrum (BIS); they also analyze Ce 4f resonant photoelectron data (RESPES) of Parks et al.\cite{6}. All three spectra are shown in Figure 2.2. Also shown in the figure are calculated spectra (represented by solid lines) from the impurity Anderson model. The authors claim that $U \approx 7eV$ and $E_m \approx -2.4eV$ give good agreement with the data. This corroborates our picture of an (relatively) energetically inaccessible 4f$^2$ configuration.

We shall thus adopt the following scenario for CeCu$_2$Si$_2$, although at the moment we are only considering a single Ce impurity in a metallic background. The 4f multiplet is described by a total angular momentum $\bar{J} = \bar{L} + \bar{S}$ ($J = 5/2$), has a degeneracy $N = 2J + 1$, and an energy $E_m$ measured relative to the chemical potential of the conduction electrons, $\mu_o$. The lowercase $m$ denotes the degenerate states that make up the multiplet. For our problem, the multiplet is rather deep (at least a couple of eV) below the chemical potential. The hybridization between a multiplet state and a conduction state of energy $\xi_k$ is represented by the anisotropic function $V_{m\sigma}(k)$, where $\sigma$ labels the conduction electron spin (see Figure 2.3). It is the large Coulomb energy, $U$, that gives rise to the strong correlations in the problem.

The Anderson impurity model, containing the basic physics we have just discussed, can now be presented:

$$H_A = \sum_{\vec{k},\sigma} \xi_{\vec{k}} c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma} + \sum_m E_m f_m^\dagger f_m + \frac{U}{2} \sum_{m \neq m'} n_m f_m^\dagger f_{m'} \left. + \frac{1}{\sqrt{N_o}} \sum_{\vec{k},\sigma,m} \left( V_{m\sigma}(\vec{k}) c_{\vec{k}\sigma}^\dagger f_m + H.c. \right) \right) \tag{2.1},$$

where $\xi_{\vec{k}} = (\hbar^2 k^2 / 2m) - \mu_o$ is the quadratic dispersion of the conduction states.
Figure 2.2:

Comparison of the spectrum calculated using the impurity Anderson model (solid lines) with the experimental spectrum (filled circles) for (a) 4f BIS, (b) 4f PES, and (c) Ce 3d XPS in CeCu$_2$Si$_2$. The experimental 4f PES spectrum was extracted from the data in reference[6]. (Taken from reference [3].)
Figure 2.3:

A schematic representation of the hybridization process, in which a conduction electron in the state $|\vec{k}\sigma> \text{ jumps into an empty } 4f \text{ orbital of total angular momentum } J = 5/2, \text{ and } z\text{-component } m \text{ described by } |m>. \text{ The matrix element is } <m|V|\vec{k}\sigma>= V_{m}\sigma(\vec{k}). \text{ If we expand the conduction state in partial waves, then only the state with total angular momentum } J = 5/2 \text{ and } z\text{-component } m \text{ would be able to hybridize. Note that the energy of the } J=7/2 \text{ excited multiplet is physically too large. It is shown thus merely to make the figure more readable. The actual size of the spin orbit coupling in CeCu}_2\text{Si}_2, \text{ should be about an order of magnitude larger than the crystal field splitting. Note, also, that the energies of the } \Gamma_6, \Gamma_7, \text{ and } \Gamma_8 \text{ states, which come from the crystal field splitting of the } J=7/2 \text{ multiplet, are not accurate. The states are shown merely to inform the reader how the } J=7/2 \text{ multiplet decomposes in cubic symmetry. See, for example, Appendix D in reference [59].}
$c^\dagger_{k\sigma}$ ($c_{k\sigma}$) are Fermionic creation (destruction) operators for conduction electrons, and $f^\dagger_m$ ($f_m$) are the corresponding operators for the $4f$ states. Note that we could also choose to use conduction electron partial wave states of total angular momentum $J = 5/2$. In this case, the operator $c_{k\sigma}$ would be replaced by $c_{k,j,m}$, where $m$ is the $z$-component of angular momentum, and $k$ represents the magnitude of the vector $\vec{k}$. It is worth noting here that the lattice version of this model, which has $N_4$ $4f$ multiplets, differs from the above only in that the $f^\dagger_m$, $f_m$ operators pickup a site index, and the hybridization term acquires a phase factor $e^{-ik\cdot \vec{R}_j}$, where $\vec{R}_j$ is the real-space vector specifying the position of the $j$-th lattice site.

The Fermionic operators in equation 2.1 satisfy the usual anticommutation relations:

$$\{c^\dagger_{k\sigma}, c_{k'\sigma'}\} = \delta_{kk'}\delta_{\sigma\sigma'}, \{c_{k\sigma}, c_{k'\sigma'}\} = \{c^\dagger_{k\sigma}, c^\dagger_{k'\sigma'}\} = 0, \quad (2.2)$$

$$\{f^\dagger_m, f_{m'}\} = \delta_{mm'}, \{f_m, f_{m'}\} = \{f^\dagger_m, f^\dagger_{m'}\} = 0. \quad (2.3)$$

The large Coulomb energy for CeCu$_2$Si$_2$ prompts us to take the limit in which $U$ goes to infinity, thereby forbidding hybridization processes that give rise to $4f^1 \rightarrow 4f^2$ valence fluctuations. This is a technical simplification for us, but even though $U$ is indeed very large by solid-state physics standards, it may be that the physics of finite $U$ is crucial to the understanding of heavy Fermions. Recently Dan Cox[7] has proposed the Quadrupolar Kondo Model (or Two-Channel Kondo Model) as an explanation of the superconductivity and of the possible non-Fermi liquid behavior in uranium based heavy Fermions. The physics needed to get non-Fermi liquid behavior derives from the existence of enough independent channels of conduction electrons to overcompensate the effective impurity spin. A finite-$U$ version of the Anderson model, as applied to
a Ce impurity, can also exhibit a two-channel Kondo effect. The crystal field split multiplet structure here is the key. Taking the $\Gamma_7$ doublet as the low-lying multiplet for the $4f^1$ configuration, and a $\Gamma_3$ (non-magnetic) doublet as the low lying multiplet for the $4f^2$ configuration (as is appropriate for cubic symmetry), a two-channel Kondo effect is possible. Conduction states of $\Gamma_8$ symmetry can mix the $4f^1$ and $4f^2$ configurations[8]. And conduction states of $\Gamma_7$ symmetry can mix the $4f^1$ and $4f^0$ configurations. If the hybridization with states of $\Gamma_8$ is the stronger of the two cases, the physics of the two-channel Kondo effect will determine the low temperature properties of the model. The pivotal question is: does this picture correspond to a dense Ce system such as CeCu$_2$Si$_2$? If so, then the finite-U Anderson model is the correct starting point for calculations. Nevertheless, the infinite $U$ limit is a reasonable simplification (at least for CeCu$_2$Si$_2$) of an already difficult problem and warrants study in its own right.

Let us rewrite equation 2.1 for the case of infinite $U$

$$H_{\infty} = \sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_m f_m^\dagger f_m$$

$$+ \sum_{k\sigma m} \left( V_{m\sigma}(\vec{k}) c_{k\sigma}^\dagger X_{om} + H.c. \right),$$

(2.4)

$X_{om} = P_0 f_m$ is the so-called Hubbard operator for the impurity[5]. It is composed of a destruction operator for an $f$ electron of angular momentum $m$ and an operator $P_0$, which projects out the $4f^0$ state. With the Hubbard operator we are guaranteed to satisfy the strict constraint, set by an infinite $U$, that the only allowed valence transitions are $4f^1 \leftrightarrow 4f^0$. 

These operators do not, however, satisfy the usual Bosonic or Fermionic commutation relations. (See, for example, pg. 317 of reference [49].)

\[ \{X_{m\sigma}, X_{o\tau}\} = X_{mm} + X_{oo} \neq 1. \quad (2.5) \]

Thus Wick’s theorem is not valid, and standard Feynman diagrammatics is not applicable. We are forced to less friendly Goldstone techniques if we are to continue along this line [18]. In the next section, we shall see how to alleviate this problem.

2.1.2 Strong-Coupling and the 1/N Expansion

It is well known that the Anderson model contains the physics of the Kondo effect, as evidenced by the fact that the Schrieffer-Wolff transformation maps the Anderson impurity onto the Kondo impurity problem [19]. This means that at low enough temperatures the 4f magnetic moments are screened by the conduction electrons, and the resulting spin singlet will require finite energy to break. This energy is denoted the Kondo energy (or temperature) \( T_K \) and is given by

\[ T_K \approx D e^{-|E_m|/(N V^2 N(0))}, \quad (2.6) \]

where \( D \) is the conduction electron bandwidth and \( N(0) \) is the density of states at the chemical potential (or Fermi energy). At high temperatures \((T \gg T_K)\) it is certainly reasonable to study the Anderson model by applying perturbation theory in the hybridization \( V \). But since the expression for \( T_K \) is non-analytic in \( V \), we see that any finite order perturbation theory won’t work for \( T < T_K \). Thus we need a procedure to handle this low temperature, strong-coupling regime.

There have been many people influential in devising an appropriate mean-field theory for the low temperature regime of the Anderson impurity model.
Anderson himself was the first to suggest an expansion in the inverse of the $4f$ multiplet degeneracy[21]. But Read and Newns were the first to develop a formal $1/N$ expansion for the Kondo limit of the Anderson model[26]. We shall discuss the results of their work in detail, since it is a useful guide when we make the jump to the lattice problem. In the lattice, we want a meaningful theory for the so-called coherent regime, wherein all the hybridization sites are phase-locked together, leading to zero resistivity at zero temperature, in accordance with Bloch’s theorem. We shall label as $T_{coh}$ the approximate temperature at which the system enters into the coherent regime and at which the resistivity starts to show a $T^2$ behavior. Our calculations for CeCu$_2$Si$_2$ will only be valid for $T<T_{coh}$. In general $T_{coh}$ is not quite an order of magnitude smaller than the Kondo temperature for the lattice, $T_o$. Recall from Chapter 1, that $T_o$ can be deduced from the quasi-elastic neutron scattering linewidth. (For CeCu$_2$Si$_2$, $T_o \approx 10$ K and $T_{coh}$ is a few Kelvin.) Fluctuations will partially destroy this coherence, giving rise to quasiparticle interactions, and $1/N$ will serve as the expansion parameter. That is, fluctuation induced quasiparticle couplings will be down by order $1/N$ from typical mean-field energies.

2.2 Slave Bosons

2.2.1 Formalities

We can be rid of the unwieldy Hubbard operators in equation 2.4 at the price of introducing a new operator, $b$, commonly called a slave Boson:

$$X_{om} \rightarrow f_m b^\dagger. \quad (2.7)$$
This technique was originally applied to the Anderson model by Barnes[22]. P. Coleman extended the idea to the low temperature, infinite U problem[20]. In equation 2.7, $b^t$ creates a $4f^0$ configuration and does not have any internal degrees of freedom (unlike the $f_m$ operators, which have N angular momentum degrees of freedom). The advantage of such a procedure is that $H_{\infty}$ now is composed entirely of Bosonic and Fermionic operators, and all the standard techniques of Feynman diagrammatics can be brought to bear.

We must realize, however, that merely making the replacement of equation 2.7 into equation 2.4 is not quite enough. The physical Fock space of our problem in the presence of infinite Coulomb repulsion corresponds to the number of $f$ electrons plus the number of slave Bosons being unity. We define a number operator

$$Q = n_f + n_b = \sum_m f_m^t f_m + b^t b.$$  \hfill (2.8)  

Thus we require that $Q=1$ at the impurity site and must project out, in some manner, the states corresponding to $Q > 1$. We shall introduce a Lagrange multiplier (or fictitious chemical potential) $\lambda$. As one might guess, for the lattice, there will be a Lagrange multiplier at each site, and equation 2.8 will pick up a site index. Exactly how we remove the unphysical states will be discussed below, but we remark here that this procedure is certainly not a new one. In fact, Abrikosov (in the 1960s) was the first to use auxiliary Fermionic fields to represent the magnetic impurity spin in the Kondo problem [23].

We now write our bosonized Hamiltonian with its Lagrange multiplier in the form

$$H_\lambda = \sum_{\vec{k}\sigma} c_{\vec{k}\sigma}^t c_{\vec{k}\sigma} + \sum_m E_m f_m^t f_m$$
\[ + \sum_{\tilde{k}\sigma m} \left( V_{m\sigma}(\tilde{k}) c_{\tilde{k}\sigma}^\dagger f_m b^\dagger + H.c. \right) + i\lambda \left( \sum_m f_m^\dagger f_m + b^\dagger b - Q \right). \] (2.9)

After some algebra, we can see that \([H_{\lambda}, Q]=0\), revealing that this new number operator is a conserved quantity. This, in turn, implies a gauge symmetry of the model. Namely, \(H_{\lambda}\) is invariant under the transformations

\[ b \to b e^{i\theta} \quad \text{and} \quad f^\dagger \to f^\dagger e^{-i\theta}. \] (2.10)

We shall discuss the consequences of this gauge symmetry shortly.

2.2.2 Calculation of the Partition Function

We compute the partition function for \(H_{\lambda}\) with the techniques of functional integrals. It certainly is possible, however, since this is a non-relativistic field theory, to retain the more standard Hamiltonian formalism, as has been done by some authors [24], [25]. The use of functional integrals in the Anderson impurity and lattice problems has been popular recently [26],[27],[28]. Perhaps the popularity stems from the following facts:

- Integrating out the Fermionic degrees of freedom is easy to do and is roughly equivalent to diagonalizing a mean-field Hamiltonian.
- The remaining Bosonic degrees of freedom (in our problem these are the slave Boson, \(b\), and the Lagrange multiplier, \(\lambda\)) are treated as static in time and uniform in space at mean-field level. A saddle point evaluation of the partition function then gives rise to a set of integral equations to be solved self-consistently.
- Fluctuations in the Boson fields, which give rise to interactions between the mean-field derived quasiparticles, are calculated from Gaussian integrals (which are user-friendly).
Since our particular calculation overtly builds upon previous work, in which the functional integral techniques were employed [29],[30],[31], we decided to do the same.

The mathematical formalism justifying this approach has been reviewed in detail elsewhere [32],[33], so we shall not spend much time discussing it. The interested reader should consult the referenced works for a rigorous introduction to functional integral techniques applied to many-body problems.

Our starting point will be equation 2.9, the last line of which represents the constraint of unit occupancy (for f-Fermions plus Bosons) at the impurity site. We write a general expression for the partition function

$$ Z = \int_{\lambda}^{i\lambda+\pi/\beta} \frac{\beta d\lambda}{2\pi} \text{Tr} e^{-\beta H}, $$

where $\beta = 1/T$ in units where Boltzmann’s constant is set to unity. The constraint is satisfied from the lambda integration, as can be seen by simply doing the integral. We find

$$ Z \approx \text{Tr} e^{-\beta H_\infty} \frac{\sin \left[ \pi(n_f + n_b - Q) \right]}{\pi(n_f + n_b - Q)}. $$

The oscillatory nature of the sine function kills off all contributions but those satisfying $n_f + n_b = Q$. At the end of the problem we let $Q \to 1$ to regain a physically meaningful answer.[9]

The trace operator in equation 2.11 can be represented as a functional integral over two kinds of fields: a complex field $(b,b^*)$ to represent the Bosons, and two independent, Grassmann fields $(c,c^*)$ and $(f,f^*)$ to represent the Fermions [33]. The Grassmann variables are rather unusual numbers that anticommute,

$$ \{ f_m, f_{m'} \} = 0, \quad f_m^2 = f_m^* f_m = 0, \quad (2.13) $$
where the variable and its conjugate are independent entities. See references [32], [33] for more properties of this uncommon algebra of anticommuting numbers.

Within this formalism, the partition function now takes the form

\[ Z = \int \frac{i^{\lambda+\pi/\beta}}{2\pi} \int D\bar{c} \int D c \int D \bar{f} \int D f \int D\bar{b} \int Db \, e^{-\int_0^\beta \mathcal{L}(\tau) d\tau}, \]  

(2.14)

where the measures are

\[ \mathcal{D} f = \prod_{m \tau} df_m(\tau), \quad \mathcal{D} c = \prod_{k \sigma \tau} dc_{k \sigma}(\tau) \quad \text{and} \quad \mathcal{D} b = \prod_{\tau} db(\tau). \]  

(2.15)

\( \mathcal{L}(\tau) \) is the Lagrangian in imaginary time \( \tau = it \)

\[ \mathcal{L}(\tau) = \sum_{k \sigma} \bar{c}_{k \sigma} \left[ \frac{\partial}{\partial \tau} + \xi_k \right] c_{k \sigma} + \bar{b} \frac{\partial}{\partial \tau} b \]

\[ + \sum_m \bar{f}_m \left[ \frac{\partial}{\partial \tau} + E_m \right] f_m \]

\[ + \frac{1}{\sqrt{N_s}} \sum_{k \sigma m} \left[ V_{m \sigma}(\bar{k}) \bar{c}_{k \sigma} f_m \bar{b} + \text{c.c.} \right] \]

\[ + i\lambda \left[ \sum_m \bar{f}_m f_m + \bar{b} \bar{b} - Q \right]. \]  

(2.16)

Before proceeding, now is a good time to discuss a technical problem inherent to this slave-Boson formalism, the so-called infrared divergence problem. We remarked immediately before equation 2.10 that there is a continuous gauge symmetry in the bosonized Anderson model which is associated with the conservation of the number operator, \( Q \). In the mean-field approximation that we will soon use, the slave boson will develop a non-zero expectation, i.e. \( \langle b \rangle \neq 0 \). This breaks the gauge symmetry, which from the Mermin-Wagner theorem, should not be broken. We have an apparent unphysical approximation. This technical difficulty has been discussed in depth by Read [34] and by Coleman [28].
The key is that the inclusion of fluctuations beyond mean-field restores the broken symmetry. Read showed that the long time \((\tau \to \infty)\) or low frequency behavior of the Boson correlation function to order \(1/N\) is

\[
\lim_{\tau \to \infty} \langle b(\tau)b(0)\rangle \approx \frac{(1-n_f)}{T_R^2} \frac{1}{|\tau|},
\]

(2.17)

where \(\alpha = n_f^2/N\). Thus the correlations do indeed (albeit slowly) decay to zero at long times, verifying that there is not true long-range order. This decay gives rise to integrals that diverge at low frequencies. Surprisingly, upon calculation of measurable quantities such as the specific heat or the static susceptibility, these divergences always cancel to give finite results [35] that agree with the exact (impurity) results from Bethe ansatz calculations [36].

Even with this check, one can ask if the mean-field analysis has any meaning, since it corresponds to an unphysical broken symmetry. Apparently, mean-field theory does well because the field theory exhibits, including fluctuations, almost long-range order, as evidenced by the algebraic temporal decay of equation 2.17. The bosonized model is as close to a true broken symmetry state as physically allowed without actually breaking the gauge symmetry. Hence the mean-field state is not a bad starting point, but the fluctuations can not be neglected (at least to order \(1/N\)).

There is yet one more subtlety with these infrared divergences. Formally we may write the complex field \(b\) in terms of an amplitude and a phase, \(b = se^{-i\theta}\) [26]. Let \(s_0\) and \(\theta_0\) be the values of these quantities at mean-field. Coleman showed (to order \(1/N\)) [28] that at long times the radial correlations showed long range order but the phase fluctuations decayed to zero:

\[
\lim_{\tau \to \infty} (s(\tau)s(0)) = s_0^2, \quad \lim_{\tau \to \infty} (\theta(\tau)\theta(0)) = \left(\frac{C}{\tau}\right)^{n_f^2/N},
\]

(2.18)
where C is a constant. It is the slave-Boson phase fluctuations that restore the broken gauge symmetry. Whereas retaining the fields $\tilde{b}$ and $b$ (the cartesian gauge) requires the cancellation of low-frequency divergences in measurable quantities, Read and Newns showed that the Bosonic phase can, in the hybridization part of the Lagrangian, be transformed away, leaving only the well-behaved radial part, $s(\tau)$. The only remaining effect of the phase, $\theta(\tau)$, is due to a phase velocity, $\dot{\theta}(\tau)$, which can be absorbed into the Lagrange multiplier, $\lambda$, raising it to the status of a dynamical field. This transformation corresponds to the so-called the radial gauge, and we shall use it for our calculations. Apparently, all sources of the low frequency divergences plaguing the untransformed problem arise from the hybridization physics, because in the radial gauge, there are no divergences. (See [34].) The next couple of pages are devoted to a derivation of the Lagrangian in the radial gauge.

To proceed, we make the following change of variables in our functional integral:

$$b(\tau) = s(\tau)e^{i\theta(\tau)} \quad \text{and} \quad f'_m(\tau) = f_m(\tau)e^{-i\theta(\tau)}.$$  \hfill (2.19)

The Jacobian for such a transformation is

$$J \left( \frac{\bar{b}b}{s\theta} \right) = \begin{vmatrix} \frac{\partial b}{\partial s} & \frac{\partial b}{\partial \theta} \\ \frac{\partial \bar{b}}{\partial s} & \frac{\partial \bar{b}}{\partial \theta} \end{vmatrix} = 2is.$$  \hfill (2.20)

The new measure for the complex (Bose) fields is

$$2is(\tau)ds(\tau)d\theta(\tau).$$  \hfill (2.21)

The transformed Lagrangian is easier to understand when broken up into the following pieces: $\mathcal{L} = \mathcal{L}_{\text{cond}} + \mathcal{L}_f + \mathcal{L}_b + \mathcal{L}_{\text{mix}} + \mathcal{L}_{\text{constraint}} = $

$$\sum_{\kappa} \bar{c}_{\kappa} \left[ \frac{\partial}{\partial \tau} + \xi_k \right] c_{\kappa} + \sum_m \bar{f}'_m e^{-i\theta} \left[ \frac{\partial}{\partial \tau} + E_m \right] f'_m e^{i\theta} + se^{-i\theta} \frac{\partial}{\partial \tau} (se^{i\theta})$$
Next, redefine the Lagrange multiplier as

\[ \lambda'(\tau) = \lambda + \dot{\theta}(\tau), \quad (2.23) \]

where the dot over \( \theta(\tau) \) denotes differentiation with respect to imaginary time. Thus the physics of a dynamic phase velocity is still present in the problem, but there are no infrared divergences with which we must contend. Then the measure for the complex fields becomes

\[ 2i\sigma(\tau)ds(\tau)d\lambda(\tau), \quad (2.24) \]

where we also define \( Ds=\prod ds \) and \( D\lambda=\prod d\lambda \). Including the term \( \sum_m i\lambda \ddot{f}_m f'_m \) with \( \mathcal{L}_f \) and using equation 2.23 gives

\[
\mathcal{L}_f = \sum_m \dddot{f}_m \left[ \frac{\partial}{\partial \tau} + E_m + i\lambda' \right] f'_m \quad \text{and} \quad (2.25)
\]

\[
\mathcal{L}_{\text{constraint}} = \left( i\lambda' - i\dot{\theta} \right) \left( s^2 - Q \right). \quad (2.26)
\]

Combining \( \mathcal{L}_b \) with equation 2.25 yields (along with other terms)

\[ ss + i\dot{\theta}Q + i\lambda' \left( s^2 - Q \right). \quad (2.27) \]

Recall from equation 2.14 that we are integrating the Lagrangian over imaginary time. For the first two terms of equation 2.27 this is easy

\[
\int_0^\beta d\tau ss = \frac{1}{2} \left[ s^2(\beta) - s^2(0) \right] = 0, \quad \text{and} \quad (2.28)
\]

\[
Q \int_0^\beta d\tau i\dot{\theta} = Q \left[ i\theta(\beta) - i\theta(0) \right] = 0, \quad (2.29)
\]
where we have treated the $Q$ as static. These results follow from the periodicity of the complex fields over the temporal range $[0,\beta]$, i.e. $\theta(\beta) = \theta(0)$ and $s(\beta) = s(0)$. Finally, dropping all the prime symbols, we are left with the following Lagrangian

$$\mathcal{L} = \mathcal{L}_{\text{cond}} + \sum_m \tilde{f}_m \left[ \frac{\partial}{\partial T} + E_m + i\lambda \right] f_m$$

$$+ \mathcal{L}_{\text{mix}} + i\lambda \left[ s^2 - Q \right].$$

(2.30)

We note in passing, that it is easy to generalize this result to the lattice. We merely include site indices on the Bose fields, $s$ and $\lambda$, and on the $f_m$ operators, and include a phase factor in the hybridizing term.

2.2.3 More Discussion of the $1/N$ Expansion

In the last part of this section, we discuss some formalities about our $1/N$ expansion [37]. Consider, first, a simple one dimensional integral

$$I(N) = \int_{-\infty}^{\infty} dt e^{-Nf(t)},$$

where $N$ is real and we assume that $f(t)$ has an absolute minimum at a point $t_o$. As $N$ gets larger the main contribution to the integrand comes from a small region about $t_o$. Expanding $f(t)$ about $t_o$ (with $\partial f/\partial t|_{t_o}=0$) gives

$$I(N) \approx e^{-Nf(t_o)} \int_{-\infty}^{\infty} dt \exp \left( -\frac{N}{2} f''(t_o)(t - t_o)^2 - \frac{N}{3!} f'''(t_o)(t - t_o)^3 \right),$$

(2.32)

where we have truncated the expansion at third order. Next, let $t' = (t - t_o)\sqrt{Nf''(t_o)}$,

$$I(N) \approx \frac{1}{\sqrt{Nf''(t_o)}} e^{-Nf(t_o)} \int_{-\infty}^{\infty} dt' \exp \left( -\frac{t'^2}{2} - \frac{1}{\sqrt{N}} t'^3 \right),$$

(2.33)
where \( C = 3!f''(t_o)^{3/2}/f^3(t_o) \). It is clear that for large \( N \) the zeroth order term dominates.

Generalizing this to the case of a function of a complex variable, we find that the simplest approximation to the integral is a saddle point approximation, wherein the argument of the exponential is made to be an extremum with respect to the variables of integration. In such a case we can write our partition function in terms of the action \((S=\int d\tau \mathcal{L}(\tau))\) as

\[
Z(N) \approx e^{-NS_0} \int DsD\lambda \exp \left( -\frac{1}{2}[\tilde{s} \lambda] \tilde{D}^{-1} \begin{bmatrix} s \\ \lambda \end{bmatrix} - \frac{1}{\sqrt{N}} O(s^3, \lambda^3, ...) \right),
\]

(2.34)

where \( S_0 \) is the action calculated from the saddle point approximation, and the first term remaining in the integral represents the Gaussian fluctuation contribution to the partition function. \( \tilde{D} \) is the dressed Bosonic propagator and because of the two Bosonic fields, \( s \) and \( \lambda \), is a \( 2 \times 2 \) matrix. Because of the complexity involved in calculating \( \tilde{D} \) in our model, we were not able to go beyond the Gaussian term. This will be discussed in detail later.

We need to make the following change of variables to get a \( 1/N \) expansion:

\[
V_{m\sigma}(\vec{k}) = \sqrt{N} \hat{V}_{m\sigma}(\vec{k}), \quad s = \tilde{s}/\sqrt{N},
\]

(2.35)

where \( \hat{V} \) and \( \tilde{s} \) are treated as order one, \( O(1) \). Further, we let \( Q = Nq \), and at the end of the day we set \( q \) to \( 1/N \). Clearly \( \mathcal{L}_{\text{cond}} \) and \( \mathcal{L}_f \) from equation 2.30 are not affected by this rescaling, but \( \mathcal{L}_{\text{mix}} \) and \( \mathcal{L}_{\text{constraint}} \) become

\[
\mathcal{L}_{\text{mix}} = \frac{1}{\sqrt{N}s} \sum_{k\sigma m} \left[ \hat{V}_{m\sigma}(\vec{k}) \hat{c}_{k\sigma} \hat{f}_m \tilde{s} + \text{c.c.} \right],
\]

(2.36)

\[
\mathcal{L}_{\text{constraint}} = N\lambda \left( \tilde{s}^2 - q \right).
\]

(2.37)
For the moment, consider the case where $V_{m\sigma}$ and $E_m$ are actually independent of $m$ (We have already assumed this for the slave Bosons, s.). Then the Lagrangian simplifies to

$$\mathcal{L} = \mathcal{L}_{\text{cond}} + N \left( \tilde{f} \left[ \frac{\partial}{\partial \tau} + E + i\lambda \right] f + \sum_{\tilde{k}, \sigma} \left[ \tilde{V}_\sigma(\tilde{k}) \tilde{c}_{\tilde{k}\sigma} f \tilde{s} + \text{c.c.} \right] + i\lambda N \left[ \tilde{s}^2 - q \right] \right). \quad (2.38)$$

As we can see, but for $\mathcal{L}_{\text{cond}}$, we have the overall prefactor of $N = 2J + 1$ that guarantees a $1/N$ expansion. Even though our multiplet energies and mixing matrix elements ($E_m$ and $V_{m\sigma}$, respectively) are not independent of the multiplet index $m$, the discussion of the previous pages should still be valid. Further, since our Lagrangian will reduce to equation 2.38 in the isotropic limit, the formal $1/N$ expansion should be well defined.

2.3 Results for the Impurity Model

In this section we shall work through a mean-field, $1/N$ calculation in detail. We shall see that in the Kondo limit, where the 4$f$ site energy $E_m$ is deep below the chemical potential, $\mu_o$, a sharp resonance in the 4$f$ density of states will appear near $\mu_o$. This resonance can, in turn, explain the large electronic effective masses seen by specific heat and static susceptibility measurements in systems with screened local moments[26].

We proceed as follows. In equation 2.38, $\tilde{s}$ and $\tilde{V}$ are assumed to be of order one. At the mean-field level, they are also assumed to be static, which we represent by a subscript "o", $\tilde{s} \rightarrow \tilde{s}_o$, $\lambda \rightarrow \lambda_o$. The $f$ and conduction propagators, $G^m_f$ and $G^s_f$, respectively, are also treated as $N$-independent. As we shall see, the Bose propagator, represented by the matrix $\hat{D}$ in equation 2.34,
Figure 2.4:

This is the simplest, order $N$ contribution to the mean-field free energy. The dashed line is the bare $f$ propagator, and the solid line is the conduction electron propagator. The Bose field $s_o$ is assumed static, and the matrix element $V_o$ is isotropic in $k$-space.

will be of order $1/N$. Thus, to construct the free energy, for example, the leading order diagrams are those with the maximum number of closed loops formed by Fermionic propagators and the minimum number of Bose propagators. This is easy to see, since closed loops constructed of the functions $G_m^o$ and $G_{k\sigma}$ will have a free sum over $m$, the angular momentum index. Thus if we represent, diagrammatically, $G_m^o$ by a dashed line and $G_{k\sigma}$ by a solid line, the diagram in Figure 2.4 will be of order $N$. Figure 2.5 shows the leading order (mean-field, order $N$) contributions to the free energy, as well as the $O(1)$ contributions. It is clear that the $O(1)$ contributions arise from diagrams with an equal number of closed Fermion loops and Bose propagators.

The mean-field Hamiltonian corresponding to the Lagrangian of equation 2.38
Figure 2.5:

Diagrams contributing to the free energy of the impurity problem. The series (a) represents the leading-$N$ diagrams. The diagrams (i), (iia), and (iii) in (b) represent the next order in $1/N$. Diagram (iib) is of still higher order in $1/N$. In (a) the full lines represent bare conduction propagators and the dashed lines represent $f$-propagators. The wavy lines represent Bose propagators, and the $\times$ represent the product $\tilde{s} \tilde{V}$. (Taken from reference [1].)
is

\[ H_{MF} = \sum_{km} \xi_k c_{km}^\dagger c_{km} + (E_m + i\lambda_o) f_m^\dagger f_m + \tilde{s}_o \tilde{V}_o \sum_{km} (c_{km}^\dagger f_m + H.c.) \]

\[ + i\lambda_o (s_o^2 - 1), \quad (2.39) \]

where the conduction electron operator, \( c_{km} \), represent partial wave conduction states with angular momentum \( J = 5/2 \) and \(-5/2 \leq J \leq 5/2\). We minimize \( H_{MF} \) with respect to the two Bose fields, \( s_o \) and \( \lambda \) to find

\[ s_o^2 = 1 - \langle n_f \rangle, \quad (2.40) \]

\[ \epsilon_m - E_m = \frac{V_o N}{s_o} \sum_{\xi} \langle f_{m}^\dagger c_{km} \rangle, \quad (2.41) \]

where we have introduced a shifted \( f \)-energy, \( \epsilon_m = E_m + i\lambda_o \). Also we have used the fact that \( \tilde{s}_o \tilde{V}_o = s_o V_o \). These equations must be solved self-consistently for \( s_o \) and \( \lambda_o \). We can proceed by calculating the hybridization dressed \( f \) propagator, \( G_m \), and the dressed, off-diagonal, propagator \( G_{mk} \). These can be easily evaluated from the Dyson equations represented in Figure 2.6. The result for the \( f \) propagator as a function of energy \( \xi \) measured relative to the chemical potential is

\[ G_m(\xi) = \frac{1}{\xi - \epsilon_m + i\pi s_o^2 V_o^2 N(0)}, \quad (2.42) \]

where \( N(0) \) is the conduction electron density of states at the chemical potential. From this expression, the \( f \) density of states is

\[ N_m(\epsilon) = \frac{-\text{Im} G_m(\xi)}{\pi} = \frac{s_o^2 V_o^2 N(0)}{\left(\xi - \epsilon_m\right)^2 + \pi^2 N^2(0)s_o^2 V_o^4}, \quad (2.43) \]

which is peaked about the shifted \( f \) energy, \( \epsilon_m \).

The \( f \) density of states can by used to calculate the average \( f \) occupancy, \( \langle n_f \rangle \) in equation 2.40. The result is

\[ \langle n_f \rangle = \frac{N}{\pi} \tan^{-1}\left(\frac{\pi s_o^2 V_o^2 N(0)}{\epsilon_m}\right), \quad (2.44) \]
at zero temperature. From the Dyson equation for the off-diagonal propagator (Figure 2.6), the expectation value in equation 2.41 can be evaluated,

\[ \sum_{\mathbf{k}} \langle f_{\mathbf{m}}^\dagger c_{\mathbf{k}m} \rangle = \frac{s \nu V_c N(0)}{2} \ln \left( \frac{\epsilon_m^2 + \pi^2 s^4 \nu^4 V_c^4 N^2(0)}{D^2} \right), \]  

(2.45)

where \( D \) is half the conduction electron bandwidth. Next we substitute the result into equation 2.41 and use the fact that the shifted \( f \) energy, \( \epsilon_m \), is generally small compared to \( D \) and \( E_m \). That is, the shifted \( f \) energy is usually near the chemical potential (which corresponds to zero energy) and hence is small, while both \( D \) and \( E_m \) are of the order of 2 eV. Thus we use the fact that \( D \gg |\epsilon_m| \) and \(|E_m| \gg |\epsilon_m|\) to simplify equation 2.41 to

\[ \epsilon_m = T_K = De^{-|E_m|/N\nu^2 N(0)}, \]  

(2.46)

which defines the impurity Kondo temperature.
We now have enough information to discuss the low temperature thermodynamics of this model. We use the approximation that the $f$ electron density of states is larger than the conduction density of states, \textit{i.e.} near the chemical potential $N_{\text{total}}(\epsilon) \approx N_{m}(\epsilon)$. For large degeneracy, $N$, the coefficient of the linear specific heat, $\gamma$, and the static susceptibility, $\chi$, are

$$\gamma = \frac{1}{3} NN_{m}(0), \quad (2.47)$$

$$\chi = \frac{1}{3} \mu_{\text{eff}}^{2} NN_{m}(0), \quad (2.48)$$

where $\mu_{\text{eff}}^{2} = g^{2} \mu_{B}^{2} J(J+1)$ is the effective magnetic moment and $\mu_{B}$ is the Bohr magneton. Since, as we have stated, the shifted $f$ energy of the impurity, $\epsilon_{m}$, is generally quite small, the density of states, $N_{m}(0)$ can be quite large. In fact, in the Kondo limit, where $\langle n_{f} \rangle \rightarrow 1$, both $\gamma$ and $\chi$ are proportional to the inverse of the Kondo temperature:

$$\gamma \approx \frac{\pi^{2}}{3T_{K}}, \quad (2.49)$$

$$\chi \approx (g\mu_{B})^{2} \frac{J(J+1)}{3T_{K}}. \quad (2.50)$$

Since the Kondo temperature can be quite small (of the order of $meV$), we see that the many-body physics of the Kondo effect can explain the enhanced values of $\gamma$ and $\chi$ measured in real systems with $4f$ moments. (See chapter 1.)

The ratio of $\gamma$ and $\chi$ is related to the famous Wilson ratio. For the mean-field, $1/N$ model, we find

$$\frac{\chi}{\gamma} = \frac{\mu_{\text{eff}}^{2}}{\pi^{2}}, \quad (2.51)$$

which corresponds to a ratio $R=1$. This is the result for non-interacting quasiparticles. We can compare this value of $R$ with the exact result from Bethe
ansatz calculations [10],[11], which give
\[
\left( \frac{\chi}{\gamma} \right)_{\text{Bethe}} = \frac{\mu_{eff}^2}{\pi^2} \left( 1 + \frac{1}{N-1} \right).
\] (2.52)

The two results are in exact agreement in the limit of infinite degeneracy. That is, the $1/N$ mean-field theory appears to be exact as $N \to \infty$.

We shall see that, in the case of the Anderson lattice, the density of states for the hybridization dressed quasiparticles (in the Kondo limit) will also be strongly peaked near the quasiparticle chemical potential. Thus the physics determining the thermodynamics of the single impurity and the lattice models is very similar. The transport properties of these two models must, of course, differ, since at low temperatures the coherent scattering of an electron off an ordered array of screened $4f$ moments will produce a resistivity that vanishes as $T \to 0$ (for a clean material).

To gauge the accuracy of the $1/N$ mean-field calculation for thermodynamic quantities, see Figure 2.7, which is taken from reference [1], and which compares the $1/N$ and Bethe ansatz results for the following quantities: the specific heat at constant volume, $C_v(T/T_K)$, the magnetic susceptibility, $\chi(T/T_K)$, and the magnetization, $M(h/T_K)$, where $h$ is the magnetic field. The $1/N$ calculation was performed for $N = 8$, and the results are represented by solid lines in the figure. The exact (Bethe ansatz) results are represented by dash-dot lines and were calculated by Rajan [12] ($C_v$ and $\chi$) and by Hewson, Rasul, and Newns [13] (the magnetization). The dots in Figure 2.7(c) are experimental data for $YbCuAl[14]$. We see that for low enough temperatures and fields ($T/T_K \leq 0.2; h/T_K \leq 0.2$) the $1/N$ technique works very well. Furthermore, the $1/N$ technique extends easily to the lattice problem (as we are about to see) and to the calculation of dynamic quantities like the magnetic susceptibility [15]). The Bethe ansatz
technique cannot be extended to the lattice or to the study of dynamics. We feel thus justified in using a $1/N$ expansion to study quasiparticle interactions in the infinite-$U$ Anderson lattice, since such a calculation will be used only for very low temperatures ($T \ll T_K$).

There is one last item in this section, which we would like to address. What happens to the mean field impurity results in the presence of crystal field splitting? We see from equation 2.46 that the Kondo temperature has a factor of $N$ in the argument of the exponential. If crystal electric fields split this $N$-fold degenerate multiplet into two separate multiplets of degeneracies $N_1$ and $N_2$ (with $N = N_1 + N_2$), what happens to the Kondo temperature? Let $\Delta_{CEF}$ be the energy difference between the two multiplets, and let $T_K^o$ be the Kondo temperature in the absence of crystal field splitting. We shall assume that $\Delta_{CEF} \gg T_K^o$, which (as we shall soon discuss) is correct for CeCu$_2$Si$_2$. In this case, the mean field Hamiltonian, when differentiated with respect to $s_o$, yields the equation

$$E_m \approx V_o^2 N(0) \left[ N_1 \ln \left( \frac{\epsilon_m}{D} \right) + N_2 \ln \left( \frac{\epsilon_m + \Delta_{CEF}}{D} \right) \right],$$

which gives a new Kondo temperature of

$$T_K = \left( \frac{D}{\Delta_{CEF}} \right)^{\frac{N_2}{N_1}} D e^{-|E_m|/NV_o^2 N(0)}. \quad (2.54)$$

With a little algebra, this can be written as

$$T_K = T_K^o \left( \frac{T_K^o}{\Delta_{CEF}} \right)^{\frac{N_2}{N_1}}. \quad (2.55)$$

If $N_2 > N_1$, and $\Delta_{CEF} \gg T_K^o$, we see that crystal fields can vastly reduce the Kondo temperature compared to the full $N$-fold degenerate multiplet.

This result is actually rather intriguing. Suppose we evaluate a fluctuation-induced diagram in spherical symmetry that represents a contribution to quasi-
Figure 2.7:

Plots of (a) Specific heat at constant volume $C_v$ in units of $T_K$ against $T$; (b) magnetic susceptibility against $T$; (c) magnetization against $h$. These are for the $N = 8$, integral-valent $U = \infty$ Anderson model. The full curves are given by the mean field solution. The exact solutions are the dot-dash curves in (a), (b) and the upper full curve in (c). In (c), the circles are experimental points for $YbCuAl$. (Taken from reference [1].)
particle interactions. Let us roughly characterize this contribution as some function of the inverse Kondo temperature, \( f(a/(T_K^n)) \), i.e. the diagram depends inversely on some power of the Kondo temperature (with \( n \geq 1 \)). Suppose we then evaluate the diagram for the lowest crystal field split multiplet. We would roughly expect a result \( f(a/(T_K^n)) \), where \( f(a/T_K) \gg f(a/T_K^n) \). The idea is that crystal field splitting could enhance the importance of the diagram in question, when compared to the case of spherical symmetry and no crystal field splitting.

We shall mention this point again in chapter 5 when we actually calculate the quasiparticle interactions, but it seems appropriate now to pique the reader's interest about the possible importance of crystal field splitting in Kondo systems.

### 2.4 Specific Models

We will now generalize equation 2.38, the Lagrangian for a single Ce impurity, to that of a lattice of Ce ions. The ease with which we can make such a generalization is a strength of the \( 1/N \) formalism. The Bose fields, \( s \) and \( \lambda \), and the \( 4f \) operators now pick up a site index, \( j \). (We use lowercase \( j \) for the site index; the angular momentum operator will always be represented by an uppercase \( J \).) There is also a phase factor, \( e^{i\vec{k}\cdot\vec{R}_j} \), that appears in the hybridization term, where \( \vec{R}_j \) denotes the real-space position of the \( j \)-th lattice site. So equation 2.38 becomes

\[
\mathcal{L} = \sum_{k\sigma} \bar{c}_{k\sigma} \left[ \frac{\partial}{\partial \tau} + \xi_k \right] c_{k\sigma} + \sum_{jm} \bar{f}_{jm} \left[ \frac{\partial}{\partial \tau} + E_m + i\lambda_j \right] f_{jm}
+ \frac{1}{\sqrt{N_s}} \sum_{k\sigma j} [V_{m\sigma}(\vec{k})\bar{c}_{k\sigma} f_{jm} \tilde{s}_j e^{i\vec{k}\cdot\vec{R}_j} + \text{c.c.}] + \sum_j i\lambda_j N \left[ \tilde{s}_j^2 - q_j \right], \tag{2.56}
\]

where the conduction states have been written in terms of the vector \( \vec{k} \) and the spin index \( \sigma = \pm 1 \).
Our knowledge of the lattice problem has been advanced by several groups. Lacroix and Cyrot[16] studied the spin-1/2 Kondo lattice by generalizing a functional integral approach to the partition function of a single impurity[17]. Andy Millis and Patrick Lee[25] and Tesanovic and Valls[24] studied the infinite-$U$ Anderson lattice thoroughly within a Hamiltonian formalism; Auerbach and Levin[29] studied the Fermi liquid properties of the Kondo lattice using functional integrals. Piers Coleman also wrote a detailed article on applications of functional integrals to various Anderson models[28]. As is often the case, much of the ground-breaking work in this area was based upon a simplified version of the Anderson lattice, the so-called SU(N) model. We briefly discuss this problem below, and then we move on to a model more suited to the heavy Fermion superconductor CeCu$_2$Si$_2$.

2.4.1 The SU(N) Model

If we assume that there are $N$ independent conduction electron states per $k$ point ($N$ is not necessarily equal to two), then the conduction electron contribution to the Lagrangian is

$$\mathcal{L}_{\text{cond}} = N \sum_{\vec{k}} \bar{c}_{\vec{k}} \left[ \frac{\partial}{\partial \tau} + \xi_{\vec{k}} \right] c_{\vec{k}}. \quad (2.57)$$

When compared with equation 2.38, we see that we can write $\mathcal{L}_{SU(N)} = N \mathcal{C}$, where the form of $\mathcal{L}$ is self-evident from equations 2.38 and 2.57. This model has been studied by several groups [29],[30],[35],[28], where they also assumed an isotropic mixing matrix element, $V_{m\sigma}(\vec{k}) \to V$. Some of these results will be discussed in later chapters. It is clear, however, that the assumption of $N$-fold degenerate conduction states could be rather dangerous. In heavy Fermions, furthermore, the mixing matrix element is not isotropic. There is motivation, therefore, to
study a more realistic model. This was first done, within the $1/N$ formalism, by F. C. Zhang and T. K. Lee [31].

2.4.2 An Anisotropic Hybridization Model

Zhang and Lee pointed out the weaknesses of the SU(N) model, so far as it has been used in calculations of heavy Fermion systems. In their work, they retained the appropriate two-fold degeneracy of the conduction electrons, and they also assumed each $4f^1$ multiplet was described by a spin-orbit coupled angular momentum, $J=5/2$. Further, they used an anisotropic hybridization of the form immortalized by Coqblin and Schrieffer [38]

$$V_{m\sigma}(\vec{k}) = -\sqrt{\frac{4\pi}{3}}(-i)^3\sigma V_k \sqrt{\frac{7-2m\sigma}{14}} Y_{3,m-\frac{5}{2}}(\hat{k}), \quad (2.58)$$

where $V_k$ represents the dependence on the magnitude of the momentum, and $\sigma=\pm1$. Their Lagrangian, which we shall call $\mathcal{L}_{ZL}$, has the same structure as equation 2.30.

As will be discussed later, the anisotropy of the quasiparticle interactions in $\mathcal{L}_{ZL}$ differs markedly from those of $\mathcal{L}_{SU(N)}$. The physics of the multiplet structure and its symmetries can have a large impact on the quasiparticle properties. It is our belief, however, that one more step needs to be taken. If we think specifically of the cerium based heavy Fermion superconductor CeCu$_2$Si$_2$, then the model of Zhang and Lee requires some further modification. We want to include the effects of crystal electric field splitting of the Ce $4f^1$ multiplet, as has been measured by inelastic neutron scattering [39]. This is the topic of the next subsection.
Figure 2.8:
The tetragonal unit cell of CeCu$_2$Si$_2$. Note there are actually two units of CeCu$_2$Si$_2$ in the cell. (From reference [55].)

2.4.3 Including Lattice Symmetries Appropriate for CeCu$_2$Si$_2$

The unit cell of CeCu$_2$Si$_2$ is tetragonal (See figure 2.8.), and we wish to study the measurable consequences of this symmetry. We start with inelastic neutron scattering measurements.

Horn et al.[39] used high energy incident neutrons to measure the inelastic magnetic scattering in CeCu$_2$Si$_2$ (see figure 2.9). The data show a clear peak at $\omega=31.5$ meV ($\approx 360$K) and a weaker peak at $\omega=12$ meV. In the presence of tetragonal symmetry, the J=5/2 manifold would be split into three doublets, which can be written as:

$$a|\pm 5/2\rangle + b|\mp 3/2\rangle$$ (2.59)

$$|\pm 1/2\rangle$$ (2.60)

$$b|\pm 5/2\rangle - a|\mp 3/2\rangle$$ (2.61)
where \( a=0.83\pm0.03 \) and \( b=0.56\pm0.04 \) would best fit the data, including the weaker peak at 12 meV.

Later, measurements of the specific heat at high temperatures [40] did not quite agree with this multiplet structure (See figure 2.10.). Bredl et al. plotted the \( 4f \) contribution to the specific heat of \( \text{CeCu}_2\text{Si}_2 \) by subtracting off the corresponding data for \( \text{LaCu}_2\text{Si}_2 \). They found they could not fit the results with two Schottky peaks, as would be expected for three crystal field doublets. Instead, the excited magnetic states behaved as if there were a four-fold degenerate multiplet about 360 K above a ground state doublet. Such a structure would be appropriate in the presence of cubic symmetry.

Further evidence for effective cubic symmetry at the cerium sites comes from the dc susceptibility measurements by Steglich and co-workers on single crystal \( \text{CeCu}_2\text{Si}_2 \) samples[41]. Their data are reproduced in Figure 2.11. They find very little difference in the temperature dependence of \( \chi_{dc} \) for a magnetic field applied parallel or perpendicular to the c-axis of the tetragonal unit cell. Note that the non-superconducting single crystal , however, shows a rather substantial anisotropy.

Also, recall from the previous chapter that we found evidence for cubic symmetry from the effective mass data of de Haas-van Alphen experiments and the isotropy of the \( H_{c2} \) data. In light of all this information, it seems acceptable to assume that the small peak in the neutron data at 12 meV is not due to crystal field excitations and to assume that there is effectively cubic symmetry at the cerium sites.

In the presence of cubic symmetry, we find the \( J=5/2 \) multiplet is split into
Figure 2.9:
Neutron Scattering Intensity for CeCu$_2$Si$_2$ and LaCu$_2$Si$_2$. Note the clear peak at $\omega=31.5$ meV and $T=10$ K due to crystal field excitations of the Ce 4$f^1$ multiplet. It is not clear if the weak peak at $\omega=12$ meV is also a crystal field excitation, since there is a similar bump in LaCu$_2$Si$_2$. $\theta=14^\circ$ is the average scattering angle. (From reference [39].)
Figure 2.10:
Specific heat vs. temperature showing Schottky peaks due to crystal field excitations. The authors claim a crystal field structure of a ground doublet and an excited quartet will fit the data. The dotted line is the attempted fit from the crystal field states of tetragonal symmetry. be the multiplet structure in the presence of cubic symmetry. (From reference [40].)
dc-susceptibility as a function of temperature for non-superconducting (ns) and superconducting (s) CeCu$_2$Si$_2$ single crystals measured with the magnetic field parallel and perpendicular to the tetragonal c-axis. (Taken from reference [41].)
a doublet of $\Gamma_7$ symmetry and a $\Gamma_8$ quartet [42]. We label the states as follows:

\begin{align}
|\Gamma_7, +1\rangle &= -\sqrt{\frac{1}{6}} | -\frac{5}{2} \rangle + \sqrt{\frac{5}{6}} |\frac{3}{2}\rangle \\
|\Gamma_7, -1\rangle &= -\sqrt{\frac{1}{6}} |\frac{5}{2}\rangle + \sqrt{\frac{5}{6}} | -\frac{3}{2}\rangle \\
|\Gamma_8, +2\rangle &= \sqrt{\frac{5}{6}} |\frac{5}{2}\rangle + \sqrt{\frac{1}{6}} | -\frac{3}{2}\rangle \\
|\Gamma_8, 1\rangle &= |\frac{1}{2}\rangle \\
|\Gamma_8, -1\rangle &= | -\frac{1}{2}\rangle \\
|\Gamma_8, -2\rangle &= \sqrt{\frac{5}{6}} | -\frac{5}{2}\rangle + \sqrt{\frac{1}{6}} |\frac{3}{2}\rangle.
\end{align}

From the neutron data we know that the ground multiplet is the doublet. Thus, without addressing the true microscopic source of the crystal fields, we deduce a multiplet structure as shown in figure 2.12, where $\Delta_{CEF}$ labels the size of the crystal field splitting. In general, equations 2.62 - 2.67 can be expressed as

$$|\Gamma, \alpha\rangle = \sum_m c_{\Gamma m} |m\rangle,$$

where the ket $|m\rangle$ are the eigenstates of $J_z$, the z-component of the total angular momentum. The coefficients $c_{\Gamma m}$ can be read directly from the equations. For example, in the $\Gamma_7$ doublet, $c_{\Gamma_{-\frac{5}{2}}} = \sqrt{1/6}$.

Next, we address the structure of the hybridization matrix element in the presence of the crystal fields. Let $\Gamma$ denote either of the two representations possible under the operations of the group $O_h$ (i.e. $\Gamma_7$ or $\Gamma_8$), and let $\alpha$ label the degenerate states within a given representation, $\Gamma$. We want to construct a matrix element $V_{\Gamma\alpha\sigma}(\vec{k})$ for hybridizing a crystal field state with quantum numbers $\Gamma$ and $\alpha$ to a conduction state with crystal momentum $\vec{k}$ and spin $\sigma$. In
Figure 2.12:

Splitting of $J=5/2$ multiplet into a $\Gamma_7$ doublet and a $\Gamma_8$ quartet due to crystal fields of cubic symmetry. Neutron scattering gives a splitting of about 360 K. (See reference [39].)

In the case of a single ion in the full $J$ manifold and plane wave conduction states, we merely use the form derived by Coqblin and Schrieffer [38] (see equation 2.58).

In our case it is trivial to generalize to the case of finite crystal field splitting, because the new 4$f$ states are just linear combinations of the $J=5/2$ states

$$V_{\Gamma\sigma}(\vec{k}) = \sum_{m=-5/2}^{5/2} c_{\Gamma\alpha m} V_{m\sigma}(\vec{k}),$$

where the $c_{\Gamma\alpha m}$ can be read directly from equations 2.62 through 2.67.

Evidently, as we generalize this result to a lattice of cerium ions at sites $\vec{R}_j$, we pick up a phase factor $e^{i\vec{k} \cdot \vec{R}_j}$, such that the mixing term in the Hamiltonian formalism becomes

$$H_{\text{mix}} = \frac{1}{\sqrt{N_s}} \sum_{\vec{k}\sigma j\Gamma} \left[ V_{\Gamma\sigma}(\vec{k}) c_{\vec{k}\sigma}^{\dagger} f_{j} c_{j\Gamma}^{\dagger} f_{j} e^{i\vec{k} \cdot \vec{R}_j} + \text{H.c.} \right].$$

The cubic symmetry is now reflected in the structure of the anisotropic function $V_{\Gamma\sigma}(\vec{k})$, which has a significantly different $\vec{k}$ dependence than Coqblin-Schrieffer form $V_{m\sigma}(\vec{k})$. This new anisotropy will have profound results on the quasiparticle interactions, as we shall see in the next chapters. First, we wish to
discuss one other important way to include the lattice symmetry of CeCu$_2$Si$_2$ in our model, through the inclusion of realistic band structure.

2.5 Inclusion of Cubic Symmetry through Band Structure

2.5.1 Introduction and Previous Work

First, a short disclaimer for this section. The broad purpose of this research project has been to quantify the effects of the crystalline symmetry on the quasiparticle interactions (within the framework of the Anderson lattice). More specifically, we wished to see if there was a superconducting instability in such a model. The use of conduction states taken from a bandstructure calculation would obviously feed information about the lattice symmetries into the Hamiltonian. We discovered, however, that the complicated structure of the three-dimensional sums over the Brillouin zone rendered the numerical solution of the mean-field self-consistency equations extremely difficult to obtain. Eventually, for the sake of pushing on, we had to abandon our original plans and revert to simple plane wave states for the conduction electrons. For the sake of completeness, however, we shall discuss the extent of our work along this line. To do so, requires a look at what had been done before.

Bandstructure calculations for CeCu$_2$Si$_2$ have been performed by several groups [43], [44],[45],[46]. For now, we shall focus on the work of Sticht, Kübler, and d’Ambrumenil[43]. As with most such calculations, the starting point is the local approximation to the density functional theory (or the LDA, for short) [47],[49]. Since this thesis is not a treatise on methods of electronic structure calculations, we shall only briefly discuss the idea behind the LDA.

Hohenberg and Kohn [50] showed that the ground state energy of a metal
was a functional of the electronic density, \( \rho(\vec{r}) \)

\[
E[\rho] = \int d^3 r V(\vec{r}) \rho(\vec{r}) + F[\rho],
\]

(2.70)

where \( V(\vec{r}) \) is an external potential and \( F[\rho] \) is an unknown functional of \( \rho(\vec{r}) \).

It is customary to break \( F \) up into various parts as

\[
F[\rho] = \frac{e^2}{2} \int d^3 r d^3 r' \rho(\vec{r}) \rho(\vec{r}') \frac{1}{|\vec{r} - \vec{r}'|} + T_o[\rho] + E_{xc}[\rho],
\]

(2.71)

where the first term is just the energy due to the Coulomb repulsion of the electrons, the term \( T_o[\rho] \) describes the kinetic energy of noninteracting electrons, and the difficult piece, \( E_{xc}[\rho] \), is called the exchange and correlation energy.

The LDA formally amounts to making a specific approximation for \( E_{xc} \), namely

\[
E_{xc}[\rho] = \int d^3 r \rho(\vec{r}) \epsilon_{xc}(\rho(\vec{r})),
\]

(2.72)

where \( \epsilon_{xc} \) is the exchange and correlation energy per electron for the homogeneous electron gas, which is assumed known. Sticht et al. include the 4\( f \) electrons in this LDA calculation; but the 4\( f \) wavefunctions are strongly localized, and it might be worrisome to assume that the average interactions in a homogeneous electron gas are applicable to the 4\( f \) electrons of CeCu\(_2\)Si\(_2\). Indeed, their results point to a deficiency in the procedure. They find that the density of states at the Fermi level is about 3.9 eV\(^{-1}\) per formula unit \( (N(0) \approx 3.9 \text{ eV}^{-1}) \), whereas a simple estimate from the specific heat (taking \( \gamma \approx 1 \text{ J/mole K}^2 \)) give \( N(0) \approx 400 \text{ eV}^{-1} \). Thus the strong correlations, which give rise to the large effective mass, have been missed.

The Fermi surface topology, since it is determined by geometry [51], is not so problematic for LDA. As one can see from Table 2.1, the LDA calculated Fermi surface areas of CeRu\(_2\)Si\(_2\) agree rather well with the corresponding de
Haas-van Alphen data. Clearly, however, more work is needed to handle the strong correlations effectively. We mention, briefly, an *ad-hoc* procedure that was developed to get effective masses of the right size for heavy Fermions: the so-called Kondo lattice *Ansatz*.

At low enough temperatures, the $4f$ moments are screened by conduction electrons. The remaining conduction electrons merely see a scattering center on the the Ce sites that causes a phase shift (as described by Nozieres [53]). For electrons with energy $\epsilon$ near the chemical potential $\mu$ we have

$$\delta^C_\sigma(\epsilon) = \delta^C_\sigma(\mu) + \frac{1}{T^*}(\epsilon - \mu),$$

(2.73)

which has two adjustable parameters, $\delta^C_\sigma(\mu)$ and $T^*$. From the Friedel sum rule, for approximately 1 $f$ electron per Ce ion, we know $\delta^C_\sigma C_e(\mu) \approx \pi/2$. The effective Kondo temperature, $T^*$, is taken from the experimental value of $\gamma$, the linear coefficient of specific heat.

The band structure is obtained from solving the KKR equations [52], and the claim is that this procedure can consistently calculate both the Fermi surface topology *and* the effective masses. This appears basically to be correct for CeRu$_2$Si$_2$, as seen again in Table 2.1 and is the state of the art in heavy Fermion bandstructure calculations.

2.5.2 Our Attempt: Simple Bandstructure and the Anderson Lattice

Our goal is slightly different from that of the electronic structure people. We wish to start from a microscopic Hamiltonian that realistically builds in strong correlations from the beginning (*i.e.* the Anderson lattice). We then do our best straightforward band structure calculation for the conduction electrons in
Table 2.1:

Comparison of de Haas-van Alphen data for CeRu$_2$Si$_2$ [52] with theoretical results. Shown are the external areas of the Fermi surface (area in megagauss) and the effective mass ratio $m^*/m_0$. Unlike LDA the renormalized band theory (RB), which makes use of the Kondo lattice Ansatz, reproduces the large observed mass anisotropies well. (From reference [49].)

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<td>4.7</td>
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<td>$\approx 10$</td>
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</tr>
<tr>
<td>$\beta$</td>
<td>(001)</td>
<td>6.1</td>
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<td>5</td>
<td>0.6</td>
<td>8</td>
<td>3.7</td>
</tr>
<tr>
<td>$\beta$</td>
<td>(110)</td>
<td>9.6</td>
<td>1.8</td>
<td>10</td>
<td>0.6</td>
<td>12</td>
<td>3</td>
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<tr>
<td>$\gamma$</td>
<td>(001)</td>
<td>10.6</td>
<td>2.6</td>
<td>10</td>
<td>0.8</td>
<td>13</td>
<td>3.5</td>
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<tr>
<td>$\gamma$</td>
<td>(110)</td>
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<td>2.3</td>
<td>16</td>
<td>0.8</td>
<td>18</td>
<td>2.6</td>
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<td>$\delta$</td>
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<td>24</td>
<td>1.5</td>
<td>26</td>
<td>2.1</td>
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<tr>
<td>$\epsilon$</td>
<td>(110)</td>
<td>25.0</td>
<td>19.7</td>
<td>23</td>
<td>1.2</td>
<td>20</td>
<td>$&gt; 20$</td>
</tr>
<tr>
<td>$\eta$</td>
<td>(001)</td>
<td>31.2</td>
<td>3.0</td>
<td>26</td>
<td>0.9</td>
<td>19</td>
<td>2.7</td>
</tr>
<tr>
<td>Z-5</td>
<td>(001)</td>
<td>—</td>
<td>—</td>
<td>250</td>
<td>4.0</td>
<td>$\approx 280$</td>
<td>$\approx 22$</td>
</tr>
<tr>
<td>Z-4</td>
<td>(001)</td>
<td>—</td>
<td>$\approx 180$</td>
<td>$\approx 5$</td>
<td>$\approx 140$</td>
<td>$&gt; 200$</td>
<td></td>
</tr>
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</table>
order to include lattice symmetries. Finally we calculate effective quasiparticle interactions in the presence of the anisotropies and the non-trivial bands.

For our purposes, it seems sufficient to take the simplest conduction states beyond those for free electrons. We assumed a weak periodic potential, $U(\vec{r})$, and make an expansion in plane waves

$$\psi_{\vec{K}}(\vec{r}) = \sum_{\vec{R}} a_{\vec{K}-\vec{R}} e^{i(\vec{K}-\vec{R}) \cdot \vec{r}}, \quad (2.74)$$

where $\vec{K}$ labels reciprocal lattice vectors, and the $a_{\vec{K}-\vec{R}}$ are the expansion coefficients. The conduction electron contribution to the Anderson lattice Hamiltonian becomes

$$H_{\text{cond}} = \sum_{\vec{k} \vec{R} \vec{R}' \sigma \sigma'} c_{\vec{k} \vec{R}, \sigma}^\dagger G_{\vec{R}, \vec{R}, \sigma, \sigma'}^{-1} c_{\vec{K} \vec{R}', \sigma'}, \quad (2.75)$$

where

$$G_{\vec{R}, \vec{R}, \sigma, \sigma'}^{-1} = \delta_{\sigma \sigma'} \left[ \xi_{\vec{k} \vec{R}} \delta_{\vec{R}, \vec{R}'} + U_{\vec{R} \vec{R}'} \right]. \quad (2.76)$$

In equations 2.75 and 2.76, $\sigma$ and $\sigma'$ are spin indices, and the Kronecker delta in front of equation 2.76 is a result of time-reversal invariance. $U_{\vec{R} \vec{R}'}$ is the Fourier transform of the lattice potential, $U(\vec{r})$. We took the lattice potential to have a screened form in real space

$$U(\vec{r}) = U_0 \frac{e^{-r/L}}{r}. \quad (2.77)$$

The length scale, $L$, is set at about the Ce-Ce separation in the plane, and the energy scale, $U_0$, is set to 0.3 eV (big enough to be of consequence, but small compared to the bandwidth).

For simplicity, we limited the number of reciprocal lattice vectors, $\vec{K}$ in equation 2.74 to seven, which are: $(0,0,0), (\pm 2,0,0), (0,\pm 2,0), (0,0,\pm 2)$, in units
Figure 2.13:
The seven large dots represent the reciprocal lattice vectors used in our band-structure calculation; note the octahedral symmetry at the $\Gamma$ point.

of $\pi/a$, where $a$ is the lattice spacing perpendicular to the c-axis ($a \approx L$). (See figure 2.13.)

Relative to the $\Gamma$ point, it is clear that this set of points transforms according to the octahedral group, $O_h$. That is, our conduction states have cubic symmetry at the zone center. Other points in the zone, however, are treated differently. For example, the zone corner, represented by $R$, is equivalent to the $\Gamma$ point from symmetry arguments. But clearly, our basis does not treat $R$ the same as $\Gamma$, and the only solution to such an inequity is to enlarge the set of lattice vectors. We decided against enlarging the basis beyond the set of seven vectors for the sake of simplicity. Clearly, to diagonalize a large Hamiltonian is time consuming, and the effects are magnified by the many instances such calculations would be needed during the course of the many-body problem. We opted, therefore, for conduction states that basically get the cubic symmetry exact near the zone center.
We can write the conduction electron contribution to the Hamiltonian as a matrix, in which we separate out the $\vec{K}=0$ part

$$\hat{H}_{\text{cond}} = \begin{pmatrix} G_{R\vec{K}}^{-1} & G_{\vec{K}0}^{-1} & V_{\vec{K}\Gamma_0} \\ (G_{\vec{K}\Gamma_0}^{-1})^* & G_{\vec{K}\Gamma_0}^{-1} & V_{\vec{K}\Gamma_0} \\ V_{\vec{K}\Gamma_0}^* & V_{\vec{K}\Gamma_0}^* & G_{\vec{K}\Gamma_0}^{-1} \end{pmatrix},$$

(2.78)

where

$$G_{\vec{K}0}^{-1} = \xi_k \delta_{\vec{K},0} + U_{-\vec{K}}$$

and

$$G_{\vec{K}\Gamma_0}^{-1} = \epsilon_\Gamma \delta_{\Gamma\Gamma'} \delta_{\alpha\alpha'}.$$  

(2.79)

(2.80)

Using a trick of Heine's [54], we can fold down the higher conduction bands and reformulate the problem as an effective f-band (with non-zero dispersion) hybridizing with the $\vec{K}=0$ plane wave band. This procedure makes use of the following identity:

$$\begin{vmatrix} A & B \\ B^t & C \end{vmatrix} = \begin{vmatrix} I & -A^{-1}B \\ -C^{-1}B^t & I \end{vmatrix} = \begin{vmatrix} A - BC^{-1}B^t & 0 \\ 0 & C - B^t A^{-1}B \end{vmatrix},$$

(2.81)

where the vertical bars imply the determinant is to be taken. A, B, and C are arbitrary matrices, and I is the identity matrix. For our problem, let $A = G_{\vec{K}\Gamma_0}^{-1} - E \delta_{\vec{K}\Gamma_0} \delta_{\sigma\sigma'}$ (which is a $12 \times 12$ matrix), and let B be the single matrix constructed from $G_{\vec{K}0}^{-1}$ and $V_{\vec{K}\Gamma_0}$ (B is as $12 \times 8$ matrix.). Finally, let

$$C = \begin{pmatrix} G_{\vec{K}0}^{-1} - E \delta_{\sigma\sigma'} & V_{\vec{K}\Gamma_0} \\ V_{\vec{K}\Gamma_0}^* & G_{\vec{K}\Gamma_0}^{-1} - E \delta_{\Gamma\Gamma'} \delta_{\alpha\alpha'} \end{pmatrix},$$

(2.82)

where C is an $8 \times 8$ matrix. The secular equation $\det(\hat{H}_{\text{cond}} - E\hat{I}) = 0$ now is equivalent to $\det(A - BC^{-1}B^t)\det(C - B^t A^{-1}B) = 0$. Taking the second term to be zero yields

$$\begin{vmatrix} \tilde{G}_{\vec{K}0}^{-1} - E\hat{I} & \tilde{V}_{\vec{K}\Gamma_0} \\ \tilde{V}_{\vec{K}\Gamma_0}^* & \tilde{G}_{\vec{K}\Gamma_0}^{-1} - E\hat{I} \end{vmatrix} = 0,$$

(2.83)
where

\[ \tilde{G}_{\sigma o}^{-1} = G_{\sigma o}^{-1} - (G_{\sigma R}^{-1})^* G_{\sigma R} R G_{\sigma o}^{-1}, \]  

\[ \tilde{V}_{o \Gamma} = V_{o \Gamma} - (G_{\sigma R}^{-1})^* G_{\sigma R} R V_{\Gamma \Gamma} \text{ and} \]  

\[ \tilde{G}_{\Gamma \Gamma'}^{-1} = G_{\Gamma \Gamma'}^{-1} - V_{\Gamma \Gamma'}^* G_{\Gamma \Gamma'} R V_{\Gamma \Gamma} \Gamma. \]  

Clearly, the dispersion of the f-band comes from the last term in equation 2.86.

After folding down, we have the following generalized Anderson lattice

\[ \tilde{H} = \sum_{k \sigma} \tilde{c}_{k \sigma}^\dagger \tilde{G}_{\sigma o}^{-1} \tilde{c}_{k \sigma} + \sum_{j \Gamma_\alpha \Gamma'_\alpha'} \tilde{f}_{j \Gamma_\alpha \Gamma'_\alpha'}^\dagger \tilde{G}_{\Gamma_\alpha \Gamma'_\alpha}^{-1} \tilde{f}_{j \Gamma_\alpha \Gamma'_\alpha} \]

\[ + \sum_{k \sigma j \Gamma_\alpha} \left[ \tilde{V}_{o \Gamma_\alpha}(k) \tilde{c}_{k \sigma}^\dagger \tilde{f}_{j \Gamma_\alpha \Gamma'_\alpha} s_j + H.c. \right] \]

\[ + \frac{1}{2} \sum_j i \lambda_j \left[ \sum_{\Gamma_\alpha} \tilde{f}_{j \Gamma_\alpha}^\dagger \tilde{f}_{j \Gamma_\alpha} + s_j^2 - Q_j \right]. \]  

We discovered that the physical importance of the higher conduction bands was not as large as we might have guessed. The effects of these bands are felt basically in two ways: at the band edges, where the bands are given a roughly quadratic dispersion; and the appearance of the dispersion in the otherwise utterly flat bands of \( \Gamma_7 \) or \( \Gamma_8 \) character. The added dispersion to the \( \Gamma_7 \) and \( \Gamma_8 \) states was not larger than the Kondo temperature itself, and so should not be of much importance. This is in agreement with the results of Zou and Anderson[58], who calculated the quasiparticle bands with the relativistic \( KKR \) equation. They also found the effects of the higher bands were small and neglectable. The quadratic downturn of the bands near the zone edges is of more importance, however. As we shall see in chapter 4, when we calculate the Bosonic self-energy, we shall need to perform numerical integrations throughout the Brillouin zone. These integrals will involve the band energies as a function of the integration.
variable $\tilde{k}$ and also as a function of the variable $\tilde{k} + \tilde{q}$, where $\tilde{q}$ is a fixed momentum. It is the energies $E_{n\tilde{k}+\tilde{q}}$ ($n$ is a band index), which are functions of the shifted momenta, that turn out to be very sensitive to this quadratic downturn in the bands. More details of this technical point, which can be easily solved, will be given in chapter 4. For now, we wish to emphasize that, but for this one instance with the Brillouin zone integrations, the higher conduction bands are basically innocuous. This is just as well, since in the next paragraph, we discuss the numerical difficulties these higher bands create, even at the mean-field level.

At the mean-field level of our $1/N$ expansion, we need to self-consistently solve a set of coupled integral equations. Physically this corresponds to minimizing the Free energy with respect to the parameters $s$ and $\lambda$. Because of the complicated $k$-dependence in equation 2.87 we found it virtually impossible to solve the self-consistency equations numerically (Finding the extremum of a function of more than one variable—numerically—quickly becomes difficult even for relatively simple functions.). We discovered that the only reliable way to find a self-consistent solution was to replace all three dimensional $k$ sums by one dimensional energy integrals over a density of states. We were not able to calculate the density of states for the Hamiltonian given by equation 2.87. Thus we were forced to return to the simpler problem of a single conduction band of free electrons.

We have discussed this extended bandstructure problem because formally it is all set up and ready to go. We were halted by the numerics, but if such a hindrance should be lessened in the future, this is a problem that should be considered. It could serve, especially in the light of our results for free elec-
trons, to quantify how much the bandstructure itself can influence quasiparticle interactions.

We close this chapter with a reminder of the actual model we used for the calculations. It is the Anderson lattice for 4f states of cubic symmetry hybridizing with free conduction electrons. Starting with equation 2.36, we generalize the rescaled slave bosons amplitude to represent the two multiplets

$$\tilde{s}_{\Gamma_7} = s_o/\sqrt{N_7} \quad \text{and} \quad \tilde{s}_{\Gamma_8} = s_o/\sqrt{N_8},$$  \hspace{1cm} (2.88)

where $N_7=2$ and $N_8=4$ are the degeneracies. Note, also, that the bare amplitude, $s_o$, is the same for both multiplets. We also assume the Lagrange multiplier, $i\lambda$, is the same for both multiplets. Thus equations 2.36 and 2.37 become:

$$L_{\text{mix}} = \frac{1}{\sqrt{N_7}} \sum_{\vec{k}\sigma j\Gamma}\left[\hat{V}_{\Gamma\alpha\sigma}(\vec{k})\tilde{c}_{\vec{k}\sigma}f_{j\Gamma\alpha}\tilde{s}_{j\Gamma} + \text{c.c.}\right]$$  \hspace{1cm} (2.89)

$$L_{\text{constraint}} = \frac{1}{2} \sum_{j\Gamma} N_{\Gamma} i\lambda_j \left(\tilde{s}_{j\Gamma}^2 - q_{j\Gamma}\right).$$  \hspace{1cm} (2.90)

In 2.89, $\hat{V}_{\Gamma\alpha\sigma} = \sqrt{N_{\Gamma}} V_{\Gamma\alpha\sigma}$. In equation 2.90, $q_{j\Gamma} = Q_j/N_{\Gamma}$. It can be seen that equation 2.90 is equivalent to 2.37 when summed freely over the multiplet index $\Gamma$.

The full Lagrangian is

$$\mathcal{L} = L_{\text{cond}} + \sum_{j\Gamma\alpha} f_{j\Gamma\alpha}\left[E_{\Gamma} + i\lambda_j\right]f_{j\Gamma\alpha}$$
$$+ \frac{1}{\sqrt{N_7}} \sum_{\vec{k}\sigma j\Gamma}\left[\hat{V}_{\Gamma\alpha\sigma}(\vec{k})\tilde{c}_{\vec{k}\sigma}f_{j\Gamma\alpha}\tilde{s}_{j\Gamma}e^{i\vec{k}\cdot\vec{A}_j} + \text{c.c.}\right]$$
$$+ \frac{1}{2} \sum_{j\Gamma} N_{\Gamma} i\lambda_j \left(\tilde{s}_{j\Gamma}^2 - q_{j\Gamma}\right).$$  \hspace{1cm} (2.91)

In the next chapter, we shall do a mean-field analysis of this system.
Chapter II REFERENCE


37. see [32] p. 120.


CHAPTER III

Mean Field Analysis in the Presence of Crystal Fields

3.1 Introduction

In this chapter, we shall use the Lagrangian of equation 2.91 to construct a mean-field action, $S_{MF}$, and a mean-field partition function $Z_{MF}$. The mean-field approximation describes non-interacting quasiparticles of energy $E_{nk}$ (where $n$ is a band index). There will also be contributions to $S_{MF}$ from terms quadratic in the Bose fields, $s$ and $\lambda$. These terms will be represented by a matrix vertex function $\hat{\Gamma}_o$. We shall see in Chapter 4, that conduction electron and f electron particle-hole excitations can dress the Bosons, giving rise to a (dressed) matrix vertex $\hat{\Gamma}$. For now, however, we shall be concerned with the mean field vertex, $\hat{\Gamma}_o$, which can be related to a Bosonic Green function, $\hat{D}_o$, via the relation

$$\hat{D}_o^{-1} \equiv -\hat{\Gamma}_o.$$  \hspace{1cm} (3.1)

The layout of this chapter is as follows. After transforming to k-space, we shall integrate out the Grassmann fields from $Z_{MF}$. Recall that these anticommuting fields arise in functional integrals to take the place of our usual anti-
commuting operators in Fock space. The resultant partition function will then contain integrals only over the complex (Bose) fields. At mean-field level, we approximate the partition function by a saddle-point evaluation of these integrals over $s_0$ and $\lambda_0$. The subscript "o" here denotes the mean-field values of these quantities. Note, also, that there is no tilde over the s field yet; that means it hasn't yet been scaled by a factor of the square root of the degeneracy.

The saddle-point evaluation boils down to requiring that the action, $S_{MF}$, be an extremum with respect to the variables $s_0$ and $\lambda_0$, bringing us to the conditions

$$\frac{\partial S_{MF}}{\partial s_0} = 0,$$  
(3.2)

$$\frac{\partial S_{MF}}{\partial \lambda_0} = 0,$$  
(3.3)

which must be solved together. At the end of this chapter, we shall discuss the numerical procedure used to find solutions to the above equations. Now, we briefly discuss the physical meaning of the mean-field parameters that emerge from a solution of these equations.

Physically, the hybridization of conduction and f electrons shifts the undispersed energies of the $\Gamma_7$ and $\Gamma_8$ multiplets, $E_7$ and $E_8$, upward toward the free electron chemical potential. The new, shifted, energies are labeled as $\epsilon_7$ and $\epsilon_8$, where $\epsilon_7 = E_7 + i\lambda_0$, and where we have assumed that the crystal field splitting is not renormalized, i.e. $|E_7 - E_8| = |\epsilon_7 - \epsilon_8|$. In the previous chapter, we discussed that $E_7 = -2.0 \text{ eV}$ and $E_8 = E_7 + \Delta_{CEF} = -1.964 \text{ eV}$ are reasonable energies for CeCu$_2$Si$_2$, where all energies are measured relative to the chemical potential of the unhybridized conduction electrons.

Also, at mean-field level, we can think of $s_0$ as renormalizing the hybridization matrix element, $V_0$ (i.e. $V \rightarrow s_0 V_0$). That $s_0$ is generally small ($s \leq 0.2$, usually)
reflects the fact that a conduction electron, because of the infinite Coulomb repulsion, can hop onto an f site only if that site is empty, which severally restricts the hopping rate.

Along with the coupled equations above, we also fix the chemical potential, $\mu$, of the quasiparticles. Numerical solution of the set of three equations then yields values for $\epsilon_7$, $\epsilon_8$, $s_0$, and $\mu$, which will be used in the next chapters to calculate interactions between the quasiparticles. We begin, by deriving the mean-field partition function, $Z_{MF}$.

3.2 The Partition Function

3.2.1 Motivation

Starting with equation 2.91 from the previous chapter, which is the Lagrangian for plane waves hybridizing with a lattice of crystal field split 4f multiplets, we perform a mean-field analysis of our model. Although this calculation uses functional integrals for the partition function, we shall also (at some places) make use of more familiar Green functions techniques within a Hamiltonian formalism. This will be sufficient to elucidate much of the physics of interest to us.

At first, we Fourier transform our Lagrangian (equation 2.91) via the following expressions:

$$\alpha_j = \sum_k \alpha_k e^{-i\vec{k} \cdot \vec{R}_j},$$

(3.4)

$$f_{j\Gamma\alpha} = \frac{1}{\sqrt{N_s}} \sum_k f_{\vec{k}\Gamma\alpha} e^{-i\vec{k} \cdot \vec{R}_j},$$

(3.5)

where $\alpha_j$ represents $i\lambda_j$ or $\delta_{j\Gamma}$ (j labels the lattice sites in real space), and $N_s$ is the number of lattice sites. Note that requiring $\delta_{j\Gamma}$ to be real means that

$$\delta^*_{\vec{k}\Gamma} = \delta_{-\vec{k}\Gamma}.$$  

(3.6)
We have assumed a single $s_j$ field can describe both $\Gamma_7$ and $\Gamma_8$ multiplets at every site. When we rescale the field by the degeneracy of the multiplets, we thus have two possibilities: $\tilde{s}_j \equiv s_j/\sqrt{2}$, or $\tilde{s}_j \equiv s_j/\sqrt{4}$. Similarly, the parameter $q$ is generally set to $1/N$, but since we have two multiplets we define $q_\Gamma \equiv 1/N_\Gamma$. We also assume (always) that $q_\Gamma$ is the same at every lattice site.

Let's look at the transformed Lagrangian term by term, starting with the site diagonal contribution from the $4f$ electrons:

$$\mathcal{L}_f = \sum_{j\Gamma\alpha} \tilde{f}_{j\Gamma\alpha} \left[ \frac{\partial}{\partial \tilde{r}} + E_\Gamma \right] f_{j\Gamma\alpha}$$

$$= \frac{1}{N_s} \sum_{j\Gamma\alpha} \sum_{\vec{k}k'} \tilde{f}_{\vec{k}\Gamma\alpha} \left[ \frac{\partial}{\partial \tilde{r}} + E_\Gamma \right] f_{\vec{k}\Gamma\alpha} e^{iR_j \cdot (\vec{k} - \vec{k}')},$$

where $E_\Gamma$ is the unshifted (bare) crystal field-split multiplet energy. Using the identity

$$\frac{1}{N_s} \sum_j e^{iR_j \cdot (\vec{k} - \vec{k}')} = \delta_{\vec{k}\vec{k}'} , \quad (3.7)$$

we find that

$$\mathcal{L}_f = \sum_{\vec{k}\Gamma\alpha} \tilde{f}_{\vec{k}\Gamma\alpha} \left[ \frac{\partial}{\partial \tilde{r}} + E_\Gamma \right] f_{\vec{k}\Gamma\alpha} . \quad (3.8)$$

Next, we look at the mixing term,

$$\mathcal{L}_{mix} = \frac{1}{\sqrt{N_s}} \sum_{k \sigma j \Gamma \alpha} \left[ \hat{V}_{\Gamma \sigma \alpha}(\vec{k}) \tilde{c}_{k \sigma} f_{j \Gamma \alpha} \tilde{s}_j \gamma e^{iR_j \cdot (\vec{k} - \vec{k}') + c.c.} \right]$$

$$= \frac{1}{N_s} \sum_{k \sigma j \Gamma \alpha} \sum_{\vec{k}' \vec{k}''} \left[ \hat{V}_{\Gamma \sigma \alpha}(\vec{k}) \tilde{c}_{k \sigma} f_{\vec{k}\Gamma\alpha} \tilde{s}_j^* e^{i\vec{R}_j \cdot (\vec{k} + \vec{k}' - \vec{k}'') + c.c.} \right] ,$$

$$\mathcal{L}_{mix} = \sum_{\vec{k}\vec{k}'\sigma \Gamma \alpha} \left[ \hat{V}_{\Gamma \sigma \alpha}(\vec{k}) \tilde{c}_{k \sigma} f_{\vec{k}\Gamma\alpha} \tilde{s}_j^* e^{i\vec{R}_j \cdot (\vec{k} - \vec{k}')} + c.c. \right] . \quad (3.9)$$

Finally, consider the constraint

$$\mathcal{L}_{constraint} = \sum_j i\lambda_j \left[ \sum_{\Gamma\alpha} \tilde{f}_{j\Gamma\alpha} f_{j\Gamma\alpha} + \frac{1}{2} \sum_{\Gamma} \left( \tilde{s}_j^2 - q_\Gamma \right) \right]$$
\[
\sum_{j,k,k',\bar{k}''} i\lambda_{\bar{k}} e^{-i\bar{k} \cdot R_j} \left[ \frac{1}{N_s} \sum_{\Gamma} \bar{f}_{\bar{k} \Gamma \alpha} f_{k'' \Gamma \alpha} e^{i R_j \cdot (\bar{k}' - \bar{k}'')} + \frac{1}{2} \sum_{\Gamma} N_{\Gamma} \tilde{s}_{\bar{k} \Gamma} \tilde{s}_{k'' \Gamma} e^{i R_j \cdot (\bar{k}' - \bar{k}'')} \right] \\
- \frac{N_s}{2} i\lambda_{\alpha} \sum_{\Gamma} q_{\Gamma},
\]

which becomes

\[
\mathcal{L}_{\text{constraint}} = \sum_{\bar{k}} i\lambda_{\bar{k}} \left[ \sum_{\Gamma} \bar{f}_{\bar{k} \Gamma \alpha} f_{k' - k \Gamma \alpha} + \frac{N_s}{2} \sum_{\Gamma} \left( \sum_{\bar{k'}} \tilde{s}_{\bar{k} \Gamma} \tilde{s}_{k' - k \Gamma} - q_{\Gamma} \right) \right].
\tag{3.10}
\]

For convenience, we rewrite the full Lagrangian once more:

\[
\mathcal{L} = \mathcal{L}_{\text{cond}} + \mathcal{L}_f + \mathcal{L}_{\text{mix}} + \mathcal{L}_{\text{constraint}}
\]

\[
= \sum \bar{c}_{k \sigma} \left[ \frac{\partial}{\partial T} + \xi_k \right] c_{k \sigma} \\
+ \sum_{\bar{k}\bar{k}' \Gamma \alpha \Gamma' \alpha'} \bar{f}_{\bar{k} \Gamma \alpha} \left[ \left( \frac{\partial}{\partial T} + E_{\Gamma} \right) \delta_{\Gamma' \Gamma} \delta_{\alpha' \alpha} \delta_{\bar{k}' \bar{k}} + i\lambda_{\bar{k} - \bar{k}'} \right] f_{\bar{k}' \Gamma' \alpha'} \\
+ \sum_{\bar{k}\bar{k}' \Gamma \alpha} \left[ \bar{V}_{\Gamma \alpha \sigma} (\bar{k}) \bar{c}_{k \sigma} f_{\bar{k} \Gamma \alpha} \tilde{s}_{k - \bar{k} \Gamma} + \text{c.c.} \right] \\
+ \frac{N_s}{2} \sum_{\bar{k} \Gamma} N_{\Gamma} i\lambda_{\bar{k}} \left[ \sum_{\bar{k'}} \tilde{s}_{\bar{k} \Gamma} \tilde{s}_{k' - \bar{k} \Gamma} - q_{\Gamma} \right],
\tag{3.11}
\]

where we have used equation 3.6 in the mixing term. The next step is to write the Lagrangian so that it is quadratic in the Grassmann fields, thereby enabling us to integrate over them.

### 3.2.2 Completing the Square

We want to integrate out the Fermionic degrees of freedom, leaving a partition function that depends only on the Bosonic fields, \( \tilde{s}_{\bar{k} \Gamma} \) and \( i\lambda_{\bar{k}} \). To proceed, we complete the square for the Grassmann fields by defining the following new field:

\[
\phi_{k \sigma} \equiv c_{k \sigma} + \sum_{\bar{k} \Gamma \alpha} \left( \frac{\partial}{\partial T} + \xi_k \right)^{-1} \bar{V}_{\Gamma \alpha \sigma} (\bar{k}) \tilde{s}_{\bar{k} \Gamma} f_{\bar{k} \Gamma \alpha}.
\tag{3.12}
\]
To see how this will work, we expand a product of two of these new fields in terms of the original Grassmann fields, \( c \) and \( f \), and compare the result with equation 3.11,

\[
\sum_{\bar{k}\sigma} \bar{\phi}_{\bar{k}\sigma} \left( \frac{\partial}{\partial \bar{T}} + \xi_{\bar{k}} \right) \phi_{\bar{k}\sigma} = \sum_{\bar{k}\sigma} \left[ \bar{c}_{\bar{k}\sigma} \left( \frac{\partial}{\partial \bar{T}} + \xi_{\bar{k}} \right) c_{\bar{k}\sigma} + \sum_{\bar{k}\Gamma'\alpha'} \bar{c}_{\bar{k}\sigma} \bar{f}_{\bar{k}\Gamma'\alpha'} \hat{s}_{\bar{k}^- \bar{k}^-} \bar{\Gamma}' \Gamma'\alpha' \bar{\Gamma}' \Gamma'\alpha' \bar{\Gamma}' \Gamma'\alpha' \bar{\Gamma}' \Gamma'\alpha' \bar{k} \right] f_{\bar{k}\Gamma'\alpha'} + \sum_{\bar{k}\Gamma'\alpha' \bar{k}'\Gamma''\alpha''} \bar{V}_{\Gamma'\Gamma''\alpha'\alpha''}^{\star} (\bar{k}) \bar{s}_{\bar{k}^- \bar{k}^-} \bar{\Gamma}' \Gamma'\alpha' \bar{\Gamma}' \Gamma'\alpha' \bar{\Gamma}' \Gamma'\alpha' \bar{k} \left( \frac{\partial}{\partial \bar{T}} + \xi_{\bar{k}} \right)^{-1} \bar{V}_{\Gamma'\Gamma''\alpha'\alpha''} (\bar{k}) \bar{s}_{\bar{k}^- \bar{k}^-} \bar{\Gamma}' \Gamma'\alpha' \bar{\Gamma}' \Gamma'\alpha' \bar{\Gamma}' \Gamma'\alpha' \bar{k} \right].
\]

(3.13)

The first three terms of the right side of equation 3.13 are just the conduction \( (L_{cond}) \) and hybridization \( (L_{mix}) \) contributions to the Lagrangian. Further, if we define a bare conduction Green function by

\[
G_{\sigma\sigma}(\bar{k}, \tau) \equiv -\left( \frac{\partial}{\partial \bar{T}} + \xi_{\bar{k}} \right)^{-1},
\]

(3.14)

then from equations 3.13 and 3.14 we can write

\[
\mathcal{L} = \sum_{\bar{k}\Gamma'\alpha'} \bar{\phi}_{\bar{k}\sigma} G_{\sigma\sigma}^{\star} (\bar{k}, \tau) \phi_{\bar{k}\sigma} - \sum_{\bar{k}\Gamma'\alpha'} \bar{f}_{\bar{k}\Gamma'\alpha'} \left( \frac{\partial}{\partial \bar{T}} + E_{\bar{T}} \right) f_{\bar{k}\Gamma'\alpha'} + \mathcal{L}_{\text{constraint}}
\]

\[
+ \bar{f}_{\bar{k}\Gamma'\alpha'} \left[ i \lambda_{\bar{k}^- \bar{k}^-} \delta_{\Gamma'\Gamma''} \delta_{\alpha'\alpha''} + \sum_{\bar{k}'\Gamma''\alpha''} \bar{V}_{\Gamma'\Gamma''\alpha'\alpha''}^{\star} (\bar{k}'') \bar{s}_{\bar{k}^- \bar{k}^-} \bar{\Gamma}' \Gamma'\alpha' \bar{\Gamma}' \Gamma'\alpha' \bar{\Gamma}' \Gamma'\alpha' \bar{k} \right] \bar{f}_{\bar{k}'\Gamma''\alpha''}.
\]

(3.15)

Since all the terms in the Lagrangian dependent upon the Grassmann fields \((\bar{\phi}, \phi)\) and \((\bar{f}, f)\) are now quadratic in these fields, we can easily integrate them out. Note that the measure for the \((\bar{\phi}, \phi)\) fields will be the same as that for the \((\bar{c}, c)\) fields since all the possible derivatives in the Jacobian dependent on both fields is unity (e.g. \( \partial c / \partial \phi = 1 \)).
Before integrating, it is convenient to perform a few further manipulations upon equation 3.15. As a first step in the mean-field analysis, let $\delta_0$ and $i\lambda_0$ represent the uniform in space and static in time limits of the fields $\delta\tilde{s}_{\Gamma\Gamma'}(\tau)$ and $i\lambda_0(\tau)$. Defining fluctuations relative to these mean-field values

$$\delta\tilde{s}_{\Gamma\Gamma'} \equiv \tilde{s}_{\Gamma\Gamma'} - \delta_0,$$  
$$i\delta\lambda_{\tilde{\kappa}} \equiv i\lambda_{\tilde{\kappa}} - i\lambda_0,$$  

means we can write

$$\tilde{s}_{\Gamma\Gamma'} = \delta_0 + \delta\tilde{s}_{\Gamma\Gamma'},$$  
$$i\lambda_{\tilde{\kappa}} = i\lambda_0 + i\delta\lambda_{\tilde{\kappa}}.$$

Substituting equations 3.18 and 3.19 into 3.15 gives

$$\mathcal{L} = \sum_{\tilde{k}\sigma} \tilde{\phi}_{\Gamma\sigma} G^{-1}_{\alpha_0}(\tilde{k}, \tau) \phi_{\Gamma\sigma} + \sum_{\tilde{k}'\alpha'} f_{\Gamma\Gamma'} \left[ \left( \frac{\partial}{\partial \tau} + E_\Gamma + i\lambda_0 \right) \delta\tilde{\Gamma}\alpha, \delta\alpha', \right]$$

$$+ \sum_{\sigma} \delta_0 \tilde{V}_{\Gamma\alpha_0\sigma}(\tilde{k}) G_{\alpha_0}(\tilde{k}, \tau) \tilde{V}_{\Gamma\alpha', \sigma}(\tilde{k}) \delta_0$$

$$+ \sum_{\tilde{k}'\Gamma\alpha'} \tilde{f}_{\Gamma\alpha'} \left[ i\delta\lambda_{\tilde{\kappa}' - \tilde{\kappa}} \delta\Gamma\alpha, \delta\alpha', + \sum_{\sigma} \delta\tilde{\sigma}_{\Gamma\sigma}(\tilde{k}) G_{\sigma\sigma}(\tilde{k}) \tilde{V}_{\Gamma\alpha', \sigma}(\tilde{k}) \delta\tilde{s}_{\Gamma\Gamma'}, \right]$$

$$+ \sum_{\tilde{k}'\Gamma\alpha'} \tilde{V}_{\Gamma\alpha_0\sigma}(\tilde{k}) G_{\sigma\sigma}(\tilde{k}) \tilde{V}_{\Gamma\alpha', \sigma}(\tilde{k}) \delta\tilde{s}_{\Gamma\Gamma'}, \right] f_{\Gamma\Gamma'} \delta_{\alpha\alpha'}. \quad (3.20)$$

For ease of writing, we define the following functions:

$$G^{-1}_{\Gamma\alpha}(\tau) \equiv - \left( \frac{\partial}{\partial \tau} + E_\Gamma + i\lambda_0 \right)^{-1},$$

$$G^{-1}_{\Gamma\alpha_0\sigma}(\tilde{k}, \tau) \equiv G^{-1}_{\Gamma\alpha}(\tau) - \Sigma_{\Gamma\alpha_0\sigma}(\tilde{k}, \tau). \quad (3.21), (3.22)$$
\[
G_{G_{\alpha}}(k, \tau) - \sum_{\alpha} \delta_{\alpha} \nu_{G_{\alpha}}(k) G_{\sigma}(k, \tau) \tilde{V}_{G_{\alpha}}(k), \tag{3.23}
\]

\[
G_{\alpha}^{B}(k, \tau) - \sum_{\sigma} \delta_{\alpha} \nu_{G_{\alpha}}(k) G_{\sigma}(k, \tau) \tilde{V}_{\alpha}(k, \tau), \tag{3.24}
\]

\[
G_{\alpha}^{C}(k, \tau) - \sum_{\alpha} \tilde{V}_{\alpha}(k) G_{\sigma}(k, \tau) V_{\alpha}^{*}(k) \delta_{\alpha}. \tag{3.25}
\]

\(G_{\alpha}(\tau)\) is the bare \(f\) electron Green function and depends on the shifted energy \(\epsilon_{\Gamma} = \epsilon_{\Gamma} + i\lambda_{\sigma}\). Equation 3.22 is just Dyson’s equation for the \(f\)-electron propagator, which we shall solve in the next section. Diagrammatically speaking, \(G_{\alpha}^{\Gamma_{\alpha}}\) is dressed to all orders by simple hybridization processes, where the self-energy has the form (see Figure 3.1)

\[
\Sigma_{\alpha}^{\Gamma_{\alpha}}(k, \tau) - \sum_{\sigma} \delta_{\sigma} \nu_{\alpha}^{\ast}(k) G_{\sigma}(k, \tau) \tilde{V}_{\alpha}(k, \tau) \tilde{\sigma} \delta_{\Gamma_{\alpha}}. \tag{3.26}
\]

Note that at the zone center, which has octahedral \((O_h)\) symmetry, the \(\Gamma_7\) and \(\Gamma_8\) multiplets cannot mix in the self-energy. That is, \(\Sigma_{\Gamma_{\alpha}}\) is diagonal in the multiplet indices. But elsewhere in the zone, the symmetry is lower than cubic, and the sum over \(\sigma\) in equation 3.26 can be nonzero for \(\Gamma \neq \Gamma'\). The reader interested in some details here should consult Table 4.2, where all unique, non-zero results for the sum

\[
\sum_{\sigma} \tilde{\sigma} \nu_{\alpha}^{\ast}(k) \tilde{V}_{\alpha}(k, \tau) \tilde{\sigma}_{\Gamma_{\alpha}}
\]

are presented. One can explicitly show that the off-diagonal expressions vanish identically at the zone center, as they must. Interestingly, because of the vanishing of the \(\Gamma_7\) matrix elements along the axes of the cubic Brillouin zone, the off-diagonal expressions also vanish along the axes. But at an arbitrary \(k\)-point in the zone, these off-diagonal terms are non-zero. We can now write the Lagrangian in a compact notation:

\[
\mathcal{L} = \mathcal{L}_{\phi} + \sum_{k \epsilon \Gamma_{\alpha} \Gamma_{\alpha}'} \tilde{f}_{\epsilon \Gamma_{\alpha}} \left[ -G_{\Gamma_{\alpha}}^{-1}(k, \tau) \delta_{k \epsilon} + i\epsilon \lambda_{k \epsilon} \delta_{\Gamma_{\alpha} \Gamma_{\alpha}'} \delta_{\alpha} \right]
\]
Dyson’s Equation for the f Green’s function:

\[
\Gamma_\alpha + \Gamma'_{\alpha'} = \Gamma_\alpha + \Gamma'_{\alpha'}
\]

\[
\begin{array}{c}
\Gamma_\alpha \\
\downarrow \\
\tilde{k}
\end{array}
\begin{array}{c}
\Gamma'_{\alpha'} \\
\downarrow \\
\tilde{k}
\end{array}
\begin{array}{c}
\Gamma_\alpha \\
\downarrow \\
\tilde{k}
\end{array}
\]

with self-energy \( \Sigma_{\Gamma_\alpha\Gamma'_{\alpha'}}(\tilde{k}) = \)

\[
\begin{array}{c}
\tilde{k}
\end{array}
\]

Figure 3.1:

A diagrammatic representation of the infinite-order summation that gives the mean-field dressed f-electron propagator. All the Green functions are defined pictorially at the top of the figure. The bare conduction electron propagator is represented by a solid line.
\[
+ \delta \tilde{s}_{\kappa - \tilde{k} \Gamma} G^{C}_{\Gamma \alpha \Gamma', \alpha'}(\kappa', \tau) + G^{B}_{\Gamma \alpha \Gamma', \alpha'}(\kappa, \tau) \delta \tilde{s}_{\kappa - \tilde{k} \Gamma'}
\]
\[
\sum_{\tilde{k}''} \delta \tilde{s}_{\tilde{k}'' \Gamma} G^{A}_{\Gamma \alpha \Gamma', \alpha'}(\tilde{k}'', \tau) \delta \tilde{s}_{\tilde{k}'' - \tilde{k} \Gamma'} f_{\tilde{k} \Gamma' \alpha'} + \mathcal{L}_{\text{constraint}},
\]  
(3.27)

where \( \mathcal{L}_{\phi} \) is the term quadratic in the \( \phi \) fields. Note that everything but the first term inside the square brackets is due to fluctuations beyond mean-field.

3.2.3 Integration over the Grassmann variables

Before integrating out the Grassmann fields, we transform all \( \tau \) dependent quantities in the Lagrangian into functions of the Matsubara quantities. Upon such a transformation, the Grassmann fields are “odd” in frequency and the complex fields are “even”:

\[
f_{\kappa \Gamma \alpha}(\tau) = \frac{1}{\sqrt{N_{\phi}}} \sum_{\omega_n} f_{\kappa \Gamma \alpha}(i \omega_n) e^{-i \omega_n \tau},
\]

(3.28)

\[
\tilde{s}_{\kappa \Gamma}(\tau) = \sum_{\nu_n} \tilde{s}_{\kappa \Gamma}(i \nu_n) e^{-i \nu_n \tau},
\]

(3.29)

where \( \nu_n = i2\pi n / \beta \) and \( \omega_n = (2n+1)i\pi / \beta \). The reader interested in more mathematical detail at this juncture, should consult chapter 2 of reference 1. During the course of this derivation, it is useful to remember the orthonormality condition for the Matsubara frequencies,

\[
\frac{1}{\beta} \int_{0}^{\beta} d\tau e^{i\tau(\omega_n - \omega_{n'})} = \delta_{nn'}.
\]

(3.30)

Recall from the previous chapter that the partition function has the general form

\[
Z = \int \mathcal{D}\phi \mathcal{D}\dot{\phi} \mathcal{D}f \mathcal{D}f' \mathcal{D}s \mathcal{D}s' e^{-\int_{0}^{\beta} d\tau \mathcal{L}(\tau)},
\]

(3.31)

where the argument of the exponential is just the negative of the action

\[
S = \int_{0}^{\beta} d\tau \mathcal{L}(\tau).
\]

(3.32)
In Matsubara space, the action is

\[ S = \sum_{k\sigma} \phi^\dagger_{k\sigma}(i\omega_n) \left[ -i\omega_n + \xi_k \right] \phi_{k\sigma}(i\omega_n) \]

\[ + \sum_{k\Gamma'\alpha'\sigma'} f^\dagger_{k\Gamma'\alpha'}(i\omega_n) \left[ -G^{-1}_{\Gamma\alpha\alpha'}(k', i\omega_n) \delta_k \delta_{\Gamma\Gamma'} \delta_{\alpha\alpha'} \right] f_{k\Gamma'\alpha'}(i\omega_n) \]

\[ + \sum_{k\Gamma\alpha\Gamma'\alpha'} f^\dagger_{k\Gamma\alpha'}(i\omega_n) \left[ i\delta\lambda_{k-k'}(i\omega_n - i\omega_n') \delta_{\Gamma\Gamma'} \delta_{\alpha\alpha'} \right] f_{k\Gamma'\alpha'}(i\omega_n') \]

\[ + \sum_{k\Gamma\alpha\Gamma'\alpha'} f^\dagger_{k\Gamma\alpha'}(i\omega_n) \left[ \delta\delta^* \delta_{k-k'}(i\omega_n + i\omega_n' - i\omega_n) G^C_{\Gamma\alpha\alpha'}(k', i\omega_n"

\[ + G^B_{\Gamma\alpha\alpha'}(k', i\omega_n"

\[ \times \delta\delta^* \delta_{k-k'}(i\omega_n - i\omega_n' - i\omega_n) \right] f_{k\Gamma'\alpha'}(i\omega_n') \right) \]

(3.33)

For simplicity of notation, we condense this expression to the following:

\[ S = S_{\phi\phi} + \text{Tr} f^\dagger_{k\Gamma\alpha}(\omega_n) \left[ -G_{\Gamma\alpha\alpha'}^{-1}(i\omega_n) + i\delta\lambda + \delta\delta^* G^C + G^B \delta\delta + \delta\delta^* G^A \delta\delta \right] f_{k\Gamma'\alpha'}(\omega_n'), \]

(3.34)

where we have not shown explicitly the momentum and frequency dependence inside the square brackets. \( S_{\phi\phi} \) is the term quadratic in the \( \phi \) fields.

We now integrate out the Grassmann fields in the action, which is just a fancy Gaussian integral of the generic form

\[ \int D\tilde{x}Dx e^{-\tilde{x}aF_{ab}x^b} = \det F = e^{\text{Tr} \ln \tilde{F}}, \]

(3.35)

and which is proved in reference [1]. \( x_a \) is a vector with Grassmann variables as components, and \( \tilde{F} \) is a matrix with indices \( a \) and \( b \). The second equality in equation 3.35 is easy to see when \( \tilde{F} \) is a diagonal matrix. In that case

\[ \text{Tr} \ln \tilde{F} = \sum_i \ln F_{ii}, \]
which gives
\[ e^{\text{Tr} \ln \hat{F}} = e^{\sum \ln F_{ii}} = \prod_i e^{\ln F_{ii}} = \prod_i F_{ii} = \det \hat{F}. \]

Generalization to a non-diagonal matrix follows from the fact that the trace keeps the same value, regardless of the basis in which the matrix is constructed.

Note in equation 3.34 that the action is separable with respect to the \( \phi \) and \( f \) fields. We can then apply equation 3.35 independently to each set of variables. The \( \phi \) fields give the following contribution to the partition function, which we label as \( Z_{\text{cond}} \) because of the presence of the conduction electron dispersion \( \xi_k \):

\[ Z_{\text{cond}} = \int \mathcal{D}\phi \mathcal{D}f \exp\left[ -\sum_{\vec{k}\sigma} \bar{\phi}_{\vec{k}\sigma}(i\omega_n)(-i\omega_n+\xi_k)\phi_{\vec{k}\sigma}(i\omega_n) \right] = e^{\text{Tr} \ln (-i\omega_n+\xi_k)}, \tag{3.36} \]

where the trace signifies the sum over \( \vec{k}, \sigma, \) and \( i\omega_n \).

Clearly, the \( f \) fields have more interesting physics, so we turn to the integral

\[ \int \mathcal{D}\tilde{f} \mathcal{D}f \exp\left[ -\sum_{\vec{k}\vec{k}'\Gamma\Gamma'\sigma'\sigma''} \bar{f}_{\vec{k}\Gamma\sigma}(i\omega_n)(-G_{\Gamma\alpha\Gamma'\alpha'}^{-1} + i\delta\lambda + \delta\bar{s}^*G^A\delta\bar{s} + G^B\delta\bar{s} + \delta\bar{s}^*G^C) f_{\vec{k}'\Gamma'\alpha'}(i\omega_{n'}) \right] \]

\[ = \exp \left[ \text{Tr} \ln \left( -G_{\Gamma\alpha\Gamma'\alpha'}^{-1} + i\delta\lambda + \delta\bar{s}^*G^A\delta\bar{s} + G^B\delta\bar{s} + \delta\bar{s}^*G^C \right) \right], \tag{3.37} \]

where the trace means we must sum over \( \vec{k}, \vec{k}', \Gamma, \Gamma', \alpha, \alpha', i\omega_n, \) and \( i\omega_{n'}. \) A slight shuffling of the argument of the exponential yields

\[ \exp \left[ \text{Tr} \ln G_{\Gamma\alpha\Gamma'\alpha'}^{-1} + \text{Tr} \ln \left[ 1 - G_{\Gamma\alpha\Gamma'\alpha'} \left( i\delta\lambda + \delta\bar{s}^*G^A\delta\bar{s} + G^B\delta\bar{s} + \delta\bar{s}^*G^C \right) \right] \right]. \tag{3.38} \]

The first term in equation 3.38 is the mean-field contribution, and the remaining terms are the fluctuations, summed to infinite order in \( \delta s \) and \( \delta \lambda \). In the next
chapter, we shall expand the logarithm to second order in the fluctuating fields, so that we can perform the resulting Gaussian integrals. For the rest of this chapter, however, we shall focus only on the mean-field physics.

We remind the reader that for the last few pages we have been looking at the contributions to the partition function from the Grassmann fields, but the Bose fields are still lurking about in the constraint term of the Lagrangian. We now define the mean field vertex, $\hat{\Gamma}_o$, mentioned in the introduction to this chapter. Substituting equations 3.16 and 3.17 into $L_{\text{constraint}}$ (equation 3.10) and combining terms gives

\[
L_{\text{constraint}} = \frac{N_s}{2} \sum_{\Gamma} N_{\Gamma} i\lambda_o \left( \delta \tilde{s}_{\Gamma}^* - q_{o\Gamma} \right) + \frac{N_s^2}{2} \sum_{k\Gamma} N_{\Gamma} \left[ \begin{array}{cc} \delta \tilde{s}_{k\Gamma}^* & i\delta \lambda_k \\ \delta \tilde{s}_{o\Gamma} & 0 \end{array} \right] \left[ \begin{array}{c} i\lambda_o \\ \delta \tilde{s}_{o\Gamma} \\ i\lambda_k \end{array} \right]. \tag{3.39}
\]

We thus define the vertex as

\[
\hat{\Gamma}_{o\Gamma} = \frac{N_{\Gamma}}{2} \left[ \begin{array}{cc} i\lambda_o & \tilde{s}_{o\Gamma} \\ \tilde{s}_{o\Gamma} & 0 \end{array} \right], \tag{3.40}
\]

where $\hat{\Gamma}_o = \sum_{\Gamma} \hat{\Gamma}_{o\Gamma}$. The corresponding Green function is

\[
\hat{D}_{o\Gamma}^{-1} = -\frac{N_{\Gamma}}{2} \left[ \begin{array}{cc} i\lambda_o & \tilde{s}_{o\Gamma} \\ \tilde{s}_{o\Gamma} & 0 \end{array} \right]. \tag{3.41}
\]

Thus, $\hat{D}_{o\Gamma}$ manifests a $1/N_{\Gamma}$ dependence. When we include the fluctuations from the second term in equation 3.38, $\hat{D}_{o\Gamma}$ will be dressed by bubble diagrams constructed from both conduction and 4f electrons. A discussion of such effects is the subject of the next chapter.

Finally, we write the partition function at the mean-field level

\[
Z_{MF} = Z_{\text{cond}} \int Ds D\lambda
\]
\[
\times \exp \left[ \text{Tr} \ln G_{\Gamma\alpha\Gamma'\alpha'}^{-1}(\vec{k}, i\omega_n) - \frac{\beta N_s}{2} \sum_{\Gamma} N_{\Gamma i} \lambda_\alpha \left( \hat{s}_{\alpha\Gamma}^2 - q_{\alpha\Gamma} \right) \right]. \quad (3.42)
\]

We shall perform a saddle-point evaluation of the remaining Bose integrals, but first we gather more information about the nature of the mean-field quasiparticle states, as deduced from the poles of the 4f Green function, \( G_{\Gamma\alpha\Gamma'\alpha'}(\vec{k}, i\omega_n) \).

### 3.3 The 4f Green Function, \( G_{\Gamma\alpha\Gamma'\alpha'}(\vec{k}, \omega) \)

In this and the next few sections, we are going to solve for the 4f Green function and the quasiparticle band energies, \( E_{n\vec{k}} \). Such calculations are most easily discussed in the usual Hamiltonian formalism, and so we shall have a respite from functional integrals for a short while.

Let the 4f Green function be a matrix in the crystal field indices. At a point in the cubic Brillouin zone not on an axis (and not at the zone center), the symmetry is lower than \( O_h \), and the self energy can mix the two multiplets, \( \Gamma_7 \) and \( \Gamma_8 \). Then the matrix Dyson’s equation

\[
G_{\Gamma\alpha\Gamma'\alpha'}^{-1}(\vec{k}, \omega) = G_{\Gamma\alpha}^{-1}(\omega) - \Sigma_{\Gamma\alpha\Gamma'\alpha'}(\vec{k}, \omega)
\]

is written, for convenience, in the shorthand notation

\[
\hat{G}^{-1} = \hat{G}_o^{-1} - \hat{\Sigma},
\]

where \( \hat{G} = G_{\Gamma\alpha\Gamma'\alpha'} \) and \( \hat{G}_o = G_{\Gamma\alpha} \). Next, we make use of the identity for generic matrices \( \hat{A}, \hat{B}, \hat{X}, \) and \( \hat{Y} \), that if \( \hat{A} = \hat{B} + \hat{X} \hat{Y} \), then

\[
\hat{A}^{-1} = \hat{B}^{-1} - \left( \hat{B}^{-1} \hat{X} \right) \left( \hat{I} + \hat{Y} \hat{B}^{-1} \hat{X} \right)^{-1} \left( \hat{Y} \hat{B}^{-1} \right).
\]

In our case, \( \hat{B} = \hat{I} \) (the unit matrix), \( \hat{X} = \hat{\Sigma} \), and \( \hat{Y} = \hat{G}_o \). Then equation 3.43 can be inverted,

\[
\hat{G} = \hat{G}_o \left( \hat{I} - \hat{\Sigma} \hat{G}_o \right)^{-1}
\]
We have seen that the 4f self-energy can be written as
\[ \Sigma_{\Gamma\alpha\Gamma'\alpha'} = \tilde{s}_{\alpha\Gamma} \tilde{V}_{\Gamma\alpha\sigma} G_{\sigma\sigma} \tilde{V}_{\alpha\Gamma'\sigma'} \tilde{s}_{\alpha'\Gamma'} . \]

In keeping with our shorthand matrix notation, we write
\[ Y_{l=V'G_{0}V} , \]
where the \( \tilde{s}_{\alpha\Gamma} \) have been absorbed into the \( \tilde{V} \) for convenience. The previous equation becomes
\[ \hat{G} = \hat{G}_{0} \left[ \hat{1} + \hat{\Sigma} \left( \hat{V}^{\dagger} \hat{G}_{\sigma\sigma} \hat{V} - \hat{V}^{\dagger} \hat{G}_{\sigma\sigma} \hat{V} \hat{G}_{\sigma\sigma} \hat{V}^{\dagger} \hat{G}_{\sigma\sigma} \hat{V} \right)^{-1} \hat{\Sigma} \hat{G}_{\sigma} \right] . \]

Following Zhang and Lee\[6\], we define the \( 2 \times 2 \) matrix
\[ \hat{\gamma} = \hat{V} \hat{G}_{\sigma} \hat{V}^{\dagger} \hat{G}_{\sigma} , \tag{3.45} \]
which produces
\[ \hat{G} = \hat{G}_{0} \left[ \hat{1} + \hat{\Sigma} \left( \hat{V}^{\dagger} \hat{G}_{\sigma\sigma} \hat{V} - \hat{V}^{\dagger} \hat{G}_{\sigma\sigma} \hat{V} \hat{G}_{\sigma\sigma} \hat{V}^{\dagger} \hat{G}_{\sigma\sigma} \hat{V} \right)^{-1} \hat{\Sigma} \hat{G}_{\sigma} \right] , \]
\[ \hat{G} = \hat{G}_{0} \left[ \hat{1} + \hat{\Sigma} \hat{V}^{-1} (\hat{1} - \hat{\gamma})^{-1} \hat{G}_{\sigma\sigma}^{-1} (\hat{V}^{\dagger})^{-1} \hat{\Sigma} \hat{G}_{\sigma} \right] , \]
\[ \hat{G} = \hat{G}_{0} \left[ \hat{1} + \hat{V}^{\dagger} \hat{G}_{\sigma\sigma}(\hat{1} - \hat{\gamma})^{-1} \hat{V} \hat{G}_{\sigma} \right] . \tag{3.46} \]

We rewrite equation 3.46 with a complex frequency, \( z \), momentum \( \vec{k} \), and and with all the subscripts shown:
\[ G_{\Gamma\alpha\Gamma'\alpha'}(\vec{k}, z) = G_{\Gamma\alpha}(z) \left[ 1 + \tilde{s}_{\alpha\Gamma} \tilde{V}_{\Gamma\alpha\sigma}(\vec{k}) G_{\sigma\sigma}(\vec{k}, z) \right. \]
\[ \times \left. \left( 1 - \gamma_{\sigma\alpha'}(\vec{k}, z) \right)^{-1} \tilde{s}_{\alpha'\Gamma'} \tilde{V}_{\Gamma'\alpha'\sigma'}(\vec{k}) G_{\Gamma'\alpha'}(z) \right] , \tag{3.47} \]
where

$$\gamma_{\alpha\sigma}(\vec{k}, z) = \sum_{\Gamma\alpha} \delta_{\alpha\Gamma} \tilde{V}_{\Gamma\alpha\sigma}(\vec{k}) G_{\Gamma\alpha}(z) \delta_{\sigma\alpha} \tilde{V}_{\Gamma\alpha\sigma}^*(\vec{k}) G_{\sigma\alpha}(\vec{k}, z). \quad (3.48)$$

By time-reversal symmetry, $\gamma$ is diagonal, so that

$$\left( i - \gamma \right)^{-1} = \begin{bmatrix} 1/1-\gamma^{++} & 0 \\ 0 & 1/1-\gamma^{--} \end{bmatrix}, \quad (3.49)$$

where

$$\gamma_{\alpha\sigma}(\vec{k}, z) = \sum_{\Gamma\alpha} \frac{\delta_{\alpha\Gamma}^2 |\tilde{V}_{\Gamma\alpha\sigma}^2(\vec{k})|^2}{(z - \xi_{\vec{k}}) (z - E_{\Gamma} - i\lambda_{\alpha})}. \quad (3.50)$$

In equation 3.50, we have used the identities

$$G_{\Gamma\alpha} = \frac{1}{z - E_{\Gamma} - i\lambda_{\alpha}}, \quad \text{and}$$

$$G_{\sigma\alpha} = \frac{1}{z - \xi_{\vec{k}}},$$

as the bare 4f and conduction electron propagators, respectively. We define the shifted energy for each crystal-field multiplet by

$$\epsilon_{\Gamma} = E_{\Gamma} + i\lambda_{\alpha}. \quad (3.51)$$

Equation 3.47 now becomes

$$G_{\Gamma\alpha\Gamma'\alpha'}(\vec{k}, z) = \frac{1}{z - \epsilon_{\Gamma}} \left[ \delta_{\Gamma\Gamma'} \delta_{\alpha\alpha'} + \frac{1}{z - \epsilon_{\Gamma'}} \frac{\delta_{\alpha\Gamma} \tilde{V}_{\Gamma\alpha\sigma} \tilde{V}_{\Gamma'\alpha'\sigma'} \delta_{\sigma\Gamma'}}{(z - \xi_{\vec{k}}) - \delta_{\alpha\Gamma} \delta_{\sigma\Gamma'}} \right], \quad (3.52)$$

where there is an implicit sum over $\sigma$ in the numerator and over $\Gamma'$, $\alpha'$ in the denominator, and where all matrix elements on the right side are functions of $\vec{k}$.

We focus momentarily on the denominator of the second term inside the square brackets. It can be written as

$$\left( z - \xi_{\vec{k}} \right) - \sum_{\alpha''} \frac{\delta_{\alpha\alpha''}^2 |\tilde{V}_{\Gamma\alpha''\sigma''}|^2}{(z - \epsilon_{\Gamma})} - \sum_{\alpha''} \frac{\delta_{\alpha''}^2 |\tilde{V}_{\Gamma\alpha''\sigma''}|^2}{(z - \epsilon_{\Gamma})} - \sum_{\alpha''} \frac{\delta_{\alpha''}^2 |\tilde{V}_{\Gamma\alpha''\sigma''}|^2}{(z - \epsilon_{\Gamma})}$$
\[
(z - \xi_r)(z - \epsilon_7)(z - \epsilon_8) - (z - \epsilon_8) \sum_{\alpha''} \tilde{s}_{\alpha 7}^2 \left| \tilde{V}_{\alpha''\sigma''\gamma} \right|^2 - \sum_{\alpha''} \tilde{s}_{\alpha 8}^2 \left| \tilde{V}_{\alpha''\sigma''\gamma} \right|^2
\]
\[
(z - \epsilon_7)(z - \epsilon_8)
\]
(3.53)

where we have used the notation \( \Gamma_7 \rightarrow 7 \) and \( \Gamma_8 \rightarrow 8 \). Note that the first sum over \( \alpha'' \) in equation 3.53 is restricted to the \( \Gamma_7 \) multiplet, and the second sum is restricted to the \( \Gamma_8 \) multiplet.

At this juncture, we claim that the roots of the numerator of equation 3.53 are the quasiparticle band energies (In the next section, we shall show it is true.). Since equation 3.53 is of third order, there are three bands, which are labeled as \( E_n(\vec{k}) \) \((n=1,2,3)\). Equation 3.53 becomes

\[
\frac{(z - E_1)(z - E_2)(z - E_3)}{(z - \epsilon_7)(z - \epsilon_8)}
\]

which finally yields the (hybridization dressed) 4f Green function

\[
G_{\Gamma \alpha \Gamma' \alpha'}(\vec{k}, z) = \frac{1}{z - \epsilon_\Gamma} \left[ \delta_{\Gamma \Gamma'} \delta_{\alpha \alpha'} + \frac{1}{z - \epsilon_\Gamma} \frac{(z - \epsilon_7)(z - \epsilon_8) \tilde{s}_{\alpha 7} \tilde{V}_{\Gamma \alpha' \sigma'}(\vec{k}) \tilde{V}_{\Gamma' \alpha' \sigma'}(\vec{k}) \tilde{s}_{\alpha' 8}}{(z - E_{1k})(z - E_{2k})(z - E_{3k})} \right].
\]

(3.54)

In the next section, we calculate the quasiparticle bands, \( E_n(\vec{k}) \), themselves.

3.4 Quasiparticle States from a Simple Matrix Diagonalization Problem

3.4.1 Mean-Field Hamiltonian

In this section, we discuss an easy way to calculate the quasiparticle band energies. We start with the mean-field Hamiltonian, in which \( \tilde{s}_{\alpha \Gamma} \) and \( \lambda_\alpha \) are uniform in space and time:

\[
H_{MF} = \sum_{\vec{k} \sigma} \xi_{\vec{k} \sigma} c_{\vec{k} \sigma}^\dagger c_{\vec{k} \sigma} + \sum_{\vec{k} \Gamma \alpha} \epsilon_\Gamma f_{\vec{k} \Gamma \alpha}^\dagger f_{\vec{k} \Gamma \alpha} + \sum_{\vec{k} \sigma \Gamma \alpha} \left[ \tilde{s}_{\sigma \alpha} \tilde{V}_{\alpha \sigma}(\vec{k}) c_{\vec{k} \sigma}^\dagger f_{\vec{k} \Gamma \alpha} + H.c. \right]
\]
\[ + \frac{N_s}{2} \sum \xi_i \lambda_i \left( \hat{\mathbf{s}}_{\mathbf{r}}^2 - q_{\alpha \mathbf{r}} \right), \]  
where \( \epsilon_i \equiv E_i + i \lambda_i \). We can easily cast equation 3.55 as a matrix multiplication problem of the form

\[ H_{MF} = \Psi^\dagger H \Psi + H_{\text{constraint}}, \]

where \( H_{\text{constraint}} \) is just the last term of equation 3.55. \( \Psi \) is an eight component column vector describing the two conduction pseudo-spin and the six 4f multiplet degrees of freedom per k point

\[ \Psi = \begin{bmatrix} c_{k+} \\ c_{k-} \\ f_{k,1} \\ \vdots \\ f_{k,6} \end{bmatrix}. \]

\( \mathcal{H} \) is an \( 8 \times 8 \) matrix, which we want to diagonalize. It turns out that we can understand the structure of the eigenvalues and eigenvectors of \( \mathcal{H} \) by solving, first, an even smaller matrix problem, namely that of a plane wave hybridizing with two non-degenerate crystal-field states. We represent this simpler problem as the following series of matrix multiplications:

\[ \begin{bmatrix} \xi_k & V_1 & V_2 \\ V_1^* & \epsilon_1 & 0 \\ V_2^* & 0 & \epsilon_2 \end{bmatrix} \begin{bmatrix} c_k \\ f_{k,1}^\dagger \\ f_{k,2}^\dagger \end{bmatrix}, \]

where the crystal field states here are labeled as "1" and "2", and where (as usual) \( \xi_k \) is the conduction electron dispersion.

It is easy to see that the secular equation for the \( 3 \times 3 \) matrix is

\[ (\xi_k - E)(\epsilon_1 - E)(\epsilon_2 - E) - |V_1|^2(\epsilon_2 - E) - |V_2|^2(\epsilon_1 - E) = 0, \]
and the eigenvector for the n-th band is

\[ |\psi_{\vec{k}n\sigma}\rangle = A_n \left[ (\vec{k}\sigma) - \frac{V_1^*}{\epsilon_1 - E_n} |1\rangle - \frac{V_2^*}{\epsilon_2 - E_n} |2\rangle \right], \]

where

\[ A_n^2 = \left[ 1 + \frac{|V_1|^2}{(\epsilon_1 - E_n)^2} + \frac{|V_2|^2}{(\epsilon_2 - E_n)^2} \right]^{-1} \]  

(3.59)
is the normalization function.

The matrix \( \mathcal{H} \) in our calculation has the same structure as the 3\times 3 matrix in equation 3.57, and so it is straightforward to generalize this solution to that of the 8 \times 8 matrix embedded in equation 3.55. Because the \( \Gamma_8 \) states are four-fold degenerate, there must be one solution of \( E = \epsilon_8 \) for every k-point. That is, there is one non-hybridizing band of \( \Gamma_8 \) symmetry. The secular equation for \( \mathcal{H} \) is

\[ (\epsilon_8 - E) \left( \xi_{\vec{k}} - E \right) - \sum_{\alpha} \frac{\delta^2_{\alpha\gamma} |\tilde{V}_{\alpha\sigma}|^2}{(\epsilon_7 - E)} - \sum_{\alpha} \frac{\delta^2_{\alpha\beta} |\tilde{V}_{\beta\alpha\sigma}|^2}{(\epsilon_8 - E)} = 0, \]  

(3.60)

which justifies equation 3.54.

The eigenvectors of \( \mathcal{H} \) are

\[ |Q_{\vec{k}n\sigma}\rangle = A_n(\vec{k}) \left[ (\vec{k}\sigma) - \sum_{\Gamma\alpha} \frac{\delta_{\alpha\Gamma} \tilde{V}_{\alpha\sigma}(|\vec{k}\rangle)}{\epsilon_\Gamma - E_{n\vec{k}}} |\Gamma\alpha\rangle \right], \]  

(3.61)

where

\[ A_n^2(\vec{k}) = \left[ 1 + \sum_{\Gamma\alpha} \frac{\delta^2_{\alpha\Gamma} |\tilde{V}_{\alpha\sigma}(\vec{k})|^2}{(\epsilon_\Gamma - E_{n\vec{k}})^2} \right]^{-1}. \]  

(3.62)

On the left-hand side of equation 3.61, \( \sigma = \pm 1 \) is the pseudo-spin variable. True spin is no longer a good quantum number in the presence of spin-orbit coupling.

The eigenvectors \( |Q_{\vec{k}n\sigma}\rangle \) can be used to construct a unitary matrix, \( U \), that diagonalizes \( \mathcal{H} \). That is, we write equation 3.55 as \( H_{MF} = \Psi^\dagger U U^\dagger \mathcal{H} U U^\dagger \Psi \), where \( U U^\dagger = 1 \). Next, define the column vector in the quasiparticle basis as \( Q = U^\dagger \Psi \).
The new Hamiltonian matrix, \( \mathcal{H}_d = U^\dagger \mathcal{H} U \) is diagonal, with the diagonal elements being the quasiparticle energies \( E_{n\mathbf{k}} \). Thus in the quasiparticle basis we have \( \mathcal{H}_{MF} = Q^\dagger \mathcal{H}_d Q \).

Using the relation \( \Psi = U \mathbf{Q} \), we can relate the creation and destruction operators in the original basis (\( \Psi \)) to the quasiparticle operators \( Q^\dagger_{k_{n\sigma}} \) and \( Q_{k_{n\sigma}} \) in the quasiparticle basis (\( Q \)). We find that

\[
\begin{align*}
    c_{\mathbf{k}\sigma} &= \sum_{n} A_n(\mathbf{k})Q_{k_{n\sigma}}, \\
    f_{\mathbf{k}\Gamma\alpha} &= -\sum_{n\sigma} \frac{A_n(\mathbf{k})\tilde{s}_{\alpha\sigma}V_{\Gamma\alpha\sigma}(\mathbf{k})}{\epsilon_{\Gamma} - E_{n\mathbf{k}}} Q_{k_{n\sigma}}.
\end{align*}
\]

These two expressions will be important in the next chapters, when we actually construct the two-quasiparticle scattering amplitude.

### 3.4.2 Nature of the Quasiparticle States

In this subsection we plot the quasiparticle bandstructure as a function of \( \mathbf{k} \). Since equation 3.60 is cubic, it is possible to write the solutions for \( E_{n}(\mathbf{k}) \) in closed form. The expressions are so cumbersome as to be effectively useless on paper, but we can easily evaluate them numerically. Figure 3.2 shows the bands along two different directions in the Brillouin zone. In Figure 3.2(a) the bands are plotted along the \( k_x \) axis, which is a special direction for cubic symmetry (i.e., the symmetry is higher along an axis than along an arbitrary direction in \( k \)-space). In general, along any of the axes, all hybridization matrix elements involving \( \Gamma_7 \) states vanish. That is, the symmetry of the \( \Gamma_7 \) states is such that \( V_{\Gamma\alpha\sigma}(\mathbf{k}) = 0 \) for any \( \mathbf{k} \) along the \( k_x, k_y \), or \( k_z \) axes. In this case, equation 3.60 reduces to the form

\[
(\epsilon_8 - E)\left[ (\xi_8 - E)(\epsilon_7 - E)(\epsilon_8 - E) - (\epsilon_7 - E)\sum_{\alpha} \tilde{s}_{\alpha\sigma} V_{\Gamma\alpha\sigma}^* \right] = 0.
\]
Thus \( E = \epsilon_8 \) and \( E = \epsilon_7 \) are solutions for all such \( k \) points. In Figure 3.2(b), we show the most general case, in which the \( \Gamma_7 \) and half of the \( \Gamma_8 \) states hybridize with the conduction states. Note that all hybridization is weak near the zone center. In fact, because of its radial \( k \)-dependence, the matrix elements \( V_{\Gamma\alpha}(\vec{k}) \) must vanish exactly at the zone center. The Coqblin-Schrieffer matrix elements[3], from which our matrix elements are constructed, depend upon the spherical Bessel function, \( j_3(\kappa r) \), which behaves like \( k^3 \) for \( k \to 0 \), thus guaranteeing that \( V \to 0 \) at the zone center.

### 3.5 Hybridization dressed Conduction Green Function, \( G_\sigma \)

In the original (undiagonalized) basis of equation 3.55, there are actually three Green functions: \( G_{\Gamma\alpha\Gamma\alpha'} \) (the \( \Gamma \) Green function); \( G_\sigma \) (the conduction Green function); and \( G_{\Gamma\alpha\sigma} \) (the off-diagonal, or mixing, Green function). All three are defined below in terms of Fock space operators

\[
G_{\Gamma\alpha\Gamma\alpha'}(\vec{k}, \tau) \equiv -(T\tau f_{\vec{k}\Gamma\alpha}(\tau) f_{\vec{k}\Gamma\alpha'}^\dagger(0)), \tag{3.65}
\]

\[
G_\sigma(\vec{k}, \tau) \equiv -(T\tau c_{\vec{k}\sigma}(\tau) c_{\vec{k}\sigma}^\dagger(0)), \tag{3.66}
\]

\[
G_{\Gamma\alpha\sigma}(\vec{k}, \tau) \equiv -(T\tau f_{\vec{k}\Gamma\alpha}(\tau) c_{\vec{k}\sigma}^\dagger(0)), \tag{3.67}
\]

where \( T\tau \) is the imaginary time ordering operator. We have already discussed the \( \Gamma \) Green function, but it will be useful to solve for the conduction and off-diagonal Green functions as well. We start with \( G_\sigma(\vec{k}, \tau) \).

In analogy to the Dyson's equation represented in Figure 3.1, we can construct a similar equation for the conduction electron propagator \( G_\sigma \) (see Figure 3.3). From Figure 3.3 we see that the self-energy for the conduction electrons...
Figure 3.2:

Schematic band structure as determined by equation [4.58] (a)-along the axes. The $\Gamma_7$ states do not hybridize and thus remain a dispersionless band as shown. $X$ is the zone boundary along the $k_x$ axis. (b) -along the diagonal of the cubic Brillouin zone. Note the $\Gamma_8$ non-hybridizing band that is always present. $R$ labels the zone boundary along the cube diagonal.
Diagrammatic representation of Dyson's equation for the conduction Green function. The double line is the hybridization dressed Green function, and $\Sigma_{\text{cc}}(\tilde{k})$ is the conduction self-energy. All other elements of the figure are as defined in Figure 3.1.
\[
\Sigma_{\sigma\sigma}(\vec{k}) = \sum_{\Gamma \alpha} \tilde{\epsilon}_{\alpha \Gamma} \tilde{V}_{\Gamma \alpha \sigma}(\vec{k}) G_{\Gamma \alpha} \tilde{V}_{\Gamma \alpha \sigma}^*(\vec{k}) \tilde{\epsilon}_{\alpha \Gamma}, \tag{3.68}
\]

where we have momentarily suppressed the frequency dependence. Once again, we have a matrix Dyson's equation to solve:

\[
\hat{G}_{\sigma}^{-1} = \hat{G}_{\sigma\sigma}^{-1} - \hat{\Sigma}_{\sigma\sigma}, \tag{3.69}
\]

where each element is a \(2 \times 2\) matrix. Only formal matrix manipulations are now needed. We can write

\[
\hat{G}_{\sigma} = \left[ (\hat{1} - \hat{V} \hat{G}_0 \hat{V}^\dagger \hat{G}_{\sigma\sigma}) \hat{G}_{\sigma\sigma}^{-1} \right]^{-1},
\]

where we are reusing a matrix notation like that used in equation 3.45.

\[
\hat{G}_{\sigma} = \hat{G}_{\sigma\sigma} \left( \hat{1} - \hat{V} \hat{G}_0 \hat{V}^\dagger \hat{G}_{\sigma\sigma} \right)^{-1}
= \hat{G}_{\sigma\sigma} + \hat{G}_{\sigma\sigma} \hat{V} \hat{G}_0 \hat{V}^\dagger \hat{G}_{\sigma\sigma} + \hat{G}_{\sigma\sigma} \hat{V} \hat{G}_0 \hat{V}^\dagger \hat{G}_{\sigma\sigma} \hat{V} \hat{G}_0 \hat{V}^\dagger \hat{G}_{\sigma\sigma} + \cdots,
\]

from a simple binomial expansion. Recognizing the \(2 \times 2\), diagonal matrix \(\hat{\gamma} = \hat{V} \hat{G}_0 \hat{V}^\dagger \hat{G}_{\sigma\sigma}\), we write

\[
\hat{G}_{\sigma} = \hat{G}_{\sigma\sigma} \left( \hat{1} + \hat{\gamma} + \hat{\gamma}^2 + \cdots \right)
= \hat{G}_{\sigma\sigma} \left( \hat{1} - \hat{\gamma} \right)^{-1}. \tag{3.70}
\]

Using what we learned about the matrix \((\hat{1} - \hat{\gamma})^{-1}\) from the calculation of the \(f\) Green function, we see that equation 3.70 is equivalent to

\[
G_{\sigma}(\vec{k}, z) = \frac{(z - \epsilon_f)(z - \epsilon_e)}{(z - E_{1\vec{k}})(z - E_{2\vec{k}})(z - E_{3\vec{k}})}. \tag{3.71}
\]
3.6 The Off-Diagonal (Mixing) Green Function, $G_{\Gamma\alpha\sigma}$

Finally, there is the off-diagonal Green function, which we calculate by the equation of motion technique. Starting with the definition (equation 3.67) we take the $\tau$ derivative of both sides to get

$$\frac{\partial G_{\Gamma\alpha\sigma}}{\partial \tau} = -\delta(\tau)\langle\{f_{\tilde{\kappa}\Gamma\alpha}(\tau), c_{\tilde{k}\sigma}^{\dagger}(0)\}\rangle - \langle T_{\tau} \frac{\partial f_{\tilde{k}\Gamma\alpha}}{\partial \tau} c_{\tilde{k}\sigma}(0) \rangle. \quad (3.72)$$

The first term on the right hand side is just the anticommutator of $f_{\tilde{k}\Gamma\alpha}(\tau)$ and $c_{\tilde{k}\sigma}^{\dagger}(0)$, which in the presence of the Dirac delta function, $\delta(\tau)$, must vanish. To evaluate the second term on the right side, we need to calculate the following derivative:

$$\frac{\partial f_{\tilde{k}\Gamma\alpha}}{\partial \tau} = -[f_{\tilde{k}\Gamma\alpha}(\tau), H_{MF}]. \quad (3.73)$$

After some algebra, we find that

$$\frac{\partial f_{\tilde{k}\Gamma\alpha}}{\partial \tau} = -\epsilon_{\Gamma} f_{\tilde{k}\Gamma\alpha}(\tau) - \sum_{\sigma'} \bar{s}_{\sigma \Gamma} \tilde{V}_{\Gamma\alpha\sigma'}(\tilde{k}) c_{\tilde{k}\sigma'}(\tau),$$

which, when substituted into equation 3.72 gives

$$\frac{\partial G_{\Gamma\alpha\sigma}}{\partial \tau} = \epsilon_{\Gamma} \langle T_{\tau} f_{\tilde{k}\Gamma\alpha}(\tau) c_{\tilde{k}\sigma}^{\dagger}(0) \rangle + \bar{s}_{\sigma \Gamma} \tilde{V}_{\Gamma\alpha\sigma}(\tilde{k}) \langle T_{\tau} c_{\tilde{k}\sigma}(\tau) c_{\tilde{k}\sigma}^{\dagger}(0) \rangle,$$

$$\frac{\partial G_{\Gamma\alpha\sigma}}{\partial \tau} = -\epsilon_{\Gamma} G_{\Gamma\alpha\sigma}(\tilde{k}, \tau) - \bar{s}_{\sigma \Gamma} \tilde{V}_{\Gamma\alpha\sigma}(\tilde{k}) G_{\sigma}(\tilde{k}, \tau). \quad (3.74)$$

In terms of a complex frequency, $z$, we have

$$G_{\Gamma\alpha\sigma}(\tilde{k}, z) = \frac{\bar{s}_{\sigma \Gamma} \tilde{V}_{\Gamma\alpha\sigma}(\tilde{k})}{z - \epsilon_{\Gamma}} G_{\sigma}(\tilde{k}, z).$$

Substituting for $G_{\sigma}$ from equation 3.71 finally gives

$$G_{\Gamma\alpha\sigma}(\tilde{k}, z) = \frac{\frac{\bar{s}_{\sigma \Gamma} \tilde{V}_{\Gamma\alpha\sigma}(\tilde{k})}{z - \epsilon_{\Gamma}}}{(z - E_{1\tilde{k}})(z - E_{2\tilde{k}})(z - E_{3\tilde{k}})}.$$
3.7 Self-Consistency Equations

3.7.1 Saddle-Point Evaluation of the Partition Function

After building some intuition from our simple matrix diagonalization problem, we return to the expression for the partition function, equation 3.42. Focusing on the first term in the argument of the exponential, we rewrite it as

\[ \sum_{\omega_n} \ln G_{\Gamma \alpha' \Gamma' \alpha}(\vec{k}, i\omega_n), \]  

(3.76)

where all sums have been shown explicitly. First we sum over the Matsubara frequencies, \( i\omega_n = (2n+1)i\pi/\beta \). It is not necessary here to show all the mathematical detail of the sum. We merely quote the result and the relegate the mathematics to Appendix A. The remaining sums over the crystal field quantum numbers now appear as sums over the band index \( n \) and the pseudo-spin index \( \sigma \):

\[ \sum_{\vec{k}\sigma n} \ln \left( 1 - e^{-\beta E_{nk}} \right) \]

So, having started with the argument of the exponential in equation 3.42, we put everything together to get a mean field action,

\[ S_{MF}(s_0, \lambda_0) = -\frac{\beta N_s}{2} \sum_{\Gamma} i\lambda_0 (s_{0\Gamma}^2 - q_{0\Gamma}) - \sum_{\vec{k}\sigma n} \ln(1 + e^{-\beta E_{nk}}). \]  

(3.77)

We perform a saddle point evaluation of the remaining complex integrals in the partition function. This means expanding equation 3.77 about its extremum with respect to the two Bose fields, \( s_0 \) and \( i\lambda_0 \). As discussed by Read and Newns[5], and as we discussed generally in the previous chapter, this comprises the lowest order (mean-field) contribution to the partition function, and hence
also to the Free energy, since \( F = -1/\beta \ln(Z) \). Requiring that
\[
\frac{\partial S_{MF}}{\partial \lambda_o} = 0
\] (3.78)
gives
\[
\frac{1}{2} \sum \Gamma N_\Gamma (\delta_{o\Gamma}^2 - q_{o\Gamma}) + \frac{1}{N_s} \sum_{k\sigma n} f(E_{nk}) \frac{\partial E_{nk}}{\partial \lambda_o} = 0.
\] (3.79)
And requiring
\[
\frac{\partial S_{MF}}{\partial s_o} = 0
\]
gives
\[
2i\lambda_os_o + \frac{1}{N_s} \sum_{k\sigma n} f(E_{nk}) \frac{\partial E_{nk}}{\partial s_o} = 0.
\] (3.80)
We also have an equation to fix the chemical potential of the quasiparticles, \( \mu \), which depends on the total number of electrons (conduction electrons, \( n_c \), and \( f \) electrons, \( n_f \)) per unit cell
\[
n_{total} = n_c + n_f = \frac{1}{N_s} \sum_{k\sigma n} f(E_{nk}).
\] (3.81)
To proceed with the self-consistent solution of equations 3.79-3.81, we need to evaluate the derivatives \( \partial E_{nk}/\partial s_o \) and \( \partial E_{nk}/\partial \lambda_o \). Starting from the secular equation (equation 3.60), we define the following quantities:
\[
\zeta_7 = \frac{1}{2} \sum_{\sigma\alpha} s_\sigma^2 |V_{7\sigma\alpha}|^2, \quad \zeta_8 = \frac{1}{2} \sum_{\sigma\alpha} s_\sigma^2 |V_{8\sigma\alpha}|^2,
\] (3.82)
where the sum over \( \alpha \) in \( \zeta_7(\zeta_8) \) represents the sum over the two(four)-fold degenerate states in the \( \Gamma_7(\Gamma_8) \) multiplet. This means that the secular equation 3.60 can be rewritten as
\[
(\xi_k - E)(\epsilon_7 - E)(\epsilon_8 - E) - \zeta_7(\epsilon_8 - E) - \zeta_8(\epsilon_7 - E) = 0.
\] (3.83)
Taking $\partial/\partial s_0$ of both sides of equation 3.83 and solving for $\partial E/\partial s_0$ gives

$$\frac{\partial E}{\partial s_0} = \frac{s_0 \sum_\sigma |V_{7\sigma\sigma}|^2(\epsilon_8 - E) + s_0 \sum_\sigma |V_{8\sigma\sigma}|^2(\epsilon_7 - E)}{\zeta_7 + \zeta_8 - (\epsilon_7 - E)(\epsilon_8 - E) - (\xi - E)[(\epsilon_7 - E) + (\epsilon_8 - E)]}.$$  

(3.84)

Also, taking $\partial/\partial \lambda_\alpha$ gives

$$\frac{\partial E}{\partial \lambda_\alpha} = \frac{-\zeta_7 \left(\frac{\epsilon_8 - E}{\epsilon_7 - E}\right) - \zeta_8 \left(\frac{\epsilon_7 - E}{\epsilon_8 - E}\right)}{\zeta_7 + \zeta_8 - (\epsilon_7 - E)(\epsilon_8 - E) - (\xi - E)[(\epsilon_7 - E) + (\epsilon_8 - E)]}.$$  

(3.85)

As we shall see, we also need $\partial E/\partial \xi$:

$$\frac{\partial E}{\partial \xi} = \frac{-(\epsilon_7 - E)(\epsilon_8 - E)}{\zeta_7 + \zeta_8 - (\epsilon_7 - E)(\epsilon_8 - E) - (\xi - E)[(\epsilon_7 - E) + (\epsilon_8 - E)]},$$  

(3.86)

where $\xi$ is the conduction electron energy.

We discovered, that to solve equations 3.79-3.81 self-consistently with a numerical algorithm was very difficult. The problem stems from the three dimensional $\vec{k}$ sums. They are evaluated numerically by dividing the cubic Brillouin zone into $N^3$ cubes and summing the contribution from each small cube. The sums require a mesh of up to $50^3$ cubes. To get self-consistent solutions, we found it necessary to write these equations in terms of energy integrals with the appropriate density of states,

$$\frac{1}{N_\sigma} \sum_{\vec{k}_\sigma} \rightarrow 2 \int d\xi N(\xi) \int \frac{d\Omega}{4\pi},$$  

(3.87)

where $N(\xi)$ is the density of states per spin for the unhybridized conduction electrons and $d\Omega$ is an element of solid angle. After all, a one dimensional integral should be easier to calculate numerically than a three dimensional integral. Note that in the SU(N) model described in the previous chapter, the spin degeneracy would contribute a prefactor of $N$ (instead of 2) in equation 3.87. For free electrons in three dimensions the density of states is

$$N(\xi) = \frac{\pi}{4\gamma^{3/2}} \sqrt{|\xi|},$$  

(3.88)
Figure 3.4:
Schematic of the quasiparticle bandstructure, showing the shifted crystal field multiplet energies ($\epsilon_7$ and $\epsilon_8$), the chemical potential ($\mu$), and the lower band edge (-D).

where $\xi$ is measured relative to the chemical potential of the free conduction electrons, and where $\gamma = \hbar^2 \pi^2 / 2ma^2 = 3.995009$ eV ($a$ is the lattice spacing, which we took to be $3.068 \text{ Å}$).

Starting with equation 3.79, which results from differentiating the action with respect to the Lagrange multiplier, $i\lambda_o$, we write it as

$$\frac{1}{2} \sum_{\Gamma} N_{\Gamma} (\delta_{o\Gamma}^2 - q_{o\Gamma}) + 2 \sum_n \int d\xi \int \frac{d\Omega}{4\pi} f(E_n) N(\xi) \frac{\partial E_n}{\partial i\lambda_o} = 0,$$

$$\frac{1}{2} \sum_{\Gamma} N_{\Gamma} (\delta_{o\Gamma}^2 - q_{o\Gamma}) + 2 \sum_n \int dE_n \int \frac{d\Omega}{4\pi} \left( \frac{\partial \xi}{\partial E_n} \right) N(\xi(E_n)) f(E_n) \frac{\partial E_n}{\partial i\lambda_o} = 0. \quad (3.89)$$
Our analysis is at zero temperature, and we choose the filling number, \( n_{\text{total}} \), so that the quasiparticle chemical potential, \( \mu \), lies near the top of the lowest band, \( E_{q} \). So only the lowest band contributes and equation 3.89 simplifies to (dropping the \( n = 1 \) subscript)

\[
\frac{1}{2} \sum_{\Gamma} N_{\Gamma}(\hat{E}_{\sigma \Gamma}^{2} - q_{\sigma \Gamma}) + 2 \int_{-D}^{\mu} dE \int \frac{d\Omega}{4\pi} N(\xi(E)) \left( \frac{\partial \xi}{\partial E} \right) \left( \frac{\partial E}{\partial \lambda_{0}} \right) = 0, \quad (3.90)
\]

where \(-D\) is the lower band edge for the quasiparticle states, and where the Fermi function has provided a sharp upper cut-off at the quasiparticle chemical potential (see Figure 3.4). The combination \( N(\xi(E))(\partial \xi/\partial E) \) can be thought of as the quasiparticle density of states. Substituting for the two derivatives in equation 3.90 from equations 3.80 and 3.85 gives

\[
\frac{1}{2} \sum_{\Gamma} (\hat{E}_{\sigma \Gamma}^{2} - q_{\sigma \Gamma}) + 2 \int_{-D}^{\mu} dE \int \frac{d\Omega}{4\pi} N(\xi(E)) \left[ \frac{\zeta_{7}}{(\epsilon_{7} - E)^{2}} + \frac{\zeta_{8}}{(\epsilon_{8} - E)^{2}} \right]. \quad (3.91)
\]

To proceed, we make one approximation. We assume that surfaces of constant energy for the quasiparticle states are spherically symmetric. Near the zone center, this is exactly correct, and there is no approximation at all. Near the zone boundary, the equal-energy surfaces become distorted from spheres due to the constraints of \( \Gamma \) symmetry. Figure 3.5 shows the projection of a constant-energy surface onto the \( k_{x}k_{y} \) plane, when the chemical potential intersects the lower band roughly as in Figure 3.4. We see that the distortion is strongest along the \( k_{x} \) and \( k_{y} \) axes.

It is important to note, that in equation 3.91, the strongest angular dependence comes from the anisotropic matrix elements in \( \zeta_{7} \) and \( \zeta_{8} \), which we treat exactly. Similarly, as we shall see later, the quasiparticle normalization \( A_{\xi}(\vec{k}) \) (equation 3.62) is strongly anisotropic, and effectively all of the anisotropy comes from the matrix elements. Thus, even though it is an approximation to assume
Figure 3.5:

Projection of a constant-energy surface onto the $k_x$-$k_y$ plane of the Brillouin zone. The filling of the quasiparticle band was chosen so that the chemical potential lies near the top of the band, where the states are mostly of $\Gamma_7$ symmetry. Note the distortion from spherical symmetry is largest near the axes.
spherical surfaces of constant energy (at least for k-points not near the zone center), we believe the angular dependence of the energies is not as important as that of the hybridization matrix elements. For example, near an axis of the Brillouin zone, the $\Gamma_7$ matrix elements are going to zero, thus forcing $\zeta_7$ also to zero. So, even if the quasiparticle energies surfaces are distorted from spheres near the axes, the sensitivity of equation 3.91 to this distortion would be lessened by the presence of the $\zeta_7$ term in the numerator. Thus, it does not seem a drastic approximation in equation 3.91 to treat $\zeta_7$ and $\zeta_8$ as having all the angular dependence.

Recall that $\zeta_7 = \frac{1}{2} \sum_{\sigma\sigma'} s_{\sigma\sigma'}^2 |V^2_{\alpha\sigma}|^2$. For a given multiplet, we can calculate the sums over $\sigma$ and $\alpha$ exactly; it is a length calculation, so the details are relegated to Appendix C. The results are:

$$\zeta_7 = \frac{2}{3} \sqrt{\pi} s_o^2 V_{k_0}^2 \left[ Y_{00} - \frac{1}{3} Y_{40}(\hat{k}) - \frac{1}{3} \sqrt{\frac{5}{14}} (Y_{44}(\hat{k}) + Y_{4-4}(\hat{k})) \right], \quad (3.92)$$

$$\zeta_8 = \frac{4}{3} \sqrt{\pi} s_o^2 V_{k_0}^2 \left[ Y_{00}(\hat{k}) + \frac{1}{6} Y_{40}(\hat{k}) + \frac{1}{6} \sqrt{\frac{5}{14}} (Y_{44}(\hat{k}) + Y_{4-4}(\hat{k})) \right], \quad (3.93)$$

where $V_{k_0}$ signifies the dependence of the hybridization upon the radial component of the momentum, which we assume is the same for both multiplets. $Y_{lm}(\hat{k})$ are the usual spherical harmonics. Except very near the zone center, the dependence of the matrix element on the radial component of momentum is very weak. Thus, it is a good approximation (away from the zone center) to write $V_{ok} = V_o$ and to think of $V_o$ as a bare hybridization strength.

Note that the combination $\zeta_7 + \zeta_8$ obeys the usual hybridization sum rule[6]

$$\zeta_7 + \zeta_8 = \frac{2}{3} \sqrt{\pi} s_o^2 V_{k_0}^2 Y_{00} = s_o^2 V_{k_0}^2, \quad (3.94)$$

where the $k$ dependence in $V_{ok}$ is important only near the zone center. We can
now integrate over the solid angle

$$\int \frac{d\Omega}{4\pi} \sum_{\alpha\sigma} |V_{7\alpha\sigma}|^2 = \frac{V_{k_0}^2}{3}, \quad (3.95)$$

$$\int \frac{d\Omega}{4\pi} \sum_{\alpha\sigma} |V_{8\alpha\sigma}|^2 = \frac{5}{3} V_{k_0}^2. \quad (3.96)$$

Equation 3.91 then becomes

$$\frac{1}{2} \sum_{\Gamma} N_\Gamma(s_{\alpha\Gamma}^2 - q_{\alpha\Gamma}) + \frac{s_o^2 V_{k_0}^2}{3} \int_{-\mu}^{\mu} dE N(\xi(E)) \left[ \frac{1}{(e_7 - E)^2} + \frac{5}{(e_8 - E)^2} \right] = 0. \quad (3.97)$$

When we analyze equations 3.80 (the $\partial/\partial s_o$ equation) and 3.81 (the chemical potential equation) similarly, we arrive at

$$2i\lambda_o - 2 \frac{V_{k_0}^2}{3} \int_{-\mu}^{\mu} dE N(\xi(E)) \left[ \frac{1}{e_7 - E} + \frac{5}{e_8 - E} \right] = 0, \quad \text{and} \quad (3.98)$$

$$n_{\text{total}} - \frac{2}{3} \int_{-\mu}^{\mu} dE N(\xi(E)) \left[ 1 + \frac{s_o^2 V_{k_0}^2}{(e_7 - E)^2} + \frac{5s_o^2 V_{k_0}^2}{(e_8 - E)^2} \right]. \quad (3.99)$$

These are the coupled equations that we must solve self-consistently.

Before discussing the formal procedure used to solve the above equations, let's see how they simplify in the limit of spherical symmetry (i.e. no crystal field splitting). Equation 3.97 becomes

$$s_o^2 - 1 + 2s_o^2 V_o^2 N(0) \int_{-\mu}^{\mu} dE \frac{1}{(e - E)^2} = 0,$$

where we have, for simplicity, assumed a structureless density of states for the free conduction electrons. Integrating gives

$$s_o^2 - 1 + 2N(0)s_o^2 V_o^2 \left[ \frac{1}{e - \mu} + \frac{1}{D + \epsilon} \right].$$

We define a lattice Kondo temperature, $T_o$, by $T_o = \epsilon - \mu$ (see Figure 3.4). Further, we expect $1/T_o >> 1/(D + \epsilon)$, since $T_o$ is of the order of meV and $D + \epsilon$ is typically of the order of eV. Thus we can approximate the result by

$$s_o^2 \left[ 1 + \frac{2N(0)V_o^2}{T_o} \right] = 1.$$
Again, because $T_o$ is small, we can neglect the one inside the brackets to get

$$s_o^2 \approx \frac{T_o}{2N(0)V_o^2}, \quad (3.100)$$

which is the usual SU(N) result for $s_o$ for $N=2[7]$.

Simplifying equation 3.98 in spherical symmetry gives

$$i\lambda_o - 2V_o^2 N(0) \int_{-D}^{\mu} dE \frac{1}{\epsilon - \mu} = 0,$$

$$i\lambda_o + 2N(0)V_o^2 \ln|\frac{T_o}{D}| = 0,$$

where we have assumed (in the case of spherical symmetry) that $D+\epsilon \approx D$. In this limit $i\lambda_o$ is the energy shift of the full (unsplit) $J=5/2$ multiplet, the unshifted energy being represented by $E_o$ with no $\Gamma$ subscript. That is, $i\lambda_o = \epsilon - E_o = -E_o = |E_o|$, where the unshifted multiplet energy, $E_o$, is generally deep below the chemical potential (e.g. $E_o \approx 2.0$ eV for Ce based materials[10]). Further, the shifted multiplet energy, $\epsilon$, is generally close to the chemical potential of the conduction electrons, at least for large $N$ ($N=6$ in this case, which is quite big). Thus $D \gg |\epsilon|$ and $|E_o| \gg \epsilon$. With these approximations we can simplify the above equation to

$$|E_o| \approx 2N(0)V_o^2 \ln|\frac{T_o}{D}|,$$

$$T_o \approx D e^{-|E_o|/2N(0)V_o^2}, \quad (3.101)$$

which is the usual SU(N) result for the Kondo temperature for $N=2[7]$. In hindsight, we now see why we defined the lattice Kondo temperature as the difference between the shifted multiplet energy and the quasiparticle chemical potential ($T_o \equiv \epsilon - \mu$). It is just this difference which is equal to the usual impurity result for the Kondo temperature, $T_K$. Thus our equations make sense in the limit of spherical symmetry, and we proceed to the actual self-consistent solution.
3.7.2 Numerical Details of Self-Consistent Solution

To solve equations 3.97-3.99 we used a "Numerical Recipes" routine named Powell[8]. In a nutshell, we are looking for the values of \( s_0, i\lambda_0, \) and \( \mu \) that solve our coupled equations. By squaring the three equations and adding them together, we construct a function, \( F \), the absolute minimum of which is zero.

Imagine plotting \( F(i\lambda_0,s_0,\mu) \) as a function of the three parameters. This gives rise to a complicated landscape, across which we are searching for the place where \( F=0 \). Numerically, this is a non-trivial calculation, since possible pathologies in the function could cause the code to get stuck in some local minimum from which it can not escape. This appeared to be the problem when the self-consistent equations were constructed from three dimensional sums over the Brillouin zone. We found the function constructed from equations 3.97-3.99, which are based upon one-dimensional energy integrals, did not cause any major problems for the algorithm Powell.

The basic idea behind Powell is to perform a succession of minimizations of the function along lines in the three dimensional parameter space (i.e. a series of one-dimensional minimizations). Powell does not, however, merely minimize consecutively along the three parameter axes (see Figure 3.6), but actually minimizes along so-called conjugate directions. Suppose we minimize the function \( F \) along some direction defined by the vector \( \vec{u} \). Then at the minimum \( \nabla F \cdot \vec{u} = 0 \). Suppose we now move along another direction defined by \( \vec{v} \), but we do not wish to ruin the minimization we have already obtained along \( \vec{u} \). We can do this if we can keep the gradient of \( F \) perpendicular to \( \vec{u} \) as we move along the new direction \( \vec{v} \). Thus \( \vec{v} \) has to be chosen with care. Here is how Powell does it.
Expand the function $F(x)$ about some origin, $\bar{x}$:

$$F(x) \approx F(\bar{x}) - \bar{b} \cdot x + \frac{1}{2} x \cdot A \cdot x, \quad (3.102)$$

where $\bar{b} = -\nabla F(\bar{x})$ and $A_{ij} = \partial^2 F/\partial x_i \partial x_j|_{\bar{x}}$. The gradient of $F$ is just $\nabla F = A \cdot \bar{x}$. Suppose we are at the point $\bar{x}_o$ on the line $\bar{u}$ at which $F$ is an extremum. Then $\nabla F = 0$, or $A \cdot \bar{x}_o = \bar{b}$. Further, as we move along the new direction $\bar{v}$, the gradient changes as $\delta(\nabla F) \approx A \cdot \bar{v}$. We want this change in the gradient to remain perpendicular to $\bar{u}$; that is, $\bar{u} \cdot \delta(\nabla F) = 0$, or

$$\bar{u} \cdot A \cdot \bar{v} = 0. \quad (3.103)$$

Within the approximation of the expansion of equation 3.102, this is the criterion for the vectors $\bar{u}$ and $\bar{v}$ to be conjugate. The algorithm finds conjugate directions and makes successive line minimizations along them. There are, of course, more details in the routine that we do not need to discuss. The interested reader is referred to the "Numerical Recipes" text[8].

We turn, now, to our results. We started with the free electron chemical potential of $\mu_o = 2.440492$ eV, which corresponds to a spherical Fermi surface containing 0.5 $N_s$ k-points. ($N_s$ is the number of lattice sites.) We took the unshifted $\Gamma_7$ multiplet energy to lie 2.0 eV below $\mu_o$, i.e. $E_7 = -2.0$ eV. With a crystal field splitting $\Delta_{CEF} = 0.036$ eV, this gives $E_8 = -1.964$. We also took a bare hybridization strength of $V_o = 0.8595$ eV. The data are gathered together and listed below:

$$\begin{align*}
\mu_o &= \text{conduction electron chemical potential} = 2.440492 \text{ eV} \\
V_o &= \text{bare hybridization strength} = 0.8595 \text{ eV} \\
n_{total} &= n_c + n_f = 1.5
\end{align*}$$
Figure 3.6:
Parameter space for minimization of a function of the variables $s_o$, $i\lambda_o$, and $\mu$. Path 1 allows for line minimizations only along the directions of the axes. Path 2 is more general and is, in principle, allowed by the minimization algorithm Powell.
\[ E_7 = \text{unshifted } \Gamma_7 \text{ doublet energy} = -2.0 \text{eV} \]

\[ E_8 = E_7 + \Delta_{CEF} = -1.964 \text{eV}. \]

The following parameters give a self-consistent solution of the mean-field equations:

\[
\begin{align*}
\epsilon_7 &= E_7 + i \lambda_0 = 0.021764775 \text{ eV} \quad (3.104) \\
\mu &= \text{quasiparticle chemical potential} = 0.020839921 \text{ eV} \quad (3.105) \\
\sigma_o &= \text{slave boson amplitude} = 0.09347194. \quad (3.106)
\end{align*}
\]

If we define a Kondo temperature as

\[ T_{o7} \equiv \epsilon_7 - \mu = 9.25 \times 10^{-4} \text{eV} \approx 9.25K, \quad (3.107) \]

we arrive at a number consistent with the experimental value for CeCu_2Si_2. Recall that from the linewidth of the quasi-elastic neutron peak we can estimate the Kondo temperature to be about 10 K[9].

As a last rough check of these parameters, we find that they can satisfy typical Kondo-esque expressions

\[
\begin{align*}
T_{o7} &\approx \frac{s_o^2 V^2}{a 2D} \approx 7.9 \times 10^{-4} \text{eV}, \text{ and} \\
T_{o7} &\approx D e^{-|E_7|^2 D/a V^2} \approx 9.3 \times 10^{-4} \text{eV},
\end{align*}
\]

where a=1.67 is a factor inserted by hand. It should not be too surprising that such a fudge factor shows up, since these analytic expression assume a constant free electron density of states, \(N(0)\), while the density of states in our numerical solution was not constant \(N(\xi) \propto \sqrt{\xi}\). Thus we have reasonable mean-field parameters that can be used in the next chapters when we calculate quasiparticle interactions. As the last section of this chapter, we wish to discuss two other sets of mean-field parameters that we have studied.
3.7.3 Other Mean-Field Parameters

We have solved the mean-field equations for different sets of parameters, which reveals some interesting results. Suppose we keep the total filling factor the same as above, \( n_{\text{total}} = n_c + n_f = 1.5 \) and adjust the free electron chemical potential to a different value; we used \( \mu_0 = 3.338556 \text{ eV} \). We also used a different bare hybridization strength \( (V_o = 0.65 \text{ eV}) \), so as to retain a Kondo temperature of about 10 K (see below):

\[
\begin{align*}
\mu_0 &= \text{conduction electron chemical potential} = 3.338556 \text{ eV} \\
V_o &= \text{bare hybridization strength} = 0.650 \text{ eV} \\
n_{\text{total}} &= n_c + n_f = 1.5 \\
E_7 &= \text{unshifted } \Gamma_7 \text{ doublet energy} = -2.0\text{eV} \\
E_8 &= E_7 + \Delta_{\text{CEF}} = -1.964\text{eV} \\
\epsilon_7 &= E_7 + i\lambda_0 = -0.84370213 \text{ eV} \\
\mu &= \text{quasiparticle chemical potential} = -0.84499898 \text{ eV} \\
s_0 &= \text{slave boson amplitude} = 0.14240942,
\end{align*}
\]

which gives a Kondo temperature of about 13.0 K. Let us call this set of parameters, mean-field parameter set (b) and call the previous set mean-field parameter set (a).

Note from Figure 3.7 that the quasiparticle bands for parameter sets (a) and (b) have just been shifted rigidly with respect to each other, with the band from parameter set (b) about 1 eV lower in energy. As a consequence of such a shift, the quasiparticle chemical potential, \( \mu \), for set (b) lies about 1 eV below the conduction electron chemical potential, and also about 1 eV below the quasiparticle chemical potential for parameter set (a). (Note that for set (a), \( \mu \) lies about 0.02
Figure 3.7:
Plot of the lowest energy band, $E_{1g}$, for the two mean-field parameter sets (labeled as (a) and (b)). In set (a), the conduction electron chemical potential is 2.44 eV, and in set (b), it is 3.33 eV. Note that the bands are just shifted with respect to each other. For set (b), the quasiparticle chemical potential, $\mu$, is fallen almost 1 eV below the reference energy, while for set (a), $\mu$ lies just above zero. For both parameter sets the unshifted $\Gamma_7$ multiplet energy sits at -2.0 eV above $\mu_0$.

That the value of $\mu$ lies so far below $\mu_0$ for set (b) is surprising, since conventional understanding of the Anderson model claims that the quasiparticle chemical potential should be near to $\mu_0$. Another way of saying the same thing, is that the shifted multiplet energy, $\epsilon_7$, should lie near $\mu_0$, rather than almost 1 eV below it.

Detailed electronic spectroscopy measurements[11] on CeCu$_2$Si$_2$ have been
studied and can perhaps be of some guidance here. Resonant photoemission (RPES) spectra on the Ce 4f electrons were measured by Parks et al.[12]. The experiment probes charge excitations from a 4f¹ to a 4f⁰ configuration and finds a peak about 2.0 eV below the Fermi energy. In the language of our calculation, we can define an energy difference \( \Delta E = |E_7 - \mu| \approx 2eV \). Note that the crystal field splitting \( \Delta_{CEF} = E_8 - E_7 \) is small on the present 2.0 eV energy scale of interest.

The numbers from mean-field parameter set (b) give \( \Delta E = 1.16 \) eV, which is a bit too small. Interestingly, if we take another parameter set (call it (c)), which is applicable to the SU(6) model, we find again different results. In this case, a filled quasiparticle band would have a filling factor of 6 particles per unit cell. The parameters for (c) are:

\[
\begin{align*}
V_o &= \text{bare hybridization strength} = 0.20 \text{ eV} \\
n_{\text{total}} &= n_c + n_f = 5.5 \\
E_7 &= \text{unshifted } \Gamma_7 \text{ doublet energy} = -2.0eV \\
E_8 &= E_7 + \Delta_{CEF} = -1.964eV \\
\epsilon_7 &= E_7 + i\lambda_o = -0.0807 \text{ eV} \\
\mu &= \text{quasiparticle chemical potential} = -0.0908 \text{ eV} \\
s_o &= \text{slave boson amplitude} = 0.393.
\end{align*}
\]

Although the Kondo temperature is a little high here, we can use the parameters to get a rough feel for what is going on. Note that the increased degeneracy (from \( N=2 \) to \( N=6 \)) has increased the energy difference to \( \Delta E = 1.92 \text{ eV} \), which is clearly in line with the expected value of about 2.0 eV for CeCu$_2$Si$_2$. Of course, this begs the question: why do the \( N=6 \) mean-field parameters agree
There is no obvious answer to the above question, but we are led to end this chapter with a short discussion of this apparent discrepancy. To be in agreement with RPES data for CeCu$_2$Si$_2$ we need an energy difference $\Delta E \approx 2.0$ eV. For $N=2$, the only way to attain such a shift, within the framework of the Anderson lattice, is (apparently) to keep the conduction electron chemical potential, $\mu_o$, small enough (i.e. $\mu_o \leq 2.5$ eV). For the SU(6) model, we found it quite easy to attain the required $\Delta E \approx 2.0$ eV. Why should we be limited to small values of $\mu_o$ for small degeneracies? (For $N=2$, the value $\mu_o=3.33$ eV produced only $\Delta E=1.2$ eV.) There is no reason a priori to believe that $\mu_o=3.33$ eV isn't a reasonable value for the conduction electron chemical potential. After all, in CeCu$_2$Si$_2$, the Cu-d and Si-p densities of states calculated in reference [11] show band widths of the order of 4 eV. We have wondered if there is some important physics missing from the Anderson model that only becomes evident for small degeneracies, but have not been able to pursue it too deeply.

We calculated the quasiparticle interactions for both mean-field parameter sets (a) and (b) and will present our results for both sets. To calculate such interactions requires knowledge of the dressed Bosonic Green function, which is the topic of the next chapter.

3.8 Effective Magnetic Moment in Cubic Symmetry

As an extra part of this chapter, we would like to discuss the paper by Zou and Anderson[13], in which they calculated the Pauli susceptibility of the Anderson lattice in the presence of spherical symmetry. Like Lee and Zhang[14] after them, they effectively used an anisotropic hybridization matrix element, $V_{m\sigma}(\vec{k})$, of the
Coqblin- Schrieffer form[3]. Their motivation for this procedure is as follows. As mentioned in the last section of Chapter 1, Anderson has suggested that the source of superconductivity in some heavy Fermion compounds might be due to localized spin fluctuations [15]. In the language of Fermi liquid theory, this means the susceptibility without (\(\chi_o\)) and with (\(\chi\)) quasiparticle interactions can be related through the expression

\[
\frac{\chi}{\chi_o} = \frac{m^*}{m} \frac{1}{1 + F_0^a},
\]

where \(F_0^a\) is the well-known Fermi liquid parameter, and where \(m^*\) is the effective mass of the quasiparticles. The Wilson ratio, which tells us how much spin fluctuations participate in the interactions as opposed to charge fluctuations, is given by

\[
R = \frac{\chi/\chi_o}{m^*/m} = \frac{1}{1 + F_0^a}.
\]

It turns out for an isolated Kondo impurity, that \(R = 2\).

On physical grounds, if spin fluctuations were responsible for the pairing in heavy Fermion superconductors, shouldn't the importance of these fluctuations be reflected in a large measured Wilson ratio (e.g. \(R > 1\))? Thus it is puzzling that most of the heavy Fermions have small Wilson ratios. For CeCu_2Si_2, \(R \approx 0.5[19]\). Zou and Anderson wished to show that the Wilson ratio, even in the presence of strong spin fluctuations, could be reduced due to the anisotropic hybridization between the conduction and the \(f\) electrons. They calculated the quasiparticle states, including spin-orbit coupling, with the procedure of Razafimandimby, Fulde, and Keller, which was discussed in Chapter 1[20]. Their results are identical to those of Lee and Zhang[14], who used a mean-field approximation to the infinite-U Anderson lattice. In spherical symmetry, for a
total angular momentum of $J = 5/2$, the quasiparticle states are

$$|Q_{k\alpha\sigma}\rangle = A_1(\vec{k}) \left[ |\vec{k}\alpha\rangle - \sum_n \frac{s_o V_m(\vec{k})}{E_{1\vec{k}}} |m\rangle \right],$$  

(3.110)

where the normalization is

$$A_1^2(\vec{k}) = \left[ 1 + \frac{s_o^2 V_o^2}{(\epsilon - E_{1\vec{k}})^2} \right].$$  

(3.111)

In the preceding equations, $E_{n\vec{k}}$ is the quasiparticle dispersion for band $n$ and $\epsilon$ is the energy of the undispersed $f$ states that do not hybridize. For the case of $J = 5/2$, the band of energy $\epsilon$ is four-fold degenerate, since two of the total six $f$ states have hybridized with the conduction states.

Zou and Anderson calculate the magnetic moment of the quasiparticle states in the lowest band,

$$\langle Q_{k\alpha\sigma} | \hat{\mu}_z | Q_{k\alpha\sigma}\rangle \equiv \mu^{\sigma\sigma'}(\vec{k}),$$  

(3.112)

where the magnetic moment operator is

$$\hat{\mu}_z = \hat{i}_z + 2\hat{s}_z = g_J \hat{J}_z.$$  

(3.113)

The effective magnetic moment is the average of $\mu^{\sigma\sigma'}$ over the spherical Fermi surface,

$$\mu_{zeff}^2 = \int \frac{d\vec{k}}{4\pi} \left[ \mu^{+1+1}_z(\vec{k})^2 + \mu^{+1-1}_z(\vec{k})^2 \right],$$  

(3.114)

and the result is $\mu_{zeff}^2 = 1.16 \mu_B^2$. $\mu_B$ is the Bohr-magneton. Note that the bare moment for a $f^1$ state is $\mu = 2.54 \mu_B$, so that hybridization has reduced the size of the moment.

The Pauli susceptibility for the quasiparticles is a function of the effective magnetic moment, $\mu_{eff}$, and the density of states at the Fermi surface, $\tilde{N}(0)$,

$$\chi_{Pauli} = 2\mu_{eff}^2 \tilde{N}(0).$$  

(3.115)
Substituting this value for the Pauli susceptibility into the expression for the Wilson ratio, equation 3.109, we get

\[ R_{\text{reduced}} = \left( \frac{\mu_{\text{eff}}}{\mu} \right)^2 \frac{1}{1 + F_0^a} = \frac{0.18}{1 + F_0^a}. \]  

(3.116)

In this way, it would be possible to have a big Stoner factor, \( 1 + F_0^a \), as befits the presence of strong spin fluctuations, but the reduced magnetic moment, could still account for a small experimentally observed Wilson ratio. It seems like a simple enough argument.

But Cox[16], Zhang and Lee[17], and Aeppli and Varma[18] point out the need to include the Van Vleck susceptibility in the calculation. The value for \( \chi \) in equation 3.109 must be the total susceptibility, as seen by experiment. In the case of the uniform susceptibility, the Van Vleck contribution represents direct transitions from the Fermi wavevector to wavevectors in higher bands. (See figure 3.8.) In this case, as we mentioned, there is a four-fold degenerate band lying at an energy \( T_0 \) above the Fermi energy. This lattice Kondo temperature, \( T_0 \), is quite small; for CeCu\(_2\)Si\(_2\) it is about 1 meV. Now the Van Vleck susceptibility will have the structure

\[ \chi_{\text{VV}}(\vec{q} = 0) = 2\mu_B^2 \sum_m \int \frac{d\vec{k}}{4\pi} \frac{|\langle Q_{E_1}\vec{\mu}_z|\vec{m} \rangle|^2}{T_0}, \]  

(3.117)

where the quasiparticle density of states \( \tilde{N}(0) \approx 1/T_0 \). This small energy denominator makes this interband contribution to the susceptibility the same size as the contribution from the Pauli susceptibility. Cox and Zhang and Lee showed that the net susceptibility was given by

\[ \chi_{\text{total}} = \chi_{\text{Pauli}} + \chi_{\text{VV}} = \frac{1}{3} g_J^2 J(J + 1)[2\tilde{N}(0)], \]  

(3.118)

which shows a dependence only on the bare magnetic moment. Thus the inclusion of the Van Vleck susceptibility negates Zou and Anderson’s argument. The
existence of a small Wilson ratio has not yet been reconciled with the assumption of strong spin fluctuations in these systems.

We now wish to discuss what happens to these arguments when crystal electric fields of cubic symmetry are added to the problem. We start, as for the $4f^1$ states of Ce, with a lattice of $J = 5/2$ multiplets and turn on the crystal fields. The resultant states of $\Gamma_7$ and $\Gamma_8$ symmetry are just equations 2.62-2.67. The quasiparticle states are given by equation 3.61, where the local crystal field states are orthonormal. That is,

$$
\langle \Gamma'\alpha'|\Gamma\alpha \rangle = \sum_{m'm} c_{\Gamma'\alpha'm'} c_{\Gamma\alpha m} \langle m'|m \rangle = \sum_m c_{\Gamma'\alpha'm} c_{\Gamma\alpha m} = \delta_{\Gamma\Gamma'} \delta_{\alpha alpha'}.
$$

In order to calculate the effective magnetic moment, we need the following ex-
pectation value:

\[ \mu_{z}^{\sigma \sigma'}(\mathbf{k}) = \langle Q_{\mathbf{k}1\sigma} | \hat{\mu}_{z} | Q_{\mathbf{k}1\sigma'} \rangle, \tag{3.120} \]

for the magnetic moment in the lowest quasiparticle band. Note that \( \sigma \) and \( \sigma' \) are pseudo-spin indices. We find that we can write equation 3.120 in the form

\[ \mu_{z}^{\sigma \sigma'}(\mathbf{k}) = A_{\mathbf{k}}^{2}(\mathbf{k}) \left[ \sigma \delta_{\sigma \sigma'} + \sum_{\Gamma' \alpha \Gamma \alpha'} \frac{g_{\Gamma \alpha' \Gamma \alpha} V_{\Gamma' \alpha' \Gamma \alpha}(\mathbf{k}) V_{\Gamma \alpha \Gamma \alpha'}(\mathbf{k}) s_{\alpha} c_{\Gamma \alpha} \right]. \tag{3.121} \]

We find that there are ten non-zero terms that contribute to the sums inside the square brackets of equation 3.121. With all such terms identified, we can calculate the effective moment through equation 3.114. We get the result

\[ \mu_{\text{cubic,eff}}^{2} = 0.583 \mu_{B}^{2}, \tag{3.122} \]

for mean-field parameter set (a). For a free \( \Gamma_{7} \) doublet the average moment is

\[ \mu_{\Gamma_{7}}^{2} = \frac{25}{49} \mu_{B}^{2}. \tag{3.123} \]

The effective magnetic moment in cubic symmetry is slightly larger than the value for a free \( \Gamma_{7} \) moment. This was expected by Cox[16], who predicted the effective moment would have the structure

\[ \mu_{\text{eff}}^{2} = \mu_{\Gamma_{7}}^{2}[1 + \alpha\sqrt{m/m^{*}}], \tag{3.124} \]

where \( \alpha \) is a prefactor that could be as big as about 10. The contributions of order \( \sqrt{m/m^{*}} \) come from the six regions on the spherical Fermi surface where the axes of the cubic Brillouin zone intersect the sphere. These are the so-called "hot-spots", which we will discuss at length in chapter 5. At these points on the Fermi surface, the plane wave conduction states and the localized \( \Gamma_{7} \) states can not hybridize. Thus one expects the \( g \)-factor at these points to go back to
the free electron value of 2. Since the effective \( g \)-factor away from these "hot-spots" is about 0.764, we expect the contribution to \( \mu_{\text{eff}} \) from the "hot-spots" to increase the effective moment above that of a free moment of \( \Gamma_7 \) symmetry.

For parameter set (a), we have

\[
\frac{m}{m^*} = \left( \frac{T_{\sigma\tau}}{s_0 V_0} \right)^2 = 1.33 \times 10^{-4}.
\]

Equation 3.124 is applicable for the quoted values of \( \mu_{\text{eff}}^2 \) and \( \mu_\gamma^2 \) if \( \alpha = 9.23 \), which is a reasonable value.

Finally, we substitute \( \mu_{\text{eff}}^2 \) into the expression for the Wilson ratio,

\[
R = \left( \frac{\pi k_B}{\mu_{\text{eff}}} \right)^2 \frac{\chi(0)}{\gamma(0)},
\]

where \( \chi(0) \) is the low temperature susceptibility, \( \gamma(0) \) is the linear coefficient of specific heat, \( k_B \) is Boltzmann's constant, and \( \mu_B \) is the Bohr magneton. Using \( \chi(0) = 0.019 \text{ emu/mole} \) (for a magnetic field along the c axis of the tetragonal unit cell)\([21]\), and \( \gamma(0) = 1000 \text{ mJ/mole-K}^2 \) \([22]\) gives \( R = 2.38 \), which is a bit large compared to the typical measured values of about 0.5 for CeCu\(_2\)Si\(_2\) \([19]\).
Chapter IV REFERENCES

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CHAPTER IV

Gaussian Fluctuations and the Slave-Boson Propagator

4.1 Introduction and a Word about Notation

This chapter consists of two main parts, in the first of which we shall calculate the Bosonic Green function through second order in the fluctuating fields, $\delta \tilde{s}_\Gamma$ and $\delta \lambda_\Gamma$. Because we are using a functional integral approach, we shall (strictly speaking) be finding the vertex function $\Gamma$, which is the inverse of the dressed Bosonic Green function. To be more specific, our vertex function will be a $2 \times 2$ matrix, which we shall write as $\hat{\Gamma}_{\Gamma \Gamma'}$. The subscripts denote the crystal field multiplet degrees of freedom. If we wish to study specific elements of this matrix, we use the following notation: $\Gamma_{ss',\Gamma\Gamma'}, \Gamma_{s\lambda,\Gamma\Gamma'}, \Gamma_{\lambda\lambda,\Gamma\Gamma'}$. As we shall see, we are allowed to sum freely over the multiplet indices, $\Gamma$, and $\Gamma'$, in the $\lambda - \lambda$ component. Call the resultant vertex, after summing, $\Gamma_{\lambda\lambda}$. With the $s$ fields, however, it is not quite so simple. Recall that, even though there is one "bare" $s$-field for both $\Gamma_7$ and $\Gamma_8$ multiplets, the scaled values are different: $\tilde{s}_{o7} = s_o/\sqrt{2}$ and $\tilde{s}_{o8} = s_o/\sqrt{4}$. Thus, for the $s - \lambda$ component of the vertex function, $\Gamma_{s\lambda,\Gamma\Gamma'}$, there is not a free sum over both $\Gamma$ and $\Gamma'$, but only over one of the two indices.
(The presence of the $\lambda$ signifies the ability to sum over one the indices.) And for the $s-s$ component, there is no free sum over $\Gamma$ and $\Gamma'$.

The dressed (matrix) Green function, $\hat{D}_{\Gamma\Gamma'}$, follows from the identity

$$ -\hat{D}^{-1}_{\Gamma\Gamma'} = \hat{\Gamma}_{\Gamma\Gamma'}. $$

(4.1)

There is also a bare vertex function denoted by $\hat{\Gamma}_{o\Gamma\Gamma'} = -\hat{D}^{-1}_{o\Gamma\Gamma'}$, with elements: $\Gamma_{o,s\Gamma\Gamma'}, \Gamma_{o,o\lambda\Gamma\Gamma'}$, and $\Gamma_{o,\lambda\lambda\Gamma\Gamma'}$. And Dyson's equation for the Bosons now takes one of two forms:

$$ \hat{\Gamma}_{\Gamma\Gamma'} = \hat{\Gamma}_{o\Gamma\Gamma'} + \hat{\Pi}_{\Gamma\Gamma'}, $$

(4.2)

$$ \hat{D}^{-1}_{\Gamma\Gamma'} = \hat{D}^{-1}_{o\Gamma\Gamma'} - \hat{\Pi}_{\Gamma\Gamma'}. $$

(4.3)

The first part of this chapter gives the detailed derivation of $\hat{D}^{-1}_{\Gamma\Gamma'}$ (or $\hat{\Gamma}_{\Gamma\Gamma'}$). For those readers wishing to forego the details, we give the results of this calculation in the next subsection, preceding the actual derivation.

In the second section of this chapter, we discuss at length the analytic tetrahedron method of k-space integration, which is the numerical procedure used to attack the complicated Brillouin zone integrals that raise their heads in the expressions for the Green function. It should become clear as we progress through the chapter, that, even in the static limit, the numerically evaluated Green functions are slow to converge—that is, they require a very fine mesh throughout the Brillouin zone.

4.2 Calculation of the Green function $\hat{D}(q)_{\Gamma\Gamma'}$.

4.2.1 Motivation

With an understanding of the mean-field quasiparticles gained in the previous chapter, we push on to study their residual interactions. The quasiparticles can
scatter off each other by exchanging a density fluctuation between them. These density fluctuations are dressed by electronic particle-hole excitations and are described by the average of combinations of the fields, $\delta \tilde{s}_{\mathbf{k}\Gamma}$ and $i\delta \lambda_{\mathbf{k}}$. Their corresponding (matrix) propagator $\hat{D}_{\Gamma\Gamma'}(\mathbf{q}, \imath \nu)$ satisfies the Dyson's equation shown above. (See equation 4.3.) In the previous chapter, we showed that the bare Boson propagator is given by

$$
\hat{D}_{\Gamma\Gamma'}^{-1} = -\frac{N_{\Gamma}}{2} \begin{pmatrix}
\imath \lambda_{\mathbf{o}} & \hat{s}_{\mathbf{o}}
\hat{s}_{\mathbf{o}} & 0
\end{pmatrix} \delta_{\Gamma\Gamma'},
$$

(4.4)

where $\hat{s}_{\mathbf{o}} = s_{\mathbf{o}}/\sqrt{N_{\Gamma}}$.

To motivate the results for $\hat{D}_{\Gamma\Gamma'}^{-1}$, before proceeding into the detailed calculations, consider the diagonal component of the matrix Dyson's equation in Figure 4.1. Taking all contributions to the self-energy of order $N_{\Gamma}$ will give a dressed propagator of order $1/N_{\Gamma}$. Here is how it works. In figure 4.1(c), the $\times$ symbols at the corners of the diagrams represent scaled hybridization matrix elements, $\hat{V}_{\Gamma\alpha}(\bar{k})$, which are of order one ($O(1)$). Thus, there is a sum over the degenerate states of the multiplet $\Gamma$ and no factor of $1/N_{\Gamma}$ from the matrix elements to cancel it. This is what we mean when we say that the Boson self-energy diagram is of order $N_{\Gamma}$. This means, also, that the external legs of the first two self-energy diagrams in figure 4.1 are constructed from the scaled fluctuations in the $s$ fields, $\delta \tilde{s}_{\mathbf{q}\Gamma}$, which are also assumed to be of order one. (See figure 4.3.) Thus, the self-energy diagrams composed of closed Fermionic loops will be most important since they have a sum over the crystal field degrees of freedom within the $\Gamma$ multiplet. We can guess in advance, without derivation, that the self-energy diagrams of interest to us are all possible closed loops, as seen in Figure 4.1. Evaluation of theses diagrams, using the mean-field Green
functions derived in the previous chapter, leads to the following results for the elements of the (inverse) Bose propagator:

\[
D^{-1}_{s\Gamma'}(\vec{q}) = 2I_{s\Gamma'}(\vec{q}),
\]

\[
D^{-1}_{s\lambda\Gamma'} = -i \left[ \frac{N}{2} \delta_{s\lambda} + \frac{x_r}{\delta_{s\lambda}} \right] \delta_{\Gamma'} + i I_{s\lambda\Gamma'}(\vec{q}),
\]

\[
D^{-1}_{\lambda\lambda\Gamma'}(\vec{q}) = -\frac{y_r}{T_{0\Gamma}} - \frac{1}{2} I_{\lambda\lambda\Gamma'}(\vec{q}),
\]

where \(x_r = 27.54, x_s = 0.0717, y_r = 0.975, y_s = 0.04029\), and where

\[
I_{s\Gamma'}(\vec{q}) = \frac{P}{N_s} \sum_{\vec{k}\vec{k}',\alpha\alpha'} f(E_{1\vec{k}})\tilde{s}_{\alpha\Gamma} \tilde{s}_{\alpha\Gamma'} \mu_{\Gamma\alpha'\alpha'}(\vec{k}') \mu_{\Gamma'\alpha'\alpha}(\vec{k}) (\epsilon_7 - E_{1\vec{k}})^2 (\epsilon_8 - E_{1\vec{k}})^2 \\
\times \frac{[\delta_{\vec{k}',\vec{k} - \vec{q}} + \delta_{\vec{k}',\vec{k} + \vec{q}}]}{(\epsilon_7 - E_{1\vec{k}})(\epsilon_7 - E_{1\vec{k}})(E_{2\vec{k}} - E_{1\vec{k}})(E_{2\vec{k}} - E_{1\vec{k}})(E_{3\vec{k}} - E_{1\vec{k}})}
\]

\[
I_{\lambda\Gamma'}(\vec{q}) = \frac{P}{N_s} \sum_{\vec{k}\vec{k}',\alpha\alpha'} \frac{f(E_{1\vec{k}})(\epsilon_7 - E_{1\vec{k}})^2 (\epsilon_8 - E_{1\vec{k}})^2}{(E_{2\vec{k}} - E_{1\vec{k}})(E_{2\vec{k}} - E_{1\vec{k}})(E_{2\vec{k}} - E_{1\vec{k}})(E_{3\vec{k}} - E_{1\vec{k}})}
\times \frac{\tilde{s}_{\alpha\Gamma} \tilde{s}_{\alpha\Gamma'} \mu_{\Gamma\alpha'\alpha'}(\vec{k}') \mu_{\Gamma'\alpha'\alpha}(\vec{k}) (\epsilon_7 - E_{1\vec{k}})}{(E_{1\vec{k}} - \epsilon_7)} \left[ \delta_{\vec{k}',\vec{k} - \vec{q}} + \delta_{\vec{k}',\vec{k} + \vec{q}} \right]
\]

\[
I_{\lambda\lambda\Gamma'}(\vec{q}) = \frac{P}{N_s} \sum_{\vec{k}\vec{k}',\alpha\alpha'} f(E_{1\vec{k}})\tilde{s}_{\alpha\Gamma} \tilde{s}_{\alpha\Gamma'} \mu_{\Gamma\alpha'\alpha'}(\vec{k}') \mu_{\Gamma'\alpha'\alpha}(\vec{k}) (\epsilon_7 - E_{1\vec{k}})^2 (\epsilon_8 - E_{1\vec{k}})^2 \\
\times \frac{[\delta_{\vec{k}',\vec{k} - \vec{q}} + \delta_{\vec{k}',\vec{k} + \vec{q}}]}{(\epsilon_7 - E_{1\vec{k}})(\epsilon_7 - E_{1\vec{k}})(E_{2\vec{k}} - E_{1\vec{k}})(E_{2\vec{k}} - E_{1\vec{k}})(E_{3\vec{k}} - E_{1\vec{k}})}
\]

In equations 4.8 - 4.10, \(E_{n\vec{k}}\) are the quasiparticle band energies. The quasiparticle chemical potential was chosen to lie in the lowest band, such that \(f(E_{1\vec{k}})\) is nonzero only for \(n = 1\). The anisotropic function \(\mu_{\Gamma\alpha'\alpha}(\vec{k})\) is defined by

\[
\mu_{\Gamma\alpha'\alpha}(\vec{k}) = \sum_{\sigma} \hat{V}_{\sigma\alpha}(\vec{k}) \hat{V}_{\sigma'\alpha'}(\vec{k}).
\]
Figure 4.1:

(a). Dyson's equation for the diagonal component (in the crystal field indices) of the inverse of the (matrix) Bosonic propagator $\hat{D}_\Gamma^{-1}$. (b). The three hybridization-dressed (mean-field) Fermionic Green functions. Note that, in general, the $f$ Green function can mix the multiplet indices at $k$-points away from the zone center. This is because away from the zone center, the symmetry is lower than cubic, allowing the crystal field indices to mix. (c). Leading contributions to the components ($ss$, $s\lambda$, and $\lambda\lambda$) of the self-energy matrix from closed Fermionic loops. The "x" symbol represents the scaled hybridization matrix element, $\tilde{V}_{\Gamma\alpha\sigma}(\tilde{k})$, which is assumed to be of order one. The external legs in the $\Gamma_{s\sigma}\Gamma\tau$ diagram come from the scaled fluctuations in the $s$ fields, $\delta\tilde{s}_{\Gamma\tau}$. 
Note the presence of the principal value integrals over the Brillouin zone. These are to be evaluated numerically, as discussed later in this chapter. As the last part of this introduction, we wish to motivate how the Bosonic Green functions can mediate quasiparticle interactions. This is most easily seen from the Hamiltonian written in the quasiparticle basis.

4.2.2 A Brief Word about Quasiparticle Interactions

Although the mathematical framework of this thesis requires we speak in terms of a Lagrangian, the physics is probably clearer to us within a Hamiltonian language. The Hamiltonian corresponding to the Lagrangian of equation 3.11 is the following:

\[
H = \sum_{k,\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{k,k',\Gamma,\alpha} f_{k\Gamma,\alpha}^\dagger \left[ E_{\Gamma} \delta_{kk'} t + i \lambda_{k-k'} \right] f_{k',\Gamma,\alpha} \\
+ \sum_{k,k',\Gamma,\alpha} \left[ \tilde{V}_{\Gamma,\alpha}(k) c_{k,\sigma}^\dagger f_{k',\Gamma,\alpha} s_{k',\Gamma,\alpha}^* + H.c. \right] \\
+ \frac{N_s}{2} \sum_{k,\Gamma} N_{\Gamma} i \lambda_{k} \left[ \sum_{k'} s_{k+k',\Gamma,\alpha}^* s_{k',\Gamma,\alpha} - q_{\Gamma} \right]. \tag{4.12}
\]

Using the transformations of equations 3.61 and 3.62, we can write \(H\) in the quasiparticle basis,

\[
H_{QP} = \sum_{k,\sigma,n,n'} \xi_n A_n^*(k) A_{n'}(k) Q_{k\sigma}^\dagger Q_{k\sigma'} + H_{\text{constraint}} \\
+ \sum_{k,k',\Gamma,n,n',\sigma} \left[ \frac{A_n^*(k) s_{n,\Gamma} \tilde{V}_{\Gamma,\alpha}(k) A_{n'}(k') s_{n',\Gamma} \tilde{V}_{\Gamma,\alpha'}(k')}{(\epsilon_{\Gamma} - E_{n,k})(\epsilon_{\Gamma} - E_{n',k'})} \right] \times Q_{k\sigma}^\dagger \left[ E_{\Gamma} \delta_{kk'} t + i \lambda_{k-k'} \right] Q_{k\sigma'} \\
+ \sum_{k,k',\Gamma,n,n',\sigma} \left[ \frac{-A_n^*(k') s_{n,\Gamma} \tilde{V}_{\Gamma,\alpha}(k') A_{n}(k) \tilde{V}_{\Gamma,\alpha'}(k)}{\epsilon_{\Gamma} - E_{n,k'}} \right] Q_{k\sigma}^\dagger Q_{k\sigma'} s_{k-k',\Gamma}^* + H.c. \right], \tag{4.13}
\]
where $H_{\text{constraint}}$ is just the last line of equation 4.12. $A_n(\vec{k})$ is the quasiparticle renormalization function and $Q_{\vec{k}n\sigma}$ is the destruction operator for a quasiparticle in band $n$, with momentum $\vec{k}$ and pseudo-spin $\sigma$. For notational simplicity we define the functions

$$
\gamma_f \Gamma(\vec{k}, \vec{k}') \equiv \frac{A_n^*(\vec{k})A_n(\vec{k}')}{\epsilon_f(n_k)}{\tilde{\epsilon}_{\vec{k}n}(\vec{k}){\bar{V}}_{\vec{k}n\sigma}(\vec{k}){\bar{V}}_{\vec{k}n\sigma}(\vec{k})},
$$

$$
\gamma_{\text{mix}} \Gamma(\vec{k}, \vec{k}') \equiv \frac{-A_n^*(\vec{k})A_n(\vec{k}')}{{\tilde{\epsilon}_{\vec{k}n}(\vec{k}){\bar{V}}_{\vec{k}n\sigma}(\vec{k}){\bar{V}}_{\vec{k}n\sigma}(\vec{k})},
$$

which means the Hamiltonian takes the form

$$
H_{\text{QP}} = \sum_{\vec{k}n\sigma} \xi_{\vec{k}} A_n^*(\vec{k}) A_n(\vec{k}) Q_{\vec{k}n\sigma}^1 Q_{\vec{k}n'\sigma}^1
$$

$$
+ \sum_{\vec{k}k_{\text{ann}}n'n'} \gamma_f \Gamma(\vec{k}, \vec{k}') Q_{\vec{k}n\sigma}^1 \left[ E_f \delta_{\vec{k}k'} + i \lambda_{\vec{k}-\vec{k}'} \right] Q_{\vec{k}n'\sigma}^1
$$

$$
+ \sum_{\vec{k}k_{\text{ann}}n'n'} \left[ \gamma_{\text{mix}} \Gamma(\vec{k}, \vec{k}') Q_{\vec{k}n\sigma}^1 Q_{\vec{k}n'\sigma}^1 \tilde{\epsilon}_{\vec{k}n}(\vec{k}) \tilde{\epsilon}_{\vec{k}n'}(\vec{k}) + H.c. \right] + H_{\text{constraint}}.
$$

Without going through all the details, we see that we can construct elementary interaction vertices from equation 4.16 that connect quasiparticle and Bose propagators. Taking the $\lambda$ fields to be represented by a curly line, and the $s$ fields to be represented by a wavy line, we construct the simple vertices seen in Figure 4.2, where the quasiparticle propagators are represented by straight lines. From these vertices, we can build the two-quasiparticle scattering amplitude (next chapter), in which the exchanged Bose propagators are those dressed by the closed Fermionic loops.

### 4.2.3 Expanding the Action

In this subsection, we begin the actual calculation of the vertex function $\hat{\Gamma}$. We shall expand the action $S$, derived in Chapter 3, up to quadratic order
Figure 4.2:
Quasiparticle interaction vertices due to the two Bose fields, $s$ and $\lambda$. The Bose field $\lambda_{\vec{k} - \vec{k}'}$ is represented by the curly line, and $\tilde{s}_{\vec{k} - \vec{k}'}$ by the wavy line. The solid, straight lines are quasiparticle propagators of momentum $\vec{k}$, band index $n$, and pseudo-spin $\sigma$. The source of the anisotropic functions $\gamma_{\text{mix}}$ and $\gamma_f$ can be intuitively understood by looking at the mean-field Hamiltonian in the quasiparticle basis.
in the fluctuations. The elements of the vertex $\Gamma_{\alpha\Gamma'}$, $\Gamma_{\lambda\Gamma'}$, and $\Gamma_{\lambda\Gamma'}$ will follow by gathering all terms of order $\delta\tilde{s}_\alpha\delta\tilde{s}_{-\alpha}$, $\delta\tilde{s}_\alpha\delta\lambda_{-\alpha}$, and $\delta\lambda_{\alpha}\delta\lambda_{-\alpha}$, respectively. At the end of this section, we shall discuss how we can sum over all the multiplet indices $\Gamma$ and $\Gamma'$. Using equations 3.36 and 3.37 in the previous chapter and after integrating out the Fermionic degrees of freedom, we write the action (momentarily suppressing the momentum and frequency dependence),

$$S = -\text{Tr} \ln G_{\Gamma_0\Gamma'_{\alpha'}}^{-1} + \frac{N_s \beta}{2} \sum_{\Gamma} N_{\Gamma} i\lambda_{\alpha} \{\tilde{s}_{\alpha\Gamma}^2 - q_{\alpha\Gamma}\}$$

$$-\text{Tr} \ln \left[1 - G_{\Gamma_0\Gamma'_{\alpha'}} \left( i\delta + \delta\tilde{s}_\alpha G^A_\alpha \delta\tilde{s}_{-\alpha} + G^B_\lambda \delta\lambda_{-\alpha} + \delta\tilde{s}_\alpha G^C_{\alpha}\right)\right]$$

$$+ \frac{N_s \beta}{2} \text{Tr} \left( \delta\tilde{s}_\alpha^* \delta\lambda \right) \tilde{\Gamma}_{\alpha\Gamma'_{\alpha'}} \left( \begin{array}{c} \delta\tilde{s}_{-\alpha} \\ \delta\lambda \end{array} \right),$$

(4.17)

where the functions $G^A$, $G^B$, and $G^C$, which were defined in the previous chapter, are given by

$$G^A_{\Gamma_0\Gamma'_{\alpha'}}(\vec{k},i\omega) \equiv \sum_\sigma \tilde{V}_{\Gamma_0\sigma}(\vec{k}) G_{\sigma\alpha}(\vec{k},i\omega) \tilde{V}_{\sigma\Gamma'_{\alpha'}}(\vec{k}),$$

(4.18)

$$G^B_{\Gamma_0\Gamma'_{\alpha'}}(\vec{k},i\omega) \equiv \delta_{\alpha\Gamma'} \tilde{G}^A_{\Gamma_0\alpha'}(\vec{k},i\omega),$$

(4.19)

$$G^C_{\Gamma_0\Gamma'_{\alpha'}}(\vec{k},i\omega) \equiv G^A_{\Gamma_0\Gamma'_{\alpha'}}(\vec{k},i\omega) \delta_{\alpha\Gamma'},$$

(4.20)

where $G_{\sigma\alpha}(\vec{k},i\omega) = 1/(i\omega - \xi_\sigma)$. Using standard field-theory notation [1], we have defined the matrix vertex function, $\tilde{\Gamma}_{\alpha\Gamma'}$, as the inverse of the bare Bose propagator, $\tilde{\Gamma}_{\alpha\Gamma'} \equiv -\tilde{D}_{\alpha\Gamma'}^{-1}$. Note that the trace means we sum over all momenta, spin, crystal-field, and Matsubara variables. In equation 4.17, $\beta$ is the inverse temperature, and $N_s$ is the number of lattice sites.

Next, expand the action so that it is a quadratic function of the $\delta\tilde{s}$ and $\delta\lambda$ variables (and call the new action $S_{\text{quad}}$). The general structure of this expression
will be, using the fact that $\delta \hat{s}_{\bar{q} \Gamma}^* (i\nu_m) = \delta \hat{s}_{-\bar{q}} (-i\nu_m)$:

$$S_{quad}(s, \lambda) = S_{MF}$$

$$+ N_s \beta \sum_{\bar{q}, \nu, \Gamma'} \left( \delta \hat{s}_{-\bar{q}^{\prime}} (-i\nu_m) \delta \lambda_{-\bar{q}} (-i\nu_m) \right) \hat{\Gamma}_{\Gamma'^{\prime}}(\bar{q}, i\nu_m) \begin{pmatrix} \delta \hat{s}_{\bar{q}^{\prime}} (i\nu_m) \\ \delta \lambda_{\bar{q}} (i\nu_m) \end{pmatrix}, \tag{4.21}$$

where the self-energy is now given by the equation

$$\hat{\Gamma}_{\Gamma'^{\prime}}(\bar{q}, i\nu_m) = \hat{\Gamma}_{0\Gamma'^{\prime}} + \hat{\Pi}_{\Gamma'^{\prime}}(\bar{q}, i\nu_m). \tag{4.22}$$

Note that the mean-field contribution to the action, $S_{MF}$, has been separated from the fluctuations. Expanding the second logarithm in equation 4.17 gives a complicated expression, which we show in all its detail in Appendix B. The reader interested in following through the mathematics should divert to the appendix at this point. It turns out, as one would intuitively expect, that the result for the Bosonic self-energy, $\hat{\Pi}_{\Gamma'^{\prime}}(\bar{q}, i\nu_m)$, which comes from gathering all terms in the expansion that are quadratic in the fluctuating Bose fields, $\delta \hat{s}_{\bar{q} \Gamma}$ and $\delta \lambda_{\bar{q}}$, is equivalent to evaluating the diagrams in figure 4.1.

### 4.2.4 Contributions to $\Gamma_{ss\Gamma'^{\prime}}(\bar{q})$

As proved in Appendix B, evaluating all terms in the expansion of the action (as discussed in the previous subsection) which are quadratic in the fluctuating $s$-fields, leads to the two self-energy diagrams in figures 4.3 and 4.4. Figure 4.3 is equivalent to the following expression:

$$\sum_{\alpha \alpha' \kappa \omega} G_{a\Gamma'^{\prime} \alpha'}(\bar{k} - \bar{q}, \omega - i\nu) \tilde{V}^*_{\bar{k} \Gamma \alpha}(\bar{k}) G_{a}(\bar{k}, \omega) \tilde{V}_{\bar{k} \alpha}(\bar{k}), \quad (4.23)$$
Figure 4.3:
A diagram contributing to the $\Gamma_{ss, s\Gamma'}(\vec{q}, i\nu)$ vertex. The wavy line represents $\delta \delta \pi(i\nu)$. All internal variables are summed over. The Fermion Green functions are the same as in figure 4.1.

where we have summed over all variables internal to the bubble diagram. The algebra of Appendix B also shows that figure 4.4 contributes to the $s - s$ component of the self-energy. The diagram gives the expression,

$$
\sum_{\alpha\sigma'\sigma'\kappa\omega} G_{\Gamma\sigma}(\vec{k} - \vec{q}, i\omega - i\nu) \tilde{V}_{\sigma\alpha'(\sigma')}(\vec{k} - \vec{q}) \delta \delta \pi(i\nu) G_{\Gamma'\sigma'\sigma}(\vec{k}, i\omega) \tilde{V}_{\sigma'\Gamma\sigma}(\vec{k}).
$$

(4.24)

Using equations 4.23, 4.24, and 4.22 the total $s - s$ component of the vertex function is thus

$$
\Gamma_{ss, s\Gamma'}(\vec{q}, i\nu) = \frac{N}{2} i\lambda \delta \pi
$$

$$
+ \frac{1}{N_s \beta} \sum_{\kappa\omega} G_{\Gamma\sigma}(\vec{k} - \vec{q}, i\omega - i\nu) \tilde{V}_{\sigma\Gamma\sigma}(\vec{k}) G_{\sigma}(\vec{k}, i\omega) \tilde{V}_{\sigma'\Gamma\sigma}(\vec{k})
$$

$$
+ \frac{1}{N_s \beta} \sum_{\kappa\omega} G_{\Gamma\sigma}(\vec{k} - \vec{q}, i\omega - i\nu) \tilde{V}_{\sigma\Gamma\sum}(\vec{k} - \vec{q}) G_{\sum\alpha''\sigma''}(\vec{k}, i\omega) \tilde{V}_{\sum\Gamma\sigma}(\vec{k}).
$$

(4.25)

Next, we sum over the Fermionic Matsubara frequencies, $i\omega_n = i\pi(2n + 1)/\beta$. 
Figure 4.4:

Another contribution to the vertex, $\Gamma_{\sigma,\Gamma'}(q, i\nu)$. The symbols are the same as in figure 4.1. The combination dashed and solid line represents the mixing Green function $G_{\Gamma_{\sigma}}$. Note there is no sum over $\Gamma$ and $\Gamma'$.

Starting with the second term in equation 4.25, we substitute for the $f$ Green function $G_{\Gamma_{\sigma}}$, and for the conduction electron Green function $G_{\sigma}$, where

$$G_{\sigma}(k, i\omega) = \frac{(i\omega - \epsilon_\tau)(i\omega - \epsilon_\delta)}{(i\omega - E_{1k})(i\omega - E_{2k})(i\omega - E_{3k})}, \quad (4.26)$$

$$G_{\Gamma_{\sigma,\Gamma'\sigma'}}(k, i\omega) = \frac{1}{i\omega - \epsilon_{\Gamma}} \left[ \delta_{\Gamma\Gamma'} \delta_{\sigma\sigma'} + \frac{1}{i\omega - \epsilon_{\Gamma'}} \frac{(i\omega - \epsilon_\tau)(i\omega - \epsilon_\delta)\delta_{\sigma\Gamma} \delta_{\sigma'\Gamma'} \hat{V}_{\Gamma_{\sigma}} \hat{V}_{\sigma'\Gamma'}'}{(i\omega - E_{1k})(i\omega - E_{2k})(i\omega - E_{3k})} \right], \quad (4.27)$$

to find

$$\frac{1}{N_{\beta}} \sum_{i\omega, \sigma, \sigma'} \frac{\hat{V}_{\Gamma_{\sigma}} \hat{V}_{\sigma\Gamma} \hat{V}_{\Gamma_{\sigma}} \hat{V}_{\sigma'\Gamma'}'}{(i\omega - E_{1k})(i\omega - E_{2k})(i\omega - E_{3k})} \delta_{\Gamma'\Gamma} \delta_{\sigma\sigma'} \frac{(i\omega - i\nu - \epsilon_\tau)(i\omega - i\nu - \epsilon_\delta)\delta_{\sigma\Gamma} \delta_{\sigma'\Gamma'} \hat{V}_{\Gamma_{\sigma}} \hat{V}_{\sigma'\Gamma'}'}{(i\omega - i\nu - \epsilon_{\Gamma})(i\omega - i\nu - E_{1k})(i\omega - i\nu - E_{3k})}, \quad (4.28)$$

For ease of writing, we define the function

$$\mu_{\Gamma_{\sigma,\Gamma'}\sigma'}(k) = \sum_{\sigma} \hat{V}_{\Gamma_{\sigma}}(k) \hat{V}_{\sigma'\Gamma'}(k). \quad (4.29)$$
We also break up equation 4.28 into two pieces, one of order $\mu$ (which means it is of order $\hat{V}^2$), and the other of order $\mu^2$ (or $\hat{V}^4$). The $O(\mu)$ term is simpler, so we look at it first:

$$\frac{1}{N_s \beta} \sum_{\mathbf{k}, \alpha, \alpha', \mathbf{i} \omega} \mu_{\Gamma' \alpha, \Gamma \alpha}(\mathbf{k}) (i \omega - \epsilon_f)(i \omega - \epsilon_s) \delta_{\Gamma' \Gamma} \delta_{\alpha \alpha'} \delta_{\mathbf{q}, \mathbf{k}, \mathbf{q}'}$$ (4.30)

We employ the standard techniques for summing over the Matsubara frequencies. It is important to note that this is a zero temperature calculation. Furthermore, we have chosen the filling factor so that the quasiparticle chemical potential lies in the lowest band, $E_{1\mathbf{k}}$ (See Figure 4.5). This ensures that the only non-zero Fermi function is $f(E_{1\mathbf{k}})$, which, since there is then only one pole in equation 4.30, is a helpful simplification. The frequency sum gives:

$$\Gamma^{(2)}_{s \Gamma' \Gamma'} = -\frac{1}{N_s} \sum_{\mathbf{k}, \alpha} \frac{f(E_{1\mathbf{k}}) \mu_{\Gamma' \alpha, \Gamma \alpha}(\mathbf{k})(\epsilon_f - E_{1\mathbf{k}})(\epsilon_s - E_{1\mathbf{k}})}{(\epsilon_f - E_{1\mathbf{k}})(E_{2\mathbf{k}} - E_{1\mathbf{k}})(E_{3\mathbf{k}} - E_{1\mathbf{k}})} \delta_{\Gamma' \Gamma'}$$ (4.31)

where the superscript $(2)$ on the left side is to denote that this term is proportional to $\hat{V}^2$.

Recall that the bare $s$ vertex function is $\Gamma_{o, s \Gamma' \Gamma'} = \frac{N_s}{2} i \lambda_o \delta_{\Gamma' \Gamma'}$, where the energy $i \lambda_o$ is of the order of an eV. We know, however, that in the Kondo regime of the Anderson model, the relevant energy scale for the quasiparticles is the Kondo temperature, $T_o$, which is of the order of meV for CeCu$_2$Si$_4$. Thus, on physical grounds, we expect that $\Gamma^{(2)}_{s \Gamma' \Gamma'}$ must somehow cancel out the large energy, $i \lambda_o$. We can see that this does indeed occur as follows.

To paraphrase the previous statement, we wish to show that $\Gamma^{(2)}_{s \Gamma' \Gamma'} + \Gamma_{o, s \Gamma' \Gamma'} = 0$. The easiest way to proceed is directly from the mean-field Hamiltonian,

$$H_{MF} = \sum_{\mathbf{k}, \sigma} \xi_{\mathbf{k}} c_{\mathbf{k} \sigma}^\dagger c_{\mathbf{k} \sigma} + \sum_{\mathbf{k}, \alpha, \Gamma} [\tilde{V}_{\Gamma \alpha, \sigma}(\mathbf{k}) \tilde{\delta}_{\alpha \sigma} c_{\mathbf{k} \sigma}^\dagger f_{\mathbf{k} \Gamma \alpha} + \tilde{V}_{\Gamma' \alpha, \sigma}(\mathbf{k}) \tilde{\delta}_{\sigma \alpha} f_{\mathbf{k} \Gamma' \alpha}^\dagger c_{\mathbf{k} \sigma}]$$
At zero temperature, we require that the energy be an extremum with respect to \( \hat{s}_\sigma \) and \( i\lambda_\alpha \). That is, we want \( \partial\langle H\rangle/\partial \hat{s}_\sigma = 0 \) and \( \partial\langle H\rangle/\partial i\lambda_\alpha = 0 \). We focus on the former condition, which gives

\[
\frac{N\Gamma}{2} i\lambda_\alpha \hat{s}_\sigma^* + \frac{1}{N_s} \sum_{k\sigma\alpha} \hat{V}_{\Gamma\alpha\sigma}(\vec{k})(c_{k\sigma}^+ f_{k\Gamma\alpha}) = 0,
\]

where \( \delta \) is an infinitesimal imaginary time interval. In terms of Matsubara frequencies, we have

\[
\frac{N\Gamma}{2} i\lambda_\alpha \hat{s}_\sigma^* + \frac{1}{N_s\beta} \sum_{k\sigma\alpha\omega} \hat{V}_{\Gamma\alpha\sigma}(\vec{k}) \lim_{\epsilon \to 0^+} G_{\Gamma\alpha\sigma}(\vec{k}, \delta) = 0,
\]

where \( \epsilon_{\Gamma^*} \) means the crystal-field multiplet "opposite" to \( \Gamma \). For example, if \( \Gamma = \Gamma_\gamma \), then \( \Gamma^* = \Gamma_8 \). Summing over \( i\omega \) yields

\[
\frac{N\Gamma}{2} i\lambda_\alpha - \frac{1}{N_s} \sum_{k\alpha} \frac{f(E_{1k}) \mu_{\Gamma\alpha}(\vec{k}) (\epsilon_{\Gamma^*} - E_{1k})}{(E_{2k} - E_{1k})(E_{3k} - E_{1k})} = 0,
\]

which is equivalent to

\[
\frac{N\Gamma}{2} i\lambda_\alpha - \frac{1}{N_s} \sum_{k\alpha} \frac{f(E_{1k}) \mu_{\Gamma\alpha}(\vec{k}) (\epsilon_{\Gamma} - E_{1k}) (\epsilon_\sigma - E_{1k})}{(\epsilon_{\Gamma} - E_{1k})(E_{2k} - E_{1k})(E_{3k} - E_{1k})} = 0. \tag{4.34}
\]
We see that equation 4.34 is just what we wanted to show. The large energy $i\lambda_o$ is canceled by the term of order $\hat{V}^2$, and only the terms of order $\hat{V}^4$ are left. (n.b. There is no contribution of order $\hat{V}^2$ from the third term in equation 4.25.)

The piece of equation 4.28 that is of order $\hat{V}^4$ is

$$\frac{1}{N_s\beta} \sum_{\vec{k}'\vec{k}'\alpha\alpha'\omega} \frac{\delta_{\alpha\gamma}\delta_{\alpha'\gamma'}\mu_{\Gamma\alpha'\Gamma'\gamma'\alpha}(\vec{k})\mu_{\Gamma\alpha'\Gamma'\gamma'\alpha}(\vec{k}') (i\omega - \epsilon_T) (i\omega - \epsilon_8)(i\omega - i\nu - \epsilon_T)}{(i\omega - E_{1\vec{k}})(i\omega - E_{2\vec{k}})(i\omega - E_{3\vec{k}})(i\omega - i\nu - \epsilon_T)(i\omega - i\nu - \epsilon_T)}$$

$$\times \frac{(i\omega - i\nu - \epsilon_8)\delta_{\vec{k}'\vec{k} - q}}{(i\omega - i\nu - E_{1\vec{k}})(i\omega - i\nu - E_{2\vec{k}})(i\omega - i\nu - E_{3\vec{k}})}.$$ 

In summing over $i\omega$, there are now two poles, since there are two factors in the denominator dependent on $E_1$, which yield the expression

$$\sum_{\vec{k}'\vec{k}'\Gamma'\alpha'\Gamma'\gamma'} \left\{ \frac{f(E_{1\vec{k}})(E_{1\vec{k}} - \epsilon_T)(E_{1\vec{k}} - \epsilon_8)\mu_{\Gamma\alpha'\Gamma'\gamma'}(\vec{k}')\mu_{\Gamma'\gamma'\alpha} (\vec{k}) \delta_{\alpha\gamma}\delta_{\alpha'\gamma'} \delta_{\vec{k}'\vec{k} - q}}{(E_{1\vec{k}} - E_{2\vec{k}})(E_{1\vec{k}} - E_{3k})(E_{1\vec{k}} - i\nu - \epsilon_T)(E_{1\vec{k}} - i\nu - \epsilon_T)} \right.$$ 

$$\times \frac{(E_{1\vec{k}} - i\nu - \epsilon_T)(E_{1\vec{k}} - i\nu - \epsilon_8)}{(E_{1\vec{k}} - E_{2\vec{k}} - i\nu)(E_{1\vec{k}} - E_{3\vec{k}} - i\nu)(E_{1\vec{k}} - E_{1\vec{k}} - i\nu)}$$

$$+ \frac{f(E_{1\vec{k}'})(E_{1\vec{k}'} - \epsilon_T)(E_{1\vec{k}'} - \epsilon_8)\mu_{\Gamma\alpha'\Gamma'\gamma'}(\vec{k}')\mu_{\Gamma'\gamma'\alpha}(\vec{k}) \delta_{\alpha\gamma}\delta_{\alpha'\gamma'} \delta_{\vec{k}'\vec{k} - q}}{(E_{1\vec{k}'} - E_{1\vec{k}} + i\nu)(E_{1\vec{k}'} - E_{2\vec{k}'})(E_{1\vec{k}'} - E_{3\vec{k}'})(E_{1\vec{k}'} - E_{3\vec{k}'})}$$

$$\times \frac{(E_{1\vec{k}'} + i\nu - \epsilon_T)(E_{1\vec{k}'} + i\nu - \epsilon_8)}{(E_{1\vec{k}'} - E_{2\vec{k}'} + i\nu)(E_{1\vec{k}'} - E_{3\vec{k}'} + i\nu)} \right\}.$$ 

In the second piece of this equation make the changes $\vec{k} \leftrightarrow \vec{k}'$, $i\nu \rightarrow -i\nu$, $\Gamma \leftrightarrow \Gamma'$, and $\alpha \rightarrow \alpha'$. Then, we analytically continue the frequency $i\nu \rightarrow \nu + i\delta$. We are working in the static limit, so set $\nu \rightarrow 0$, and take the real part of the result to get

$$P \sum_{\vec{k}'\vec{k}'\alpha\alpha'} \frac{f(E_{1\vec{k}})\delta_{\alpha\gamma}\delta_{\alpha'\gamma'} \mu_{\Gamma\alpha'\Gamma'\gamma'}(\vec{k}') \mu_{\Gamma'\gamma'\alpha}(\vec{k}) (\epsilon_T - E_{1\vec{k}})^2 (\epsilon_8 - E_{1\vec{k}})^2}{(E_{1\vec{k}'} - E_{1\vec{k}})(E_{2\vec{k}'} - E_{1\vec{k}})(E_{3\vec{k}'} - E_{1\vec{k}})(E_{2\vec{k}'} - E_{1\vec{k}})(E_{3\vec{k}'} - E_{1\vec{k}})}$$

$$\times \frac{[\delta_{\vec{k}',\vec{k} - q} + \delta_{\vec{k}',\vec{k} + q}]}{(\epsilon_T - E_{1\vec{k}})(\epsilon_T - E_{1\vec{k}})},$$

(4.35)
where $P$ denotes the principal value is to be taken.

There is also the result represented by Figure 4.4, which comes from the expression

$$
\frac{1}{N_s \beta} \sum_{k'k'\alpha'\alpha'i\omega} \tilde{V}_{\alpha'\Gamma_\alpha}(\tilde{k}) G_{\Gamma_\alpha}(\tilde{k}, i\omega - i\nu) \tilde{V}_{\alpha'\Gamma_\alpha'}(\tilde{k}') G_{\Gamma_\alpha'}(\tilde{k}', i\omega) \delta_{\tilde{k}', \tilde{k} - \tilde{q}}
$$

and which is equivalent to the third term in equation 4.25. Recall from Chapter 3 that

$$
G_{\Gamma_\alpha}(\tilde{k}, i\omega) = \frac{\tilde{s}_{\alpha'} \tilde{V}_{\alpha'\Gamma_\alpha}(\tilde{k})(i\omega - \epsilon_{\Gamma'})}{(i\omega - E_{1\tilde{k}})(i\omega - E_{2\tilde{k}})(i\omega - E_{3\tilde{k}})}.
$$

(4.36)

When substituted above this gives

$$
\frac{1}{N_s \beta} \sum_{k'k'\alpha'\alpha'i\omega} \frac{\tilde{s}_{\alpha'} \tilde{s}_{\alpha'} \mu_{\Gamma_\alpha'\Gamma_\alpha'}(\tilde{k}') \mu_{\Gamma_\alpha'\Gamma_\alpha}(\tilde{k})(i\omega - i\nu - \epsilon_{\Gamma'})(i\omega - \epsilon_{\Gamma'}) \delta_{\tilde{k}', \tilde{k} - \tilde{q}}}{(i\omega - E_{1\tilde{k}})(i\omega - E_{2\tilde{k}})(i\omega - E_{3\tilde{k}})}
$$

(4.37)

Although it is not obvious, after summing over the frequencies, $i\omega$, and in the static limit ($\nu \to 0$), equation 4.37 becomes equation 4.35. Direct comparison with equation 4.35 will show the results are equivalent. Finally, the expression for $\Gamma_{ss\Gamma\nu^*}(\tilde{q})$ can be written as

$$
\Gamma_{ss\Gamma\nu^*}(\tilde{q}) = -2I_{ss\Gamma\nu^*}(\tilde{q}),
$$

(4.38)

where we have defined

$$
I_{ss\Gamma\nu^*}(\tilde{q}) \equiv \frac{P}{N_s} \sum_{k'k'\alpha'\alpha'} \frac{f(E_{1\tilde{k}}) \tilde{s}_{\alpha'} \tilde{s}_{\alpha'} \mu_{\Gamma_\alpha'\Gamma_\alpha'}(\tilde{k}') \mu_{\Gamma_\alpha'\Gamma_\alpha}(\tilde{k})(\epsilon_{\Gamma'} - E_{1\tilde{k}})^2(\epsilon_{\nu} - E_{1\tilde{k}})^2}{(E_{1\tilde{k}'} - E_{1\tilde{k}})(E_{2\tilde{k}'} - E_{1\tilde{k}})(E_{3\tilde{k}'} - E_{1\tilde{k}})(E_{2\tilde{k}} - E_{1\tilde{k}})}
$$

$$
\times \frac{[\delta_{\tilde{k}', \tilde{k} - \tilde{q}} + \delta_{\tilde{k}', \tilde{k} + \tilde{q}}]}{(\epsilon_{\Gamma} - E_{1\tilde{k}})(\epsilon_{\Gamma'} - E_{1\tilde{k}})(E_{3\tilde{k}} - E_{1\tilde{k}})}.
$$

(4.39)

The factor of two in equation 4.38 comes from the equivalence of equations 4.35 and 4.37.
4.2.5 Contributions to $\Gamma_{\lambda \Gamma'}(\vec{q})$.

From the expansion of the action (Appendix B), there are two equivalent terms that contribute to the off-diagonal component of the vertex function, $\Gamma_{\lambda \Gamma'}$. We focus on one term and double it:

$$G_{\Gamma \Gamma'}(\vec{k} - \vec{q}, i\omega - i\nu)\tilde{s}_{\alpha \sigma'}\tilde{V}_{\Gamma' \sigma'}(\vec{k} - \vec{q})G_{\sigma \sigma}(\vec{k} - \vec{q}, i\omega - i\nu)\tilde{V}_{\sigma' \alpha}(\vec{k} - \vec{q})$$

which is equivalent to

$$G_{\Gamma \sigma}(\vec{k} - \vec{q}, i\omega - i\nu)\tilde{V}_{\sigma' \sigma}(\vec{k} - \vec{q})\delta_{\tilde{s}_{\Gamma'}}(i\nu)G_{\Gamma' \sigma}(\vec{k} - \vec{q}, i\omega)\delta_{\lambda}(i\nu). \quad (4.40)$$

Substituting for the Green functions in equation 4.41 gives an expression that again can be divided into a $\tilde{V}^2$ piece and a $\tilde{V}^4$ piece. We start with the $\tilde{V}^2$ term,
which is

\[
\frac{i}{N_s\beta} \sum_{k\bar{k}',\alpha\alpha',\omega} \frac{\delta_{\alpha\Gamma}\mu_{\Gamma_0\Gamma_0'}(i\omega - \epsilon_{\Gamma'})\delta_{\Gamma\Gamma'}\delta_{\alpha\alpha'}\delta_{\bar{k}',\bar{k}-\bar{q}}}{(i\omega - E_{1\bar{k}})(i\omega - E_{2\bar{k}})(i\omega - E_{3\bar{k}})(i\omega - i\nu - \epsilon_{\Gamma'})}.
\] (4.42)

Summing over the Matsubara frequencies and taking the static limit gives

\[
\frac{i}{N_s\beta} \sum_{k\bar{k},\alpha\alpha'} f(E_{1\bar{k}})\delta_{\alpha\Gamma}\mu_{\Gamma_0\Gamma_0'}(i\omega - E_{1\bar{k}})\delta_{\Gamma\Gamma'}\delta_{\alpha\alpha'}
\]

\[
\frac{1}{(E_{2\bar{k}} - E_{1\bar{k}})(E_{3\bar{k}} - E_{1\bar{k}})(\epsilon_{\Gamma'} - E_{1\bar{k}})}.
\] (4.43)

The sums in equation 4.43 are all well-defined. There are no poles due to a term in the denominator like \(E_{1\bar{k}+q} - E_{1\bar{k}}\), as appears in equation 4.39. Thus it is not difficult to evaluate the expression numerically by carving the Brillouin zone into \(N^3\) cubes. This was done for both mean-field parameter set (a) and (b), which were introduced in the previous chapter. The results are listed below:

- for parameter set (a)
  
  \[
  \mu_0 = 2.440942 \text{ eV}
  \]
  
  \[
  E_\tau = -2.0 \text{ eV}
  \]
  
  \[
  V_0 = 0.8595 \text{ eV}
  \]
  
  \[
  n_{\text{total}} = 1.5
  \]
  
  \[
  \mu = 0.0208399
  \]
  
  \[
  \epsilon_\tau = 0.0217648
  \]
  
  \[
  s_\tau = 0.0934719,
  \]

we find \(\Gamma^{(2)}_{\alpha\lambda,\tau\tau}=27.54\) and \(\Gamma^{(2)}_{\alpha\lambda,88}=1.535\) for \(N=51\). It is interesting to note, that \(2/\delta_{\alpha\tau}=30.26\), which is actually in very good agreement with the numerical result for \(\Gamma^{(2)}_{\alpha\lambda,77}+\Gamma^{(2)}_{\alpha\lambda,88}\).

- For parameter set (b),
  
  \[
  \mu_0 = 3.338556 \text{ eV}
  \]
\[ E_7 = -2.0 \text{ eV} \]
\[ V_0 = 0.65 \text{ eV} \]
\[ n_{\text{total}} = 1.5 \]
\[ \mu = -0.8449990 \]
\[ \epsilon_7 = -0.84370213 \]
\[ s_0 = 0.14240942 \]

we find that \( \Gamma_{s\lambda,77}^{(2)} = 17.168 \) and \( \Gamma_{s\lambda,88}^{(2)} = 1.333 \) for \( N=51 \). Again, we note that \( 2/\tilde{s}_\sigma=19.86 \) and is in good agreement with the numerical result for the sum \( \Gamma_{s\lambda,77}^{(2)} + \Gamma_{s\lambda,88}^{(2)} \). In fact, this leads us to rewrite equation 4.43 as follows:

\[ \Gamma_{s\lambda,77}^{(2)} = \frac{i\pi_7}{\tilde{s}_\sigma}, \quad (4.44) \]

where for set (a) \( \pi_7 = 1.82, \pi_8 = 0.0717 \), and for set (b) \( \pi_7 = 1.729, \pi_8 = 0.0949 \).

Even thought the \( k \)-integral has not been difficult to evaluate, we found it instructive to simplify equation 4.43 so as to be able to evaluate everything analytically. We can then compare the approximate analytic result with the numerical result, giving us a way to judge the consequences of the approximations used. We begin by writing the \( k \)-sum as an energy integral,

\[ i \sum_{\alpha\sigma} N(0) \int_{-D}^{\mu} dE_1 \left( \frac{\partial \xi}{\partial E_1} \frac{\xi_7 - E_1}{E_3 - E_2} \right) \tilde{s}_\sigma |\tilde{V}_{\alpha\sigma}(\tilde{k})|^2, \]

where we have assumed a uniform density of states, \( N(0) \), for the free conduction electrons, and where \( \xi_7 \) is the free electron dispersion. The lower quasiparticle band edge is \( -D \). Next, we approximate the derivative \( \partial \xi / \partial E_1 \approx (E_3 - E_1) / (\epsilon_8 - E_1) \), which is the result for the SU(2) problem when \( E_1 \) and \( E_3 \) are the two hybridizing bands. This amounts to neglecting the middle hybridizing band that crosses over from \( \Gamma_7 \) to \( \Gamma_8 \) character as we move away from the zone center.
Finally, summing over the crystal field indices and assuming spherical symmetry gives

\[ i2N(0)\tilde{s}_o \tilde{V}_o^2 \int_{-D}^{\mu} dE_1 \frac{1}{(\epsilon_7 - E_1)(E_2 - E_1)} \]

\[ + i4N(0)\tilde{s}_{o8} \tilde{V}_{o8}^2 \int_{-D}^{\mu} dE_1 \frac{(\epsilon_7 - E_1)}{(\epsilon_8 - E_1)^2(E_2 - E_1)}. \]  (4.45)

Note that the energy band \( E_2 \) is basically equal to the energy \( \epsilon_7 \) for most momenta less than the Fermi momentum. (See Figure 4.6.) Thus we let \( E_2 \rightarrow \epsilon_7 \) in equation 4.45 to get

\[ i2N(0)\left[ \tilde{s}_o \tilde{V}_o^2 \left( \frac{1}{T_{o7}} - \frac{1}{D + \epsilon_7} \right) + 2\tilde{s}_{o8} \tilde{V}_{o8}^2 \left( \frac{1}{T_{o8}} - \frac{1}{D + \epsilon_8} \right) \right], \]

where we have defined the Kondo temperatures \( T_{o\Gamma} = \epsilon_\Gamma - \mu \). Since \( T_{o7} = 1.29 \) meV, \( T_{o8} = 3.73 \times 10^{-2} \) eV, and \( D + \epsilon_7 \approx D + \epsilon_8 \approx 2.5 \) eV, it is okay to drop the terms dependent on D. We are left with

\[ \Gamma^{(2)}_{s^\lambda} \approx 2iN(0)\left[ \tilde{s}_o \tilde{V}_o^2 \frac{1}{T_{o7}} + 2\tilde{s}_{o8} \tilde{V}_{o8}^2 \frac{1}{T_{o8}} \right], \]  (4.46)

where the superscript (2) on the left side means the term is of order \( \tilde{V}_o^2 \). In the limit of zero crystal field splitting this reduces to

\[ \frac{iNN(0)\tilde{s}_o \tilde{V}_o^2}{T_o} = \frac{i\sqrt{NN(0)Ns_oV_o^2}}{T_o}, \]  (4.47)

where \( N \) is now the degeneracy of the \( J_z \) multiplet and \( T_o \) is the Kondo temperature in the absence of crystal field splitting. Using that for spherical symmetry \( N(0)Ns_o^2V_o^2 \approx T_o \), equation 4.47 reduces further to

\[ \frac{i\sqrt{N}}{s_o}. \]  (4.48)
Figure 4.6:

Note that it is a good approximation to set $E_n \rightarrow \epsilon_7$ for most values of $|\vec{k}| < k_F$. The energy $\epsilon_7$ is represented by the dashed line.
This limit of $\Gamma_{s\lambda}^{(2)}$ is in agreement with the result of Zhang and Lee [2], who performed a $1/N$ calculation for the case of no crystal-field splitting, and who assumed an anisotropic hybridization matrix element of the Coqblin-Schrieffer form. (See equation 6 in reference [2] and note that the symbol $\alpha$ in their paper corresponds to $s_o V_o$ in our work.)

Before going on to the $\bar{V}^4$ term in $\Gamma_{s\lambda\Gamma'}$, let's gather all contributions to the $\Gamma_{s\lambda\Gamma'}$ so far. Within the framework of the approximations used, these are

$$\Gamma_{s\lambda\Gamma'}^{\text{partial}}(\bar{q}) = i\left(\frac{N_\Gamma}{2} \bar{s}_{0\Gamma} + \frac{T_0}{\bar{s}_{0\Gamma}}\right)\delta_{\Gamma'}$$

(4.49)

where the subscript "partial" is meant as a reminder that the $\bar{V}^4$ term has not yet been included. Using our mean-field values for the parameters $s_o$, $V_o$, and $T_{0\Gamma}$, in set (a) we can substitute numbers into the first two terms of equation 4.49. With

$$s_o = 0.0934719$$
$$V_o = 0.8595 \text{ eV}$$
$$T_{07} = 9.25 \times 10^{-4} \text{ eV}$$
$$T_{08} = 3.692 \times 10^{-2} \text{ eV},$$

we find that

$$N_7 \bar{s}_{07} = 0.1322$$
$$N_8 \bar{s}_{08} = 0.1869$$
$$\frac{x_7}{\bar{s}_{07}} = 27.54 \text{ eV}$$
$$\frac{x_8}{\bar{s}_{08}} = 1.535 \text{ eV}$$

It is clear that the dominant terms are

$$\frac{x_\Gamma}{\bar{s}_{0\Gamma}}.$$
Next, we return to the $\hat{V}^4$ term in $\Gamma_{s\Lambda\Gamma'}$, which is

\[
i \frac{1}{N_s \beta} \sum_{\vec{k} \vec{k'}, \alpha \alpha'} (i\omega - i\nu - \epsilon_\tau)(i\omega - i\nu - \epsilon_\omega) \frac{\tilde{s}_{\alpha \Gamma} \tilde{s}_{\alpha' \Gamma'} \delta_{\vec{k}, \vec{\epsilon} - \vec{q}}}{(i\omega - i\nu - E_{2\vec{k}})(i\omega - i\nu - E_{2\vec{k}'})(i\omega - i\nu - E_{2\vec{k}'})(i\omega - i\nu - E_{2\vec{k}})} \times \left[ \frac{\tilde{s}_{\alpha \Gamma} \mu_{\alpha \Gamma} \tilde{\epsilon}_{\alpha'}(\vec{k}) \mu_{\alpha' \Gamma'} \tilde{\epsilon}_{\alpha'}(\vec{k}')}{(i\omega - i\nu - E_{3\vec{k}})(i\omega - i\nu - \epsilon_\tau)(i\omega - i\nu - \epsilon_{\Gamma'})} \right]
\]
\[
\times \left[ \frac{\tilde{s}_{\alpha' \Gamma} \mu_{\alpha' \Gamma} \tilde{\epsilon}_{\alpha}(\vec{k}) \mu_{\alpha \Gamma'} \tilde{\epsilon}_{\alpha'}(\vec{k}')}{(i\omega - i\nu - E_{3\vec{k}'})(i\omega - i\nu - \epsilon_\tau)(i\omega - i\nu - \epsilon_{\Gamma'})} \right] \left[ \delta_{\vec{k}' - \vec{q}, \vec{k} - \vec{q}} + \delta_{\vec{k}' + \vec{q}, \vec{k} - \vec{q}} \right].
\]

Summing over the Matsubara frequencies and taking the limit as $\nu \to 0$:

\[
I_{s\Lambda\Gamma'}(\vec{q}) \equiv \frac{P}{N_s} \sum_{\vec{k}, \vec{k'}} \frac{f(E_{1\vec{k}})(\epsilon_\tau - E_{1\vec{k}})^2(\epsilon_\omega - E_{1\vec{k}})^2}{(E_{2\vec{k}} - E_{1\vec{k}})(E_{3\vec{k}} - E_{1\vec{k}})(E_{2\vec{k}'} - E_{1\vec{k}})(E_{3\vec{k}'} - E_{1\vec{k}})} \times \sum_{\alpha \alpha'} \frac{\tilde{s}_{\alpha \Gamma} \tilde{s}_{\alpha' \Gamma'}}{(E_{1\vec{k}} - \epsilon_\tau)(E_{1\vec{k}} - \epsilon_{\Gamma'})} \left[ \frac{\tilde{s}_{\alpha \Gamma} \mu_{\alpha \Gamma} \tilde{\epsilon}_{\alpha'}(\vec{k}) \mu_{\alpha' \Gamma'} \tilde{\epsilon}_{\alpha'}(\vec{k}')}{(E_{1\vec{k}} - \epsilon_\tau)} \right] \delta_{\vec{k}', \vec{q} - \vec{q}} + \delta_{\vec{k}', \vec{k} + \vec{q}}.
\]

Thus the off-diagonal vertex function is

\[
\Gamma_{s\Lambda\Gamma'}(\vec{q}) = i \left( \frac{N_f}{2} \tilde{s}_{\alpha \Gamma} + \frac{x_{\Gamma}}{\tilde{s}_{\alpha \Gamma}} \right) \delta_{\Gamma'} - iI_{s\Lambda\Gamma'}(\vec{q}).
\]

### 4.2.6 Contributions to $\Gamma_{s\Lambda\Gamma'}(\vec{q})$

There is only one term that contributes to $\Gamma_{s\Lambda\Gamma'}$, namely,

\[
\frac{1}{2} (i \cdot i) G_{\Gamma \alpha \Gamma'}(\vec{k} - \vec{q}, i\omega - i\nu) \delta \lambda_{\vec{q}}(i\nu) G_{\Gamma' \alpha \Gamma}(k, i\omega) \delta \lambda_{-\vec{q}}(-i\nu),
\]

which is represented diagrammatically in Figure 4.7. As before, upon substitution for the $f$ Green function, we have a complicated expression, which can be subdivided into two equivalent (in the static limit) pieces of order $\mu$ (that is, $\hat{V}^2$), one piece of order $\mu^2$ ($\hat{V}^4$), and even one piece of order $\mu^0$. The $\mu^0$ term...
Figure 4.7:
Contribution to the $\lambda$ vertex, $\Gamma_{\lambda\lambda,\Gamma'}(\vec{q}, i\nu)$.

will vanish when we sum over the Matsubara frequencies, since it will not have a Fermi function dependent upon the lowest energy band, $E_{1k}$.

Focus, next, on the $V^2$ term, which is

$$\frac{-1}{N_s\beta} \sum_{\vec{k}\vec{k}',\alpha\alpha'} (i\omega - i\nu - \epsilon_{\Gamma})(i\omega - \epsilon_{\Gamma'})(i\omega - E_{1\vec{k}})(i\omega - E_{2\vec{k}})(i\omega - E_{3\vec{k}}).$$

After summing over $i\omega$, we have

$$-\frac{P}{N_s} \sum_{\vec{k}'\alpha\alpha'} \frac{f(E_{1\vec{k}})\delta_{\alpha\alpha'} \delta_{\Gamma\Gamma'} \delta_{\vec{k}\vec{k}'} \delta_{\Gamma\Gamma'} (E_{1\vec{k}} - \epsilon_{\Gamma})(E_{1\vec{k}} - \epsilon_{\Gamma'})}{(E_{1\vec{k}} - \epsilon_{\Gamma})^2(E_{1\vec{k}} - \epsilon_{\Gamma'})(E_{1\vec{k}} - E_{2\vec{k}})(E_{1\vec{k}} - E_{3\vec{k}})}$$

$$\Gamma^{(2)}_{\lambda\lambda,\Gamma'} = \frac{1}{N_s} \sum_{\alpha} \frac{f(E_{1\vec{k}})\delta_{\alpha\alpha'} \delta_{\Gamma\Gamma'} (\epsilon_{\Gamma - E_{1\vec{k}}})(\epsilon_{\Gamma - E_{1\vec{k}}})^3 \delta_{\Gamma\Gamma'}}{(E_{2\vec{k}} - E_{1\vec{k}})(E_{3\vec{k}} - E_{1\vec{k}})(\epsilon_{\Gamma - E_{1\vec{k}}})^3} \delta_{\Gamma\Gamma'}.$$  (4.53)

As we did with equation 4.43, we evaluate the $k$-sum in equation 4.53 numerically. We find $\Gamma^{(2)}_{\lambda\lambda,77}=1053.6 \ (eV)^{-1}$, $\Gamma^{(2)}_{\lambda\lambda,88}=1.091\ (eV)^{-1}$ (with $N=51$) for parameter set (a), and $\Gamma^{(2)}_{\lambda\lambda,77}=714.8\ (eV)^{-1}$, $\Gamma^{(2)}_{\lambda\lambda,88}=1.336\ (eV)^{-1}$ for set (b). Recalling that $T_{\sigma\tau}=9.25 \times 10^{-4} \ eV$ for set (a), and $T_{\sigma\tau}=1.297 \times 10^{-3} \ eV$ for set (b),
means that we can write
\[ \Gamma^{(2)}_{\lambda\lambda\Gamma\Gamma'} = \frac{y_7}{T_0^\Gamma}, \quad (4.54) \]
where \( y_7 = 0.975, y_8 = 0.04029 \) for set (a), and \( y_7 = 0.925, y_8 = 0.0498 \) for set (b).

As we also did for equation 4.43, we approximate this integral to make it analytically tractable. As an energy integral, it takes the form
\[ N(0) \sum_{\Gamma_\alpha} \int_{-\mathcal{D}}^\mu dE_1 \frac{\partial \xi}{\partial E_1} \left| \frac{\tilde{V}_{\Gamma_\alpha\sigma}}{s_{\sigma\Gamma}} \right|^2 (\epsilon_7 - E_1)(\epsilon_8 - E_1) \]
\[ \frac{(\epsilon_2 - E_1)(\epsilon_3 - E_1)(\epsilon_\Gamma - E_1)^2}{(E_2 - E_1)(E_3 - E_1)} \quad (4.55) \]
The simplifications are: \( \partial \xi / \partial E_1 \approx (E_3 - E_1) / (\epsilon_8 - E_1) \); \( (E_2 - E_1) \rightarrow (\epsilon_7 - E_1) \) in the denominator of equation 4.55; and \( s_{\sigma\Gamma}\tilde{V}_{\sigma\Gamma}^2 \) is made spherically symmetric. The integral then simplifies to
\[ 2N(0) \int_{-\mathcal{D}}^\mu dE_1 \left[ \frac{s_{\sigma\Gamma}^2 \tilde{V}_{\sigma\Gamma}^2}{(\epsilon_7 - E_1)^3} + 2 \frac{s_{\sigma\Gamma}^2 \tilde{V}_{\sigma\Gamma}^2}{(\epsilon_8 - E_1)^3} \right] \]
\[ = 2N(0) \left[ \frac{s_{\sigma\Gamma}^2 \tilde{V}_{\sigma\Gamma}^2}{T_{\sigma\Gamma}^2} + 2 \frac{s_{\sigma\Gamma}^2 \tilde{V}_{\sigma\Gamma}^2}{T_{\sigma\Gamma}^2} \right], \quad (4.56) \]
where \( T_{\sigma\Gamma} = \epsilon_\Gamma - \mu \). (The reader is reminded that the tilde over a variable means it has been rescaled by a factor of \( \sqrt{N_\Gamma} \), i.e. \( s_{\sigma\Gamma} = s_\sigma / \sqrt{N_\Gamma} \) and \( \tilde{V}_{\sigma\Gamma} = \sqrt{N_\Gamma} V_\sigma \).)

To arrive at equation 4.56 we have dropped the terms \( 1/(\mathcal{D} + \epsilon_7) \) and \( 1/(\mathcal{D} + \epsilon_8) \).

Using that \( s_{\sigma\Gamma}^2 \tilde{V}_{\sigma\Gamma}^2 = s_\sigma^2 V_\sigma^2 \), gives
\[ \frac{2N(0)s_\sigma^2 V_\sigma^2}{2} \left[ \frac{1}{T_{\sigma\Gamma}^2} + \frac{2}{T_{\sigma\Gamma}^2} \right]. \quad (4.57) \]

From our mean-field analysis, we know that \( 2N(0)s_\sigma^2 V_\sigma^2 \approx T_{\sigma\Gamma} \), which leaves
\[ \frac{1}{2} \left[ \frac{1}{T_{\sigma\Gamma}^2} + \frac{2T_{\sigma\Gamma}}{T_{\sigma\Gamma}^2} \right] = \frac{1}{2} \left[ 1081.1 + 1.36 \right], \]
where the mean-fields values of parameter set (a) were used to get the numbers on the right side. This shows us that the second term above may be neglected, and our analytic approximation leads to
\[ \Gamma^{(2)}_{\lambda\lambda} = \frac{1}{2T_{\sigma\Gamma}^\Gamma}. \]
As before, we see that the approximations employed to evaluate equation 4.53 analytically are not too bad. Recall that the numerical evaluation of the k-space sum yielded approximately $1/T_\alpha$.

The order $\hat{V}^4$ contribution to $\Gamma_{\lambda\lambda'\Gamma'}$ is

$$\frac{-1}{2N_s\beta} \sum_{\vec{k}\vec{k}'\alpha\alpha'} \frac{\delta_{\alpha\alpha'} \delta_{\alpha\alpha'} \mu_{\alpha\alpha'}(\vec{k}') \mu_{\alpha\alpha'}(\vec{k}) (i\omega - \epsilon_\tau)(i\omega - \epsilon_8) \delta_{\vec{k},\vec{k}'} \delta_{\vec{k}'} \delta_{\vec{k}'-\vec{q}}}{(i\omega - E_{1\vec{k}})(i\omega - E_{2\vec{k}})(i\omega - E_{3\vec{k}})(i\omega - \nu - E_{1\vec{k}}')(i\omega - \nu - E_{2\vec{k}}')}
\times \frac{(i\omega - \nu - \epsilon_\tau)(i\omega - \nu - \epsilon_8)}{(i\omega - \nu - E_{3\vec{k}}')(i\omega - \nu - \epsilon_\tau')(i\omega - \nu - \epsilon_\tau')(i\omega - \epsilon_\tau')}. \quad (4.58)$$

The Matsubara sum, in the static limit, gives

$$\Gamma^{(4)}_{\lambda\lambda'\Gamma'} = \frac{P}{2N_s} \sum_{\vec{k}\vec{k}'\alpha\alpha'} \frac{f(E_{1\vec{k}})^2 \delta_{\alpha\alpha'} \delta_{\alpha\alpha'} \mu_{\alpha\alpha'}(\vec{k}') \mu_{\alpha\alpha'}(\vec{k}) [\delta_{\vec{k},\vec{k}+\vec{q}} + \delta_{\vec{k}',\vec{k}-\vec{q}}]}{(E_{1\vec{k}} - E_{1\vec{k}})(E_{2\vec{k}} - E_{1\vec{k}}')(E_{3\vec{k}} - E_{1\vec{k}}')(E_{2\vec{k}} - E_{1\vec{k}}')}
\times \frac{(\epsilon_\tau - E_{1\vec{k}})^2 \epsilon_8 - E_{1\vec{k}})^2}{(\epsilon_\tau - E_{1\vec{k}})^2 (\epsilon_\tau' - E_{1\vec{k}}')^2 (E_{3\vec{k}} - E_{1\vec{k}})^2 (E_{2\vec{k}} - E_{1\vec{k}})}. \quad (4.59)$$

We define the function $I_{\lambda\lambda'\Gamma'}(\vec{q})$ by equation 4.59 and the following equality:

$$\Gamma^{(4)}_{\lambda\lambda'\Gamma'}(\vec{q}) = \frac{1}{2} I_{\lambda\lambda'\Gamma'}(\vec{q}). \quad (4.60)$$

Thus, the total contribution to $\Gamma_{\lambda\lambda'\Gamma'}$ is

$$\Gamma_{\lambda\lambda'\Gamma'}(\vec{q}) = \frac{y_\Gamma}{T_\alpha} \delta_{\Gamma\Gamma'} + \frac{1}{2} I_{\lambda\lambda'\Gamma'}(\vec{q}). \quad (4.61)$$

4.2.7 The Dressed Green Function, $\hat{D}_{\Gamma\Gamma'}(\vec{q})$.

As we near the end of this first section of the chapter, we can now present the dressed Bosonic Green function. In matrix form, we define

$$\hat{D}^{-1}_{\Gamma\Gamma'}(\vec{q}) = -\hat{\Gamma}_{\Gamma\Gamma'}(\vec{q}), \quad (4.62)$$

which gives

$$D^{-1}_{\alpha\alpha'\Gamma'}(\vec{q}) = 2I_{\alpha\alpha'\Gamma'}(\vec{q}), \quad (4.63)$$
\[ D_{s}^{-1}(q) = -i \left( \frac{N_f}{2} s_{\delta \Omega} \right) \delta_{\Gamma \Gamma'} + i I_{s \lambda \Gamma \Gamma'}(q), \quad (4.64) \]

\[ D_{\lambda \lambda \Gamma \Gamma'}^{-1}(q) = -\frac{y_{\Gamma}}{T_{0 \Omega}} \delta_{\Gamma \Gamma'} - \frac{1}{2} I_{\lambda \lambda \Gamma \Gamma'}(q), \quad (4.65) \]

where \( I_{s \lambda \Gamma \Gamma'} \) is defined in equation 4.39, \( I_{s \lambda \Gamma \Gamma'} \) in equation 4.50, and \( I_{\lambda \lambda \Gamma \Gamma'} \) in equation 4.59.

### 4.2.8 Summing over the Crystal Field Multiplet Indices

It is convenient to define a Bose propagator \( \hat{D} \), that is independent of the crystal field indices. To do this, look at the last term of the action 4.21,

\[ \sum_{\Gamma \Gamma'} \left( \delta \delta_{\Gamma} \delta \lambda \right) \hat{G}_{\Gamma \Gamma'} \left( \delta \delta_{\Gamma'} \right), \quad (4.66) \]

where, for convenience, we have not shown the momentum or frequency dependence. Recalling that \( \delta \delta_{\Gamma} = \delta s / \sqrt{N_{\Gamma}} \), where \( \delta s \) is independent of the crystal field multiplet, means we can expand the products in equation 4.66 as follows:

\[ \sum_{\Gamma \Gamma'} \left( \delta s \frac{\Gamma_{s \lambda \Gamma \Gamma'}}{\sqrt{N_{\Gamma} N_{\Gamma'}}} \delta s + \delta \delta_{\Gamma} \delta \lambda \frac{\Gamma_{s \lambda \Gamma \Gamma'}}{\sqrt{N_{\Gamma} N_{\Gamma'}}} \delta s + \delta \lambda \frac{\Gamma_{s \lambda \Gamma \Gamma'}}{\sqrt{N_{\Gamma} N_{\Gamma'}}} \delta \lambda \frac{\Gamma_{s \lambda \Gamma \Gamma'}}{\sqrt{N_{\Gamma} N_{\Gamma'}}} \delta \lambda \right). \quad (4.67) \]

Because all the Bosonic fields are now independent of \( \Gamma \) and \( \Gamma' \), we can write equation 4.66 as

\[ \left( \delta s \delta \lambda \right) \hat{G} \left( \delta s \delta \lambda \right), \quad (4.68) \]

where

\[ \hat{G} = \left( \frac{\sum_{\Gamma \Gamma'} \frac{\Gamma_{s \lambda \Gamma \Gamma'}}{\sqrt{N_{\Gamma} N_{\Gamma'}}}}{\sum_{\Gamma \Gamma'} \frac{\Gamma_{s \lambda \Gamma \Gamma'}}{\sqrt{N_{\Gamma} N_{\Gamma'}}}} \frac{\sum_{\Gamma \Gamma'} \frac{\Gamma_{s \lambda \Gamma \Gamma'}}{\sqrt{N_{\Gamma} N_{\Gamma'}}}}{\sum_{\Gamma \Gamma'} \frac{\Gamma_{s \lambda \Gamma \Gamma'}}{\sqrt{N_{\Gamma} N_{\Gamma'}}}}, \quad (4.69) \]

Let us define a Bose propagator, $\hat{D}(\vec{q})$ by the following, where we shall suppress the temporal dependence:

$$\hat{D}(\vec{q}) = -\hat{\Gamma}(\vec{q}) = \left( \begin{array}{c}
\langle \delta s_{-\vec{q}} \delta s_{\vec{q}} \rangle \\
\langle \delta \lambda_{-\vec{q}} \delta s_{\vec{q}} \rangle \\
\end{array} \right). \tag{4.70}$$

Then we see that the crystal field dependent propagator $\hat{D}_{\Gamma \Gamma'}(\vec{q})$, can be related to the elements of this new propagator as follows:

$$D_{ss\Gamma \Gamma'}(\vec{q}) = \langle \delta \tilde{s}_{-\vec{q}} \delta \tilde{s}_{\vec{q}} \rangle = \frac{\langle \delta s_{-\vec{q}} \delta s_{\vec{q}} \rangle}{\sqrt{N_\Gamma \sqrt{N_{\Gamma'}}}} = \frac{D_{ss}(\vec{q})}{\sqrt{N_\Gamma \sqrt{N_{\Gamma'}}}}, \tag{4.71}$$

and

$$D_{s\lambda \Gamma}(\vec{q}) = \langle \delta \tilde{s}_{-\vec{q}} \delta \lambda_{\vec{q}} \rangle = \frac{\langle \delta s_{-\vec{q}} \delta \lambda_{\vec{q}} \rangle}{\sqrt{N_\Gamma}} = \frac{D_{s\lambda}(\vec{q})}{\sqrt{N_\Gamma}}. \tag{4.72}$$

$D_{\lambda \lambda}(\vec{q})$ has no factors of $N$ to worry about; that is, $D_{\lambda \lambda}(\vec{q}) = D_{\lambda \lambda}(\vec{q})$. We shall see $D_{ss\Gamma \Gamma'}(\vec{q})$, $D_{s\lambda \Gamma}(\vec{q})$, and $D_{\lambda \lambda}(\vec{q})$ again in the next chapter, when we construct the quasiparticle scattering amplitude.

Please note, that we will not always include the explicit momentum vector, $\vec{q}$, in the arguments of the Bosonic Green functions. The argument $\vec{q}$ will be written when we wish to emphasize the momentum dependence.

4.2.9 Simplifications in Absence of Crystal Field Splitting.

In the last part of this section, we show that in the limit of spherical symmetry at the 4f sites our Bose propagator (as given by equations 4.63-4.65) reduces to that calculated by Zhang and Lee[2] in their earlier work. As discussed in chapter 2, they did not include crystal field splittings in their $1/N$ expansion, but they did use an anisotropic hybridization matrix element of the Coqblin-Schrieffer form[3], $V_{mc}(\vec{k})$, where $m$ labels the $N$ degenerate $J_z$ states of the
lowest spin-orbit coupled multiplet. Conforming to Zhang and Lee's notation, we define

$$V_{m\sigma}(\vec{k}) = V_{ok}\beta(\vec{k}), \quad (4.73)$$

where $V_{ok}$ carries the dependence on the radial component of $\vec{k}$, and the angular dependence is inside $\beta(\vec{k})$,

$$\beta_{m\sigma}(\vec{k}) = -\sqrt{\frac{4\pi}{3}} (-i)^3 \sigma \sqrt{\frac{7 - 2m\sigma}{14}} Y_{3,m - \frac{3}{2}}(\vec{k}), \quad (4.74)$$

with $\sigma = \pm 1$ is the pseudo-spin index.

We begin with $D_{ss}^{-1}(\vec{q})$. In spherical symmetry our function $I_{ss}^{G\Gamma'}(\vec{q})$ reduces to

$$I_{sphere}^{ss} = \sum_{\vec{k}\vec{k}'} f(E_{1\vec{k}}) \delta_0^2 V_o^4 \sum_{mm's\sigma'} \beta^*_{m\sigma}(\vec{k}) \beta_{m's\sigma'}(\vec{k}) \beta^*_{m's\sigma'}(\vec{k}') \beta_{m\sigma}(\vec{k}') \delta_{\vec{k}',\vec{k}+\vec{q}}. \quad (4.75)$$

For simplicity, we define

$$B(\vec{k} \cdot \vec{k}') = \sum_{mm's\sigma'} \beta^*_{m\sigma}(\vec{k}) \beta_{m's\sigma}(\vec{k}) \beta^*_{m's\sigma}(\vec{k}') \beta_{m\sigma}(\vec{k}'). \quad (4.76)$$

which depends only on the angle between the vectors $\vec{k}$ and $\vec{k}'$.

There are only two hybridizing bands in this problem, which are described by

$$E_{n\vec{k}} = \frac{\xi_{\vec{k}} + \epsilon \pm \sqrt{(\xi_{\vec{k}} - \epsilon)^2 + 4s^2 V_o^2}}{2}, \quad (4.77)$$

where the non-hybridizing bands have energy $\epsilon$, and $\xi_{\vec{k}}$ is the dispersion for the free electrons. Using equation 4.77 it is easy to prove the following identity:

$$(E_{2\vec{k}'} - E_{1\vec{k}})(E_{1\vec{k}'} - E_{1\vec{k}}) = (\xi_{\vec{k}'} - \xi_{\vec{k}})(\epsilon - E_{1\vec{k}}), \quad (4.78)$$

(see Appendix D for the proof). The identity substituted into equation 4.75 yields

$$I_{sphere}^{ss} = \sum_{\vec{k}\vec{k}'} \frac{f(E_{1\vec{k}}) \delta_0^2 V_o^4 B(\vec{k} \cdot \vec{k}') \delta_{\vec{k}',\vec{k}+\vec{q}}}{(E_{2\vec{k}'} - E_{1\vec{k}})(\xi_{\vec{k}'} - \xi_{\vec{k}})(\epsilon - E_{1\vec{k}})}.$$
Figure 4.8:
A schematic quasiparticle band structure in the absence of crystal field splitting. These bands result from the hybridization of free electrons with 6-fold degenerate, J=5/2 multiplets at each lattice site. Note the presence of the 4 non-hybridizing bands of energy $\epsilon$. This is the band structure appropriate for the calculation of Zhang and Lee[2].
Next, given that \( N(0)s_o^2V_o^2 \approx T_0 \), we can write

\[
\frac{NV_o^2}{N(0)} \sum_{kk'} \frac{f(E_{1k})T_0 B(\hat{k} \cdot \hat{k}') \delta_{k',k \pm q}}{(E_{2k} - E_{1k})(\xi_{k'} - \xi_k)(\epsilon - E_{1k})}.
\]

Following Zhang and Lee, define

\[
J_n(\tilde{q}) = \frac{n}{N^2(0)} \sum_{kk'} \frac{f(E_{1k})T_0 T_n B(\hat{k} \cdot \hat{k}') \delta_{k',k \pm q}}{(E_{2k} - E_{1k})(\xi_{k'} - \xi_k)(\epsilon - E_{1k})^n}.
\]

Finally we have

\[
I_{sphere}^{ss} = NV_o^2N(0)J_1(\tilde{q}),
\]

which means that

\[
D_{ss}^{-1}(\tilde{q}) = 2NV_o^2N(0)J_1(\tilde{q}).
\]

Equation 4.80 agrees with equation 6 of Zhang and Lee, which shows that our result reduces to the correct expression in the limit of spherical symmetry.

Next, we look at the off-diagonal propagator. Starting from equation 4.50, we rewrite \( I_{\lambda\mu \Gamma \Gamma'} \) in spherical symmetry,

\[
I_{sphere}^{ss} = 2i\tilde{s}_o^3\tilde{V}_o^4 \sum_{kk'} \frac{f(E_{1k})B(\hat{k} \cdot \hat{k}') \delta_{k',k \pm q}}{(E_{2k} - E_{1k})(E_{1k} - E_{1k})(E_{2k} - E_{1k})(E_{1k} - \epsilon)}
\]

\[
= -2i\tilde{s}_o^3\tilde{V}_o^4 \sum_{kk'} \frac{f(E_{1k})B(\hat{k} \cdot \hat{k}') \delta_{k',k \pm q}}{(E_{2k} - E_{1k})(\xi_{k'} - \xi_k)(\epsilon - E_{1k})^2},
\]

where equation 4.78 was used. Now \( \tilde{s}_o^4\tilde{V}_o^4 = s_o^4V_o^4 = T_0^2/N^2(0) \). Thus we have

\[
I_{sphere}^{ss} = \frac{-2i}{\tilde{s}_o N^2(0)} \sum_{kk'} \frac{f(E_{1k})T_0^2 B(\hat{k} \cdot \hat{k}') \delta_{k',k \pm q}}{(E_{2k} - E_{1k})(\xi_{k'} - \xi_k)(\epsilon - E_{1k})^2}
\]

\[
= -\tilde{s} J_2(\tilde{q}).
\]
So, in spherical symmetry

\[ D_{s\lambda}^{-1}(\bar{q}) = \frac{-2i}{\bar{s}_o} \left( 1 + \frac{1}{2} J_2(\bar{q}) \right), \]  

(4.81)

which (to within a factor of 2) agrees with Zhand and Lee. (n. b. Zhang and Lee include an extra factor of \(\sqrt{2/N}\) in their definition of \(V_{m\sigma}(\vec{k})\), which we have not done.)

Finally, what happens to \(D_{s\lambda}^{-1}(\bar{q})\)? From equation 4.59 we have

\[
I_{\lambda\lambda}^{\text{sphere}} = \frac{1}{2} s^4 V_o^4 \sum_{k,k'} \frac{f(E_{1k}) B(\vec{k} \cdot \vec{k'}) \delta_{\vec{k},\vec{k}\pm\vec{q}}}{(E_{1k'} - E_{1k})(E_{2k'} - E_{1k})(E_{2\bar{k}} - E_{1\bar{k}})(\epsilon - E_{1\bar{k}})^2}
\]

\[
= \frac{1}{2} s^4 V_o^4 \sum_{k,k'} \frac{f(E_{1\bar{k}}) B(\vec{k} \cdot \vec{k'}) \delta_{\vec{k},\vec{k}\pm\vec{q}}}{(E_{2\bar{k}} - E_{1\bar{k}})(\xi_{k'} - \xi_{\bar{k}})(\epsilon - E_{1\bar{k}})^3}.
\]

Using \(s^4 V_o^4 = T_o^2 / N^2(0)\), we can write

\[
I_{\lambda\lambda}^{\text{sphere}} = \frac{1}{2T_o N^2(0)} \sum_{k,k'} \frac{f(E_{1\bar{k}}) T_o^3 B(\vec{k} \cdot \vec{k'}) \delta_{\vec{k},\vec{k}\pm\vec{q}}}{(E_{2\bar{k}} - E_{1\bar{k}})(\xi_{k'} - \xi_{\bar{k}})(\epsilon - E_{1\bar{k}})^3}
\]

= \frac{1}{6T_o} J_3(\bar{q}).

So, in spherical symmetry,

\[ D_{s\lambda}^{-1}(\bar{q}) = \frac{-1}{T_o} \left( 1 + \frac{1}{6} J_3(\bar{q}) \right), \]  

(4.82)

which shows agreement (with Zhang and Lee).

A wonderful consequence of spherical symmetry is the appearance of the term \(\xi_{k'} - \xi_{\bar{k}}\) in the denominators of equations 4.80-4.82. This term is the source of all the divergences in the propagator. (i.e., whenever a \(\vec{k} + \vec{q}\) is selected such that \(\xi_{k+\bar{q}} = \xi_{\bar{k}}\)) Handling the principal value nature of these poles is greatly facilitated if the integration can be performed analytically. It turns out, that analytic integration is possible when \(\xi_{\bar{k}}\) has a quadratic dispersion.
To be more specific, suppose we fix \( \vec{q} = q \hat{z} \). Then \( \vec{k} \cdot \vec{q} = k q \cos \theta \), and

\[
\xi_{\vec{k}'} - \xi_{\vec{k}} = \gamma q^2 (1 + \frac{2k}{q} \cos \theta),
\]

(4.83)

where \( \gamma = \hbar^2 \pi^2 / 2ma \) (\( a \) is the lattice spacing). Further, the sums buried inside the function \( B(\vec{k} \cdot \vec{k}') \) can be evaluated exactly to give[2] (see Appendix A):

\[
\frac{1}{3} P_o(\vec{k} \cdot \vec{k}') + \frac{8}{21} P_2(\vec{k} \cdot \vec{k}') + \frac{2}{7} P_4(\vec{k} \cdot \vec{k}'),
\]

(4.84)

where \( P_n(\vec{k} \cdot \vec{k}') \) is the \( nth \) Legendre polynomial evaluated at the angle between \( \vec{k} \) and \( \vec{k}' \). Using equations 4.83 and 4.84, the angular integrals in the \( J_n \) functions can be done analytically, leaving a relatively simple radial integral to do numerically.

In our problem, the anisotropy due to the cubic symmetry destroys the possibility of performing any part of the \( \vec{k} \)-sums in the \( I_{\delta \Gamma'}, I_{\delta \Gamma'}, \) and \( I_{\Lambda \Gamma'} \) functions analytically. Further, because of the singular nature of the integrands, we do not wish to make any approximations. Thus we are made to calculate numerically the three dimensional principal-value sums in equations 4.80 -4.82. The remainder of this chapter is devoted to a discussion of our procedure for doing these sums. We make use of the so-called analytic tetrahedron method, which was originally used in concert with band structure calculations to find the density of states[4] and the real part of the dynamic susceptibility[5] for elemental metals.
4.3 The Analytic Tetrahedron Method

4.3.1 Introduction

We can write the expressions for our Bosonic Green functions so that they look like spectral functions of the form

$$
\Phi(E) = \frac{1}{N_s} \sum_{\vec{k}} \frac{M(\vec{k})}{E - E_{n\vec{k}} - i\delta},
$$

where $M(\vec{k})$ is a matrix element which can be a complicated function of $\vec{k}$, and where $E_{n\vec{k}}$ is the dispersion of the $n$-th energy band. Generally, the numerical evaluation of such an expression can be challenging. In terms of real and imaginary parts, equation 4.85 is equivalent to

$$
\Phi'(E) = \text{Re}\Phi(E) = P \frac{1}{N_s} \sum_{\vec{k}} \frac{M(\vec{k})}{E - E_{n\vec{k}}},
$$

$$
\Phi''(E) = \text{Im}\Phi(E) = \frac{\pi}{N_s} \sum_{\vec{k}} M(\vec{k}) \delta(E - E_{n\vec{k}}).
$$

In the absence of $M(\vec{k})$, $\Phi''(E)$ is just a density of states, while $\Phi'$ looks like the real part of a dynamic susceptibility. Handled numerically, the principal value nature of the sum in equation 4.86 makes it non-trivial. In fact, if we tried to do the sum by simply evaluating the function at many points throughout the zone, and then multiplying by a weighting factor, we would find an essentially infinite variance. That is, upon averaging the result over many different mesh sizes, the variance of the mean would be huge compared to the mean-value itself[6]. Thus some thought is required as how to proceed.
4.3.2 Linear Interpolation of the Energy inside Cubic and Tetrahedral Microzones.

An advance in this field of computation was made in the late 1960s by Gilat and Raubenheimer [4], who wished to calculate the phonon density of states in solids. Let us focus, momentarily, on equation 4.87 and write it specifically as a density of states, \( N(E) \):

\[
N(E) = \frac{1}{N_s} \sum_k \delta(E - E_{nk}) = \int_{E_{nk}=E} \frac{dS}{|\nabla_k E|}, \tag{4.88}
\]

where \( dS \) is an element of surface area, and the integral is over a surface of constant energy, \( E \).

Calculations of the density of states up to the time of Gilat and Raubenheimer's work had leaned upon a sampling method in which one calculates the energy eigenvalues at many different \( \vec{k} \)-points of the irreducible Brillouin zone and then sorts them into bins of some energy width \( \Delta E \), thereby creating a histogram, the height of which gives the number of states with a certain energy. (n.b. The irreducible Brillouin zone is the smallest part of the zone that can be used, under the operations of the appropriate symmetry group, to generate the entire Brillouin zone.) The disadvantage of such a sampling technique is the need for a very fine mesh of \( \vec{k} \) points to yield enough detail in the calculated density of states[7].

With Gilat and Raubenheimer's procedure, we break up the Brillouin zone into \( n_{mesh}^2 \) cubes and calculate the energy eigenvalues at the center of each cube. Call these energies \( E_{nk_c} \), where \( \vec{k}_c \) defines the center of a cube. If energies are needed on a finer scale than that set by the sub-cubes, the energies are
interpolated from the nearest cube center,

\[ E_{n\vec{k}} = E_{n\vec{k}_c} + \nabla_{\vec{k}} E_{n\vec{k}_c} \cdot (\vec{k} - \vec{k}_c), \]  

which thus requires knowledge of the gradients of the energy bands. Clearly, the choice of mesh size must be made wisely, since it won’t work to interpolate in regions of k-space where the bands are too rapidly changing. A reasonable choice for \( n_{\text{mesh}} \) will depend on the nature of the problem to be solved. Once \( n_{\text{mesh}} \) is fixed, however, all energies away from cube center, \( \vec{k}_c \), are calculated from equation 4.89.

Because of the linear interpolation, the surfaces of constant energy are just planes, since they will be defined as the set of k-points satisfying

\[ \nabla_{\vec{k}} E_{n\vec{k}_c} \cdot (\vec{k} - \vec{k}_c) = 0. \]  

For a given energy, say \( E^* \), the area integral in equation 4.88 now follows by finding the amount of area, \( S(E^*) \), that lies within each of the \( n_{\text{mesh}}^3 \) cubes. Since all the areas are planar, this reduces to the geometry problem of finding the possible areas of intersection between a plane and a cube, which Gilat and Raubenheimer calculated exactly. Thus this procedure is basically an exact calculation of the density of states, since the only approximation is that which comes from using linearly interpolated energies.

Of course, no procedure is flawless. When the bands are rapidly varying, equation 4.89 must be used judiciously, since the true surfaces of constant of energy may not be very planar. Further, this procedure requires calculation of the energy gradients at the \( n_{\text{mesh}}^3 \) cube centers. The advantages of such an analytic procedure, however, can oftentimes outweigh the disadvantages just mentioned [8],[9],[10], and variations of Gilat and Raubenheimer’s ideas are today ubiquitous.
Another advance came when Jepsen and Andersen[11] and (independently) Lehmann, Rennert, Taut, and Wonn[12] discovered the advantages of dividing the Brillouin zone into tetrahedra, as opposed to cubes. If \( \vec{k}_i \) \((i=1,2,3,4)\) label the four corners of a tetrahedron, then it is possible to interpolate the energy for any k-point inside the tetrahedron by knowing only the energies at the four corners, \( E_i \equiv E_{\vec{k}_i} \). For example, starting with the energy \( E_4 \), we can write[13]

\[
E_k = E_4 + \vec{b} \cdot (\vec{k} - \vec{k}_4),
\]

where the effective energy gradient, \( \vec{b} \), depends only on the set of \( \vec{k}_i \) and \( E_i \) as follows:

\[
\vec{b} = \sum_{i=1}^{3} [E_i - E_4] \vec{r}_i.
\]

The vector \( \vec{r}_1 \) is defined by \( \vec{r}_1 = \vec{k}_2 \times \vec{k}_3 / v \), where \( v \) is six times the volume of one tetrahedron and \( \vec{k}_1 = \vec{k} - \vec{k}_4 \). Note, also, that the vectors \( \vec{r}_2 \) and \( \vec{r}_3 \) follow from cyclic permutations of the indices in the definition of \( \vec{r}_1 \). By this interpolation method, we do not need to know both the energies, \( E_k \), and the gradients, \( \nabla_k E \).

Another advantage tetrahedra have over cubes is their ability to tile any Brillouin zone, not just a zone of cubic symmetry; and the tetrahedra inside a zone need not all be congruent (although it probably would be nice if they were all congruent). Finally, the analytic expressions for the areas of intersection, \( S(E) \), of a plane and a tetrahedron are slightly simpler than those of a plane and a cube. The interested reader is referred to references [4],[11], and [13] for a comparison of the expressions for these areas.

Rath and Freeman[5], and independently Lingård[14], were the first to apply these ideas to calculate the real part of the spectral function (equation 4.86). Since such physically useful quantities as the magnetic susceptibility and the
dielectric function can be calculated from equation 4.86, it is useful to have a procedure in hand that is able to handle the principal value nature of the k-sum. We shall discuss the work of Rath And Freeman in detail, since their results were used as a template when we constructed our code to calculate the Bosonic propagators.

We are able to cast our functions \( I_{ab}(\vec{q}) \) in the following susceptibility-like form:

\[
I_{ab}(\vec{q}) = \frac{P}{N_s} \sum_{\vec{k},\vec{k}'} f(E_{1\vec{k}}) a_{ab}(\vec{k}, \vec{k}') \frac{M_{ab}(\vec{k}, \vec{k}')}{E_{1\vec{k}'} - E_{1\vec{k}}},
\]

(4.93)

where the matrix element is a complicated function and will be presented later, and where \( a, b \) can represent \( ss, s, \lambda, \) or \( \lambda, \lambda \). The Fermi function, of course, restricts us to only the volume below the Fermi surface. Since the surfaces of constant energy are planar, we want to know the possible unique ways a plane can cut through a tetrahedron. It turns out, fortunately, that there are only three such ways; and furthermore, in each of the three cases, the two subdivided volumes of the intersected tetrahedron (the volume above the Fermi surface and the volume below the Fermi surface) are themselves either a single tetrahedron or a composite of three tetrahedra. We never deal with anything but tetrahedra.

Since they are a pivotal part of the procedure, we now study these three cases in detail. As before, let \( \vec{k}_i \) (i=1,2,3,4) label the four corners of a tetrahedron and \( E_i \) be the corresponding energies of the lowest band (\( n = 1 \)). Following Rath and Freeman[5], we assume the energies are ordered so that

\[
E_4 < E_3 < E_2 < E_1.
\]

(4.94)

Consider, first, the case where the Fermi surface intersects the tetrahedron, with the Fermi energy \( E_F \) of a size such that

\[
E_4 < E_F < E_3 < E_2 < E_1.
\]

(4.95)
Figure 4.9:
Intersection of the Fermi surface (plane) with the tetrahedron for the case $E_4 < E_F < E_3 < E_2 < E_1$. The occupied region of the tetrahedron (denoted by O) is also a tetrahedron: $(\vec{k}_4, \vec{K}_1, \vec{K}_2, \vec{K}_3)$. The unoccupied region (U) is a sum of three tetrahedra. (From reference [5])

(See Figure 4.9.) The points at which the planar Fermi surface intersects the tetrahedron are labeled $\vec{K}_1, \vec{K}_2,$ and $\vec{K}_3$. The Fermi function then tells us that we must include the contribution from the smaller (occupied) tetrahedron defined by the points $\vec{k}_4, \vec{K}_1, \vec{K}_2,$ and $\vec{K}_3$.

For the second case, suppose the Fermi surface intersects the tetrahedron so that $E_4 < E_3 < E_F < E_2 < E_1$. (See Figure 4.10.) If the intersection points are called $\vec{K}_1, \vec{K}_2, \vec{K}_3,$ and $\vec{K}_4$, then the volume beneath the Fermi surface will consist of three tetrahedra, which are themselves defined by: $(\vec{k}_4, \vec{K}_3, \vec{K}_1, \vec{K}_2)$, $(\vec{k}_3, \vec{K}_2, \vec{K}_3, \vec{K}_1)$, and $(\vec{k}_3, \vec{K}_1, \vec{K}_3, \vec{K}_4)$.

Finally, if $E_4 < E_3 < E_2 < E_F < E_1$, then once again the volume below the Fermi surface is the sum of three tetrahedra. (See Figure 4.11.) If $\vec{K}_1, \vec{K}_2, \vec{K}_3,$ and $\vec{K}_4$ are the points of intersection, then the three tetrahedra are: $(\vec{k}_3, \vec{K}_4, \vec{K}_2, \vec{K}_3)$, $(\vec{k}_4, \vec{K}_1, \vec{K}_2, \vec{K}_3)$, and $(\vec{k}_4, \vec{K}_2, \vec{K}_2, \vec{K}_3)$. Of course, there are also
Figure 4.10:
Intersection of the Fermi surface with the tetrahedron for the case $E_4 < E_3 < E_F < E_2 < E_1$. The occupied region (O) is a sum of three tetrahedra: $(\vec{k}_4, \vec{k}_3, \vec{K}_1, \vec{K}_2)$, $(\vec{k}_3, \vec{K}_2, \vec{K}_3, \vec{K}_1)$, $(\vec{k}_3, \vec{K}_1, \vec{K}_3, \vec{K}_4)$. The unoccupied region (U) is also a sum of three tetrahedra. (From reference [5])

the two trivial cases: if $E_4 < E_F$, then none of the tetrahedron can contribute to the sum, and if $E_1 > E_F$, the all of it can contribute.

We assume that the matrix element, $M_{ab}(\vec{k}, \vec{k}')$, is constant throughout a given tetrahedron, as is almost always done in susceptibility calculations[15],[16]. The consequences of this assumption will be discussed later. At present, we see that we need the following integral over a tetrahedron:

$$ I = \int_{\text{tetra}} \frac{d^3k}{E_{1\vec{k}'} - E_{1\vec{k}}}, $$

(4.96)

where $\vec{k}' = \vec{k} \pm \vec{q}$. For simplicity, we use the same geometry as Rath and Freeman.

Let the corners of the tetrahedron have the coordinates

$$ \vec{k}_1 = (0, 0, 0) $$

(4.97)

$$ \vec{k}_2 = (X_1, 0, 0) $$

(4.98)
Figure 4.11:
Intersection of the Fermi surface with the tetrahedron for the case $E_4 < E_3 < E_2 < E_F < E_1$. The occupied region of the tetrahedron (O) is a sum of three tetrahedra: $(\vec{k}_3, \vec{k}_4, \vec{K}_3, \vec{k}_2), (\vec{k}_4, \vec{K}_1, \vec{K}_2, \vec{K}_3), (\vec{k}_4, \vec{k}_2, \vec{K}_2, \vec{K}_3)$. The unoccupied region is a tetrahedron. (from reference [5])

$$\vec{k}_3 = (X_2, Y_2, 0) \quad (4.99)$$
$$\vec{k}_4 = (X_3, Y_3, Z_3). \quad (4.100)$$

(See Figure 4.12.) Next, we define the energy differences at the four corners,

$$V_i = E_{1\vec{k}_i} - E_{1\vec{k}_1}, \quad (4.101)$$

and proceed to interpolate both $E_{1\vec{k}_i}$ and $E_{1\vec{k}_1}$ into the tetrahedron, relative to the corner at the origin. This means, for a $\vec{k}$ inside the tetrahedron, that

$$E_{\vec{k}} = E_{\vec{k}_1} + \vec{b} \cdot (\vec{k} - \vec{k}_1), \quad (4.102)$$

$$E_{\vec{k}'} = E_{\vec{k}_1} + \vec{b}' \cdot (\vec{k} - \vec{k}_1), \quad (4.103)$$

where we have dropped the band index for simplicity, and where we have used the fact that $\vec{k}' - \vec{k}_1 = \vec{k} - \vec{k}_1$. From equation 4.92 we know that the effective
Figure 4.12:
Chosen geometry for the k-space integral over a tetrahedron.

gradient takes the form
\[
\vec{b} = \sum_{i=2}^{4} (E_{\vec{k}_i} - E_{\vec{k}_1}) \cdot \vec{r}_i, \tag{4.104}
\]

\[
\vec{b}' = \sum_{i=2}^{4} (E_{\vec{k}'_i} - E_{\vec{k}'_1}) \cdot \vec{r}_i. \tag{4.105}
\]

Subtracting equations 4.103 and 4.102 then gives
\[
E_{\vec{k}'} - E_{\vec{k}} = V_1 + \sum_{i=2}^{4} (V_i - V_1) \vec{r}_i \cdot (\vec{k} - \vec{k}_1). \tag{4.106}
\]

Using the four vectors $\vec{k}_i$ defined by equations 4.97-4.100, we find, after some algebra, that
\[
E_{\vec{k}'} - E_{\vec{k}} = A + Bk_x + Ck_y + Dk_z, \tag{4.107}
\]

where

\[
V_1 = A \tag{4.108}
\]

\[
V_2 = A + BX_1 \tag{4.109}
\]

\[
V_3 = A + BX_2 + CX_3 \tag{4.110}
\]
\[ V_4 = A + BX_3 + CY_3 + DZ_3. \] (4.111)

The integral can now be written in the form
\[ I = \int_{tetra} d^3k \frac{1}{A + Bk_x + Ck_y + Dk_z}, \] (4.112)
which depends only on the set of \( V_i \) and the volume of the tetrahedron. The result is, using the notation of Rath and Freeman[5]:
\[ I = 3v_{tet} \left( \frac{V_1^2}{D_1} \ln \left| \frac{V_1}{V_4} \right| + \frac{V_2^2}{D_2} \ln \left| \frac{V_2}{V_4} \right| + \frac{V_3^2}{D_3} \ln \left| \frac{V_3}{V_4} \right| \right), \] (4.113)
where \( v_{tet} \) is the volume of the tetrahedron, and where
\[ D_1 = (V_1 - V_4)(V_1 - V_2)(V_1 - V_2) \] (4.114)
\[ D_2 = (V_2 - V_4)(V_2 - V_3)(V_2 - V_1) \] (4.115)
\[ D_3 = (V_3 - V_4)(V_3 - V_2)(V_3 - V_1). \] (4.116)

We must study equation 4.113 carefully in the limits where some of the \( V_i \)'s are equal to each other or are equal to zero. It turns out that there are quite a few such cases, which leads to many cumbersome logic statements in the actual computer code.

For example, consider the case where the energy differences at corners 1 and 2 are degenerate to each other, and (separately) the differences at corners 3 and 4 are degenerate, i.e. \( V_1 = V_2 \) and \( V_3 = V_4 \). Let \( V_2 = V_1 + x \) and \( V_4 = V_3 + y \), where \(|x| << |V_1| \) and \(|y| << |V_3| \). Substituting into equation 4.113, we find (after some algebra)
\[ \frac{I}{3v_{tet}} \rightarrow \frac{-V_1^2}{(V_1 - V_3)^3} \left( \frac{y}{x} \right) \ln \left| \frac{V_1}{V_3} \right| + \frac{V_1}{(V_1 - V_3)^2} \left[ \frac{2(V_1 - V_3) - 2V_1 + \frac{x}{y}V_1}{V_1 - V_3} \right] \ln \left| \frac{V_1}{V_3} \right| \]
\[ + \frac{V_1 + V_3}{(V_1 - V_3)^2}. \]
Taking the limits as \(x \to 0\) and \(y \to 0\) such that \(x/y \to 1\) gives us

\[
\frac{I}{3v_{tet}} = \frac{V_1 + V_3}{(V_1 - V_3)^2} - \frac{2V_1V_3}{(V_1 - V_3)^3} \ln \left| \frac{V_1}{V_3} \right|,
\]

which reduces to \(1/V_3\) when \(V_1 \to 0\) and to \(1/V_1\) when \(V_3 \to 0\). There are other cases, which we shall not derive here. See Table 4.1 for a listing of all the limits of equation 4.113. It is important to note, that whenever an expression for the integral occurs that would diverge as the result of a particular limit, the tetrahedron for which that limit applies is neglected.

Note in Table 4.1 that we have done a bit more than consider just the cases where \(V_i = V_j\) exactly. (Exactly, here, means that \(|V_i - V_j|/|V_i| = \delta\), where \(\delta\) is some very small number like \(10^{-5}\).) Instead, we made the substitution \(V_i = V_j + x\), where \(|x|\) is small compared to \(|V_j|\) and expanded equation 4.113 to second order in \(x\). For the first case in Table 4.1, where \(V_1 \to V_2 \to V_3 \to V_4\), there are three such small parameters, labeled by \(x\), \(y\), and \(z\), and we explicitly show the result of such an expansion in terms of these quantities. For the remaining cases, the algebraic expressions are too cumbersome to be of value in the table, but we remind the reader that the terms are present by including a \(+O(x, y, \cdots)\) after the zeroth order term. The motivation was, that by including these higher order terms the \textit{true} behavior of the integral might better (and more smoothly) be approximated, since then we can avoid sharply defined boundaries among the cases[17].

Before proceeding directly to our own self-energy calculations, we must check our integration code. We do so by calculating the static susceptibility of the free electron gas. The solution [18], in three dimensions, is given by the famous Lindhard function[19], and so we have an analytical check of our numerics. We
Table 4.1:
Various non-zero limiting cases of equation 4.113. Note that Cases II, III, and IV are valid for all possible permutations of the \( V_i \). Any combination of the \( V_i \) not present in the table have a zero contribution to the integral over the tetrahedron. Also, note that \( x_{ij} \equiv V_i - V_j \).

<table>
<thead>
<tr>
<th>Case</th>
<th>Restriction</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>I. ( V_1 = V_2 = V_3 = V_4 )</td>
<td>( V_1 \neq 0 )</td>
<td>( \frac{1}{V_1} - \frac{x_{14} + x_{24} + x_{34}}{4V_1^2} + \mathcal{O}(x^2) )</td>
</tr>
<tr>
<td></td>
<td>( V_3 \neq 0 )</td>
<td>( \frac{V_2^2 \ln \left</td>
</tr>
<tr>
<td>II. ( V_1 = V_2 = V_3 )</td>
<td>( V_4 \neq 0 )</td>
<td>( \frac{V_2^2 - 4V_3V_4 + 3V_4^2}{2(V_3 - V_4)^3} + \mathcal{O}(x_{13}, x_{23}) )</td>
</tr>
<tr>
<td></td>
<td>( V_3 \neq 0 )</td>
<td>( \frac{1}{2V_3} + \mathcal{O}(x_{13}, x_{23}) )</td>
</tr>
<tr>
<td>III. ( V_1 = V_2, V_3 = V_4 )</td>
<td>( V_2 \neq 0 )</td>
<td>( \frac{V_2^2 - V_2^2 - 2V_2V_4 \ln \left</td>
</tr>
<tr>
<td></td>
<td>( V_4 \neq 0 )</td>
<td>( \frac{1}{V_4} + \mathcal{O}(x_{12}, x_{34}) )</td>
</tr>
<tr>
<td></td>
<td>( V_2 = 0, V_4 \neq 0 )</td>
<td>( \frac{1}{V_2} + \mathcal{O}(x_{12}, x_{34}) )</td>
</tr>
<tr>
<td></td>
<td>( V_2 \neq 0, V_4 = 0 )</td>
<td>( \frac{1}{V_2} + \mathcal{O}(x_{12}, x_{34}) )</td>
</tr>
<tr>
<td>IV. ( V_1 = V_2 \neq V_3 \neq V_4 )</td>
<td>( V_2 \neq 0, V_3 \neq 0, V_4 \neq 0 )</td>
<td>( \frac{V_2}{(V_2 - V_3)(V_2 - V_4)} + \frac{V_2 \ln \left</td>
</tr>
<tr>
<td></td>
<td>( V_2 = 0, V_3 \neq 0, V_4 \neq 0 )</td>
<td>( \frac{\ln \left</td>
</tr>
<tr>
<td></td>
<td>( V_2 \neq 0, V_3 = 0, V_4 \neq 0 )</td>
<td>( \frac{1}{V_2 - V_4} + \frac{V_4 \ln \left</td>
</tr>
<tr>
<td></td>
<td>( V_2 \neq 0, V_3 \neq 0, V_4 = 0 )</td>
<td>( \frac{1}{V_2 - V_3} + \frac{V_3 \ln \left</td>
</tr>
<tr>
<td></td>
<td>( V_2 \neq 0, V_3 = 0, V_4 = 0 )</td>
<td>( \frac{1}{V_2} + \mathcal{O}(x_{12}) )</td>
</tr>
</tbody>
</table>
know that

\[
\int d^3 k \frac{f(\xi_k)}{\xi_{k+q} - \xi_k} = \frac{\pi}{\gamma q} \left[ \frac{k_F^2 - \frac{q^2}{4}}{2} \ln \left| \frac{k_F + \frac{q}{2}}{k_F - \frac{q}{2}} \right| + \frac{q k_F}{2} \right],
\]

(4.118)

where \( \gamma = \hbar^2 \pi^2 / 2 ma \), \( \xi_k = k^2 - \mu_o \), \( \mu_o \) is the chemical potential, and where we assumed \( \tilde{q} = q \tilde{z} \). For a Fermi momentum of \( k_F = 0.84 \), in units of \( \pi / a \), we evaluated equation 4.118 for many values of \( q \). As can be seen from Figure 4.13, the code handles this test case fine. Note that in the figure, the line represents the analytical result, while the open circles are the numerical data, which we obtained by breaking the Brillouin zone into \( 8 \times 51^3 \) tetrahedra. That is, the zone was divided into \( 51^3 \) cubes, and each cube was divided into eight tetrahedra. Although deceptively simple in appearance, this integral represents a non-trivial check of the code, since there is an entire surface of poles inside the Brillouin zone (defined by the relation \( k_z = -q/2 \)) that must be handled properly.

In contrast, a one-dimensional principal value integral can be regularized numerically by basically subtracting off the divergence[20], and such a procedure is facilitated by the relatively small number of poles throughout the domain of integration. In our three-dimensional integral for the free-electron gas, there are \( n_{\text{mesh}}^2 \) poles, which clearly gets large as \( n_{\text{mesh}} \) increases, and it is no longer possible to regularize the integral in a simple way. The large quantity of work done by (mostly) electronic structure physicists in this field of numerical k-space sums, is indicative of the degree of complexity inherent to these problems [9],[10].

### 4.3.3 Numerical Evaluation of the Dressed Bosonic Propagator

Having tested the code on the free-electron gas, we turn back to equations 4.63 - 4.65. For convenience we rewrite the dressed Bosonic Green function below:

\[
D^{-1}_{\omega \Gamma'}(\bar{q}) = 2 I_{\omega \Gamma'}(\bar{q}),
\]

(4.119)
Figure 4.13:
A calculation of the Lindhard function as a function of momentum, \( q \), along the \( z \) direction. The line is the analytical result, and the circles—calculated by the analytic tetrahedron method—are the numerical results. The integration mesh consisted of \( 8 \times 51^3 \) tetrahedra throughout the entire Brillouin zone.
\[ D^{-1}_{s\lambda\Gamma'}(\tilde{q}) = -i \left( \frac{N_{f \Gamma} \delta_{o\Gamma} + \pi_{\Gamma}}{\delta_{o\Gamma}} \right) \delta_{\Gamma'} + i J_{s\lambda\Gamma'}(\tilde{q}), \quad (4.120) \]

\[ D^{-1}_{\lambda\Lambda\Gamma'}(\tilde{q}) = -\frac{y_{\Gamma}}{\lambda_{\Gamma}} \delta_{\Gamma'} - \frac{1}{2} I_{\lambda\Lambda\Gamma'}(\tilde{q}). \quad (4.121) \]

If we define

\[ I_{\Gamma\Gamma'}(\tilde{k}, \tilde{k}') = \frac{\delta_{o\Gamma} \delta_{o\Gamma'} (\delta_{\tilde{k}, \tilde{k} + \tilde{q}} + \delta_{\tilde{k}', \tilde{k} - \tilde{q}})}{(E_{\tilde{k}'} - E_{\tilde{k}})(E_{3\tilde{k}'} - E_{2\tilde{k}})(E_{2\tilde{k}} - E_{1\tilde{k}})(E_{3\tilde{k}} - E_{1\tilde{k}})} \times \frac{(\epsilon_{\tilde{k}} - E_{1\tilde{k}})^2(\epsilon_{\tilde{k}'} - E_{1\tilde{k}})^2}{(\epsilon_{\tilde{k}} - E_{1\tilde{k}})(\epsilon_{\tilde{k}'} - E_{1\tilde{k}})}, \quad (4.122) \]

then

\[ I_{s\lambda\Gamma'}(\tilde{q}) = \sum_{\tilde{k} \tilde{k}' \alpha \alpha'} \frac{f(E_{1\tilde{k}}) I_{\Gamma\Gamma'}(\tilde{k}, \tilde{k}') \mu_{\Gamma \alpha \Gamma' \alpha'}(\tilde{k}) \mu_{\Gamma' \alpha' \Gamma \alpha}(\tilde{k}')} {E_{1\tilde{k}} - E_{1\tilde{k}'}}, \quad (4.123) \]

\[ I_{\lambda\Lambda\Gamma'}(\tilde{q}) = \sum_{\tilde{k} \tilde{k}' \alpha \alpha'} \frac{f(E_{1\tilde{k}}) I_{\Gamma\Gamma'}(\tilde{k}, \tilde{k}') \left[ \frac{\delta_{o\Gamma} \delta_{o\Gamma'} \mu_{\Gamma \alpha \Gamma' \alpha'}(\tilde{k}) \mu_{\Gamma' \alpha' \Gamma \alpha}(\tilde{k}')}{E_{1\tilde{k}} - \epsilon_{\Gamma'}} \right]} {E_{1\tilde{k}} - \epsilon_{\Gamma'}}, \quad (4.124) \]

\[ I_{\lambda\Lambda\Gamma'}(\tilde{q}) = \frac{1}{2} \sum_{\tilde{k} \tilde{k}' \alpha \alpha'} \frac{f(E_{1\tilde{k}}) I_{\Gamma\Gamma'}(\tilde{k}, \tilde{k}') \delta_{o\Gamma} \delta_{o\Gamma'} \mu_{\Gamma \alpha \Gamma' \alpha'}(\tilde{k}) \mu_{\Gamma' \alpha' \Gamma \alpha}(\tilde{k}')} {(\epsilon_{\Gamma} - E_{1\tilde{k}})(\epsilon_{\Gamma'} - E_{1\tilde{k}})(E_{1\tilde{k}} - E_{1\tilde{k}'})}. \quad (4.125) \]

We focus, first, on \( I_{s\lambda\Gamma'}(\tilde{q}) \). Casting equation 4.123 in the form of a spectral function (equation 4.93), it is clear that the effective matrix element is

\[ M_{s\lambda\Gamma'}(\tilde{k}, \tilde{k}') = \sum_{\alpha \alpha'} I_{\Gamma\Gamma'}(\tilde{k}, \tilde{k}') \mu_{\Gamma \alpha \Gamma' \alpha'}(\tilde{k}) \mu_{\Gamma' \alpha' \Gamma \alpha}(\tilde{k}'), \quad (4.126) \]

which, underneath all the notation, is a complicated function of momentum. We begin our study of equation 4.126 by looking only at a piece of it, namely, the combination of hybridization matrix elements,

\[ \mu_{\Gamma \alpha \Gamma' \alpha'}(\tilde{k}) \mu_{\Gamma' \alpha' \Gamma \alpha}(\tilde{k}') = \sum_{\sigma \sigma'} \tilde{V}_{\Gamma \alpha}(\tilde{k}) \tilde{V}_{\Gamma' \alpha'}(\tilde{k}) \tilde{V}_{\Gamma' \alpha'}(\tilde{k}') \tilde{V}_{\Gamma \alpha}(\tilde{k}'). \quad (4.127) \]
For given values of $\Gamma, \alpha, \Gamma'$, and $\alpha'$, the sums over $\sigma$ and $\sigma'$ in equation 4.127 can be computed exactly (See Appendix A). If $\Gamma = \Gamma' = \Gamma_7$ and $\alpha = \alpha' = +1$, this corresponds to the crystal-field state $|\Gamma_7, +1\rangle = -\sqrt{\frac{1}{6}} | -\frac{5}{2} \rangle + \sqrt{\frac{5}{6}} | \frac{3}{2} \rangle$. (See equation 2.62.) In this case, we find that

$$\begin{align*}
\mu_{\Gamma_7, +1, \Gamma_7, +1}(\vec{k}) & = \hat{V}_{\Gamma_7}(\vec{k}) \sum_{\sigma, \sigma'} \left[ Y_{00}^*(\vec{k}) - \frac{1}{3} Y_{40}^*(\vec{k}) - \frac{1}{3} \sqrt{\frac{5}{14}} (Y_{44}^*(\vec{k}) + Y_{44}^*(\vec{k}')) \right] \\
& \quad \times \hat{V}_{\Gamma_7}(\vec{k}) \sum_{\sigma, \sigma'} \left[ Y_{00}(\vec{k}') - \frac{1}{3} Y_{40}(\vec{k}') - \frac{1}{3} \sqrt{\frac{5}{14}} (Y_{44}(\vec{k}') + Y_{44}(\vec{k}')) \right].
\end{align*}$$

(4.128)

Note that $\hat{V}_{\sigma}(\vec{k})$ represents the dependence of the scaled (by $1/\sqrt{N_{\Gamma}}$) hybridization matrix element on the radial component of the momentum.

It is possible to do a similar calculation for all the other combinations of crystal-field quantum numbers. The results are presented in Table 4.2. All of these cases are then used to perform the sums over $\Gamma, \alpha, \Gamma'$, and $\alpha'$ in equation 4.126, leaving us with a matrix element, $M_{ss}(\vec{k}, \vec{k}')$, that is a function of momentum only. Thus we end up back with the expression

$$I_{s\Gamma s' \Gamma'}(\vec{q}) = \frac{P}{N_s} \sum_{\vec{k}, \vec{k}'} \frac{f(E_{1\vec{k}})M_{ss' \Gamma s' \Gamma'}(\vec{k}, \vec{k}')}{E_{1\vec{k}} - E_{1\vec{k}'}}. \quad (4.129)$$

We now turn to technical matters pertaining to the numerical evaluation of equation 4.129.

4.3.4 Technical Matters.

To begin, we mention briefly that we do not restrict our calculation to the irreducible wedge of the cubic Brillouin zone. A possible definition of the wedge is all the $k$-points satisfying

$$1 \geq k_x \geq k_y \geq k_z \geq 0, \quad (4.130)$$
Table 4.2:

Functional forms for the angular dependence of $\mu_{\Gamma\alpha\Gamma'\alpha'}$ for all possible combinations of the crystal field quantum numbers $\Gamma, \alpha, \Gamma', \alpha'$. Note, that by time-reversal symmetry, $\mu_{\Gamma\alpha\Gamma'\alpha'}=\mu_{\Gamma'\alpha'\Gamma\alpha}$, where the * denotes the time-reversed pair. For example, $\mu_{71,71} = \mu_{7,-1,7,-1}$. Note, also, that $V_{\alpha}(|k|)$ represents the dependence on the radial component of $k$. Any combination of quantum numbers not present in the table or not the time-reversed pair of quantum numbers in the table, will vanish upon summing over the pseudo-spin indices.

| $\Gamma, \alpha$ | $\Gamma', \alpha'$ | $\frac{\mu_{\Gamma\alpha\Gamma'\alpha'}(|k|)}{V_{\alpha}(|k|) V_{\alpha'}(|k|)}$ |
|------------------|------------------|----------------------------------|
| $7,1$            | $7,1$            | $-\frac{2\sqrt{\pi}}{3} [Y_{00} - \frac{1}{3} Y_{40} - \frac{1}{3} \sqrt{\frac{5}{14}} (Y_{44} + Y_{4-4})]$ |
| $8,2$            | $8,2$            | $-\frac{2\sqrt{\pi}}{3} [Y_{00} - \frac{8}{7} \sqrt{\frac{1}{5}} Y_{40} + \frac{1}{21} Y_{44} + \frac{1}{3} \sqrt{\frac{5}{14}} (Y_{44} + Y_{4-4})]$ |
| $8,1$            | $8,1$            | $-\frac{2\sqrt{\pi}}{3} [Y_{00} + \frac{8}{7} \sqrt{\frac{1}{5}} Y_{40} + \frac{2}{7} Y_{40}]$ |
| $8,2$            | $8,1$            | $\frac{10}{21} \sqrt{\frac{2\pi}{5}} [Y_{22} + \frac{3}{5} Y_{2-2} - \frac{\sqrt{3}}{2} Y_{42} + \frac{\sqrt{3}}{6} Y_{4-2}]$ |
| $8,1$            | $8,2$            | $\frac{10}{21} \sqrt{\frac{2\pi}{5}} [Y_{2-2} + \frac{3}{5} Y_{22} - \frac{\sqrt{3}}{2} Y_{4-2} + \frac{\sqrt{3}}{6} Y_{42}]$ |
| $8,2$            | $8,-1$           | $-\frac{4}{21} \sqrt{\frac{2\pi}{5}} [Y_{2-1} + \frac{5}{6} \sqrt{\frac{1}{2}} Y_{4-1} - \frac{5}{6} \sqrt{\frac{21}{2}} Y_{43}]$ |
| $8,-1$           | $8,2$            | $\frac{4}{21} \sqrt{\frac{2\pi}{5}} [Y_{21} + \frac{5}{6} \sqrt{\frac{3}{2}} Y_{4-1} - \frac{5}{6} \sqrt{\frac{21}{2}} Y_{4-3}]$ |
| $7,1$            | $8,2$            | $\frac{4}{21} \sqrt{6\pi} [Y_{2-1} - \frac{1}{6} Y_{4-1}]$ |
| $8,1$            | $7,1$            | $-\frac{4}{21} \sqrt{6\pi} [Y_{21} - \sqrt{\frac{1}{6}} Y_{41}]$ |
| $7,1$            | $8,1$            | $-\frac{4}{21} \sqrt{2\pi} [Y_{21} + \frac{1}{6} \sqrt{\frac{21}{2}} Y_{4-3} + \frac{5}{6} \sqrt{\frac{3}{2}} Y_{41}]$ |
| $8,1$            | $7,1$            | $-\frac{4}{21} \sqrt{2\pi} [Y_{2-1} + \frac{1}{6} \sqrt{212} Y_{43} + \frac{5}{6} \sqrt{\frac{3}{2}} Y_{4-1}]$ |
| $7,1$            | $8,-1$           | $\frac{2}{21} \sqrt{18\pi} [Y_{22} - \frac{1}{3} Y_{2-2} + \frac{1}{6} \sqrt{\frac{3}{2}} Y_{4-2} + \frac{5}{6} \sqrt{\frac{3}{2}} Y_{42}]$ |
| $8,-1$           | $7,1$            | $\frac{2}{21} \sqrt{18\pi} [Y_{2-2} - \frac{1}{3} Y_{22} + \frac{1}{2\sqrt{3}} Y_{42} + \frac{5}{6} \sqrt{\frac{3}{2}} Y_{4-2}]$ |
| $7,1$            | $8,-2$           | $-\frac{4}{21} \sqrt{\pi} [Y_{20} - \frac{\sqrt{2}}{3} Y_{40} + \frac{5}{6} \sqrt{\frac{7}{2}} Y_{4-4} - \frac{1}{6} \sqrt{\frac{7}{2}} Y_{44}]$ |
| $8,-2$           | $7,1$            | $-\frac{4}{21} \sqrt{\pi} [Y_{20} - \frac{\sqrt{2}}{3} Y_{40} + \frac{5}{6} \sqrt{\frac{7}{2}} Y_{44} - \frac{1}{6} \sqrt{\frac{7}{2}} Y_{4-4}]$ |
which corresponds to $1/48$ of the full zone. Of course, reducing the domain of integration by a factor of 48 seems useful, but the presence of the wavevector $\vec{q}$ ($\vec{k}' = \vec{k} \pm \vec{q}$) complicates things. If we wish to restrict the $k$-points to the irreducible wedge, then we must also sum over all momenta in the star of $\vec{q}$[21]. That is, we must include a sum over all momenta that can be obtained from $\vec{q}$ by the operations of cubic symmetry. (In this case, the symmetry group is $O_h$, the octahedral group.)

We can motivate this restriction with a toy example. Consider a two dimensional square lattice, as shown in Figure 4.14, and a vector $\vec{k} = (0.9, 0.1)$, which we shall take to lie in the irreducible wedge of the square Brillouin zone. Let there also be a vector $\vec{q} = (0.4, 0.0)$. If the function to be integrated were a function of $\vec{k}$ alone, then we could sum just over the $k$-points in the wedge and multiply the answer by the number of elements in the star of $\vec{k}$. The star of $\vec{k}$, denoted by $\{\vec{k}^*\}$, is the set of vectors equivalent to $\vec{k}$ under the operations of the symmetry group of the problem. We take $N_k$ to signify the number of $k$-points in that set. (For our 2D example, $N_k=8$.) Because our function is not a function of $\vec{k}$ alone, but depends also on $\vec{q}$, we need to think carefully how the irreducible wedge of the Brillouin zone should be used.

Consider each element in the star of $\vec{k}$, which are marked by $\times$s in Figure 4.14. For every such $\vec{k}$, we find $\vec{k} + \vec{q}$ and then, by using operations of square symmetry, we bring $\vec{k} + \vec{q}$ back to the irreducible wedge. For the given $\vec{q}$, and for all eight elements in the star of $\vec{k}$, there are four unique points in the irreducible wedge at which we end up. These four points are marked as open circles in Figure 4.14. Since $N_k=8$, each open circle stands for two of the eight elements in the set formed by $\{\vec{k}^*\} + \vec{q}$.
Figure 4.14:
Brillouin zone for a two dimensional square lattice. $\times$ labels the members of the star of $\bar{k}$. The filled in circle labels the members of the star of $\bar{q}$. 
Next, fix $\vec{k}$ at the original value of $\vec{k}=(0.9, 0.1)$, and sum over all elements in \{\vec{q}^*\}, of which there are four, and which are represented by filled-in circles in Figure 4.14. In this case, returning all values of $\vec{k}+\{\vec{q}^*\}$ to the irreducible wedge, we find that the open circles are still the equivalent points. Thus, in summing over all elements in \{\vec{q}^*\} is equivalent to summing over the elements of \{\vec{k}^*\}, if we multiply the \{\vec{q}^*\} sum by two. Using this fact, we jump to the general result

$$
\sum_{\vec{k}} \frac{1}{E_{\vec{k}+\vec{q}} - E_{\vec{k}}} = \frac{\mathcal{N}_k}{\mathcal{N}_q} \sum_{\vec{k} \in IW} \sum_{\{\vec{q}^*\}} \frac{1}{E_{\vec{k}+\vec{q}} - E_{\vec{k}}},
$$

(4.131)

where $\vec{k} \in IW$ denotes the k-points in the irreducible wedge.

For a given $\vec{k}$, we gain an advantage with this procedure only if $\vec{q}$ has higher symmetry than $\vec{k}$ so that $\mathcal{N}_k/\mathcal{N}_q > 1$. For the majority of $\vec{k}$ and $\vec{q}$, this inequality is not satisfied. That is, in three dimensions, for a general $\vec{k}$ not on an axis or at a zone corner (or center) $\mathcal{N}_k=48$. This is also true for general $\vec{q}$. Thus, for most possible combinations of $\vec{k}$ and $\vec{q}$, $\mathcal{N}_k/\mathcal{N}_q=1$. Furthermore, consideration only of the irreducible wedge in three dimensions would considerably complicate the geometry, since then we would have to worry about tetrahedra protruding partially out of or into the wedge. Thus it was not clear that enough was to be gained by working only in the irreducible wedge.

As the next technical point, consider again the following integral for the free electron gas:

$$
P \int d^3k \frac{1}{\xi_{\vec{k}+\vec{q}} - \xi_{\vec{k}}},
$$

where we assume $\vec{q} = q\hat{z}$. We know that the poles will occur at all k-points satisfying $k_z + (q/2) = 0$, which describes a plane perpendicular to the $k_z$ axis. We also know, empirically, that the tetrahedron method works best if the poles of the integrand happen to be directly at—or very close to—the corner of a tetra-
hedron, because then no linear interpolation of the energies is necessary. The best convergence for the free electron gas occurs when the mesh is chosen so that only boundaries of the tetrahedra lie against the plane defined by \( k_z + (q/2) = 0 \), i.e. no tetrahedron is intersected by the plane, except possibly at one of its four corners.

Interestingly enough, we find this exact same criterion works very well in the case of crystal field splitting. In Figure 4.15, we plot the numerical value of the integral

\[
\int d^3k \frac{f(E_{1\bar{k}+\bar{q}})}{E_{1\bar{k}+\bar{q}} - E_{1\bar{k}}} \tag{4.132}
\]

for \( \bar{q} = 0.5\bar{z} \) and as a function of the mesh parameter, \( n_{\text{mesh}} \). (Recall that \( 8 \times n_{\text{mesh}}^3 \) is the total number of tetrahedra throughout the Brillouin zone.) The solid line in the figure shows the results for a uniform mesh along the \( z \) direction, and the dashed line shows the results for an adaptive mesh along the \( z \) direction, satisfying the condition that no tetrahedron cuts the plane of \( k_z + (q/2) = 0 \). We used parameter set (b) to produce this plot. Except for the peaks around \( n_{\text{mesh}} = 28 \) and \( n_{\text{mesh}} = 42 \), it is clear that the adaptive mesh works remarkably well. The uniform mesh (solid line) is oscillating a great deal around a mean value of about 1200 (don’t worry about the units for now), while the adaptive mesh quickly converges to about 1200. The oscillations are probably due to the interpolation of the sharp Fermi surface near the plane \( k_z + (q/2) = 0 \). The adaptive mesh does not have to interpolate the energies for \( k \)-points on this plane, and it clearly does not suffer from the same “ringing”.

We have also checked this result by performing the integral in equation 4.132 but using the energies from the SU(2) problem, which are given by

\[
E_{1\bar{k}} = \frac{\xi_{\bar{k}} + \epsilon - \sqrt{(\xi_{\bar{k}} - \epsilon)^2 + 4s^2V^2_0}}{2}, \tag{4.133}
\]
Figure 4.15:
Comparison of evaluations of equation 4.132 using two different mesh types. The solid line represents a uniform mesh along all three principal axes of the Brillouin zone. The dotted line is the result of using an adaptive mesh along the z-direction ($\tilde{q} = 0.5\tilde{z}$) such that no tetrahedron cuts the plane defined by $k_z + 0.25 = 0$. Clearly the adaptive mesh is much the better.
and where all the symbols have been previously defined. A plot similar to that in Figure 4.15 is obtained. It is clear that an adaptive mesh that can handle an arbitrary \( \tilde{q} \), not just a vector with a non-zero \( z \)-component only, can be constructed and will handle well the principal value nature of our self-energy integrals. The fly in the ointment, however, remains: we must deal with the complicated “matrix elements”. We need to study the convergence properties of the integral when the matrix elements are included, but since they are so complicated, we shall break them up into simpler portions and study them piece by piece.

Recall that equation 4.126 is the matrix element for the propagator \( D_{ss}^{-1} \). There also are the matrix elements \( M_{s\lambda} \) and \( M_{\lambda\lambda} \), corresponding to the other two components of the Green function. We begin studying these functions by assuming a simplified version of them applicable to the SU(2) problem:

\[
I_{ss}^{\text{sphere}} = \int d^3k \frac{f(E_{1k}) s^2 V_o^4}{(E_{1k+q} - E_{1k})(E_{1k} - \epsilon)^2}, \tag{4.134}
\]

\[
I_{s\lambda}^{\text{sphere}} = \int d^3k \frac{f(E_{1k}) s^3 V_o^4}{(E_{1k+q} - E_{1k})(E_{1k} - \epsilon)^3}, \tag{4.135}
\]

\[
I_{\lambda\lambda}^{\text{sphere}} = \int d^3k \frac{f(E_{1k}) s^4 V_o^4}{(E_{1k+q} - E_{1k})(E_{1k} - \epsilon)^4}, \tag{4.136}
\]

where the mean-field parameters used are:

\[
\epsilon = -0.704086 \text{ eV}
\]

\[
\mu = -0.7150 \text{ eV}
\]

\[
s_o = 0.24639
\]

\[
V_o = 0.375 \text{ eV}
\]

\[
T_o (\text{Kondo temperature}) = \epsilon - \mu = 10.9 \text{ meV}.
\]
These numbers correspond to a very large Kondo scale of around 100K and hence a quasiparticle band that is not very flat near the chemical potential. In this case, we can estimate that the ratios of these integrals will be \((I_{ss}^{\text{sphere}} / I_{s\lambda}^{\text{sphere}}) \approx (I_{s\lambda}^{\text{sphere}} / I_{s\lambda}) \approx (s_o / T_o) \approx 22.6\), independent of the mesh parameter, \(n_{\text{mesh}}\). In Figure 4.16 we see that \((I_{\lambda\lambda}^{\text{sphere}} / I_{s\lambda}^{\text{sphere}}) \approx 19\) and \((I_{s\lambda}^{\text{sphere}} / I_{ss}^{\text{sphere}}) \approx 18\), which isn’t bad agreement. Also, we see that the ratio is largely independent of \(n_{\text{mesh}}\).

Thus even if the separate integrals \(I_{ss}^{\text{sphere}}\), \(I_{s\lambda}^{\text{sphere}}\), and \(I_{\lambda\lambda}^{\text{sphere}}\) have not converged as of \(n_{\text{mesh}} = 50\), their behavior is understandable and basically predictable, which is reassuring. As a matter of fact, this leads us to use the following criterion for our analysis of the rest of the pieces of the matrix elements: if the ratio of two different matrix elements is well behaved as a function of the mesh parameter \(n_{\text{mesh}}\), then we believe those matrix elements themselves are well behaved and will (given a large enough mesh) lead to a converged result for the integrals of which they are constituent parts. Note that we are not commenting on how large of a mesh is needed to get convergence. The necessary mesh size for convergence appears to be quite large indeed and is the main hindrance to a successful completion of this calculation.

We return to the crystal field problem and define three integrals that are analogous to equations 4.134- 4.136:

\[
I'_{ss} = \int d^3k \frac{f(E_{1\bar{k}})s_o^3V_o^4}{(E_{1\bar{k}+\bar{q}} - E_{\bar{k}})} \left[ (E_{1\bar{k}} - \epsilon_8)^2 + 2(E_{1\bar{k}} - \epsilon_7)(E_{1\bar{k}} - \epsilon_8) + (E_{1\bar{k}} - \epsilon_7)^2 \right], \quad (4.137)
\]

\[
I'_{s\lambda} = \int d^3k \frac{f(E_{1\bar{k}})s_o^3V_o^4}{(E_{1\bar{k}+\bar{q}} - E_{1\bar{k}})} \left[ \frac{(E_{1\bar{k}} - \epsilon_8)^2}{E_{1\bar{k}} - \epsilon_7} + (E_{1\bar{k}} - \epsilon_8) + (E_{1\bar{k}} - \epsilon_7) + \frac{(E_{1\bar{k}} - \epsilon_7)^2}{E_{1\bar{k}} - \epsilon_8} \right], \quad (4.138)
\]

\[
I'_{\lambda\lambda} = \int d^3k \frac{f(E_{1\bar{k}})s_o^3V_o^4}{(E_{1\bar{k}+\bar{q}} - E_{1\bar{k}})} \left[ \left( \frac{E_{1\bar{k}} - \epsilon_8}{E_{1\bar{k}} - \epsilon_7} \right)^2 + 2 + \left( \frac{E_{1\bar{k}} - \epsilon_7}{E_{1\bar{k}} - \epsilon_8} \right)^2 \right]. \quad (4.139)
\]

Just for convenience of checking the matrix elements, we have freely summed
Figure 4.16:
Ratios of the integrals \( \frac{I_{\lambda\lambda}}{I_{s\lambda}} \) and \( \frac{I_{s\lambda}}{I_{ss}} \) in the SU(2) model as a function of mesh parameter, \( n_{\text{mesh}} \).
Figure 4.17:
Ratios of the functions \( I'_{\lambda\lambda}/I'_{\lambda\lambda} \) and \( I'_{\lambda\lambda}/I'_{\lambda\lambda} \) in the presence of crystal fields as a function of the mesh parameter, \( n_{\text{mesh}} \). The functions \( I'_{\lambda\lambda}, I'_{\lambda\lambda}, \) and \( I'_{\lambda\lambda} \) are defined in the text. This figure is a check of the contribution (to the full matrix elements \( M_{ab} \)) of the hybridization matrix elements as a function of mesh size.

over all multiplet indices in equation 4.137-4.139. The mean-field parameters in this case are from set (b). Figure 4.17 shows that \( I'_{\lambda\lambda}/I'_{\lambda\lambda} \) and \( I'_{\lambda\lambda}/I'_{\lambda\lambda} \) are behaving reasonably well as a function of mesh size, since the plot shows nice horizontal lines.

This procedure can be generalized to study any combination of terms in the matrix elements. In fact, this was done with many different combinations, and
the only problem arose with the following functions:

\[
I''_{ss} = \int d^3k \frac{I'_{ss}}{E_{3\vec{k}+\vec{q}} - E_{1\vec{k}}},
\]

(4.140)

\[
I''_{s\lambda} = \int d^3k \frac{I'_{s\lambda}}{E_{3\vec{k}+\vec{q}} - E_{1\vec{k}}},
\]

(4.141)

\[
I''_{\lambda\lambda} = \int d^3k \frac{I'_{\lambda\lambda}}{E_{3\vec{k}+\vec{q}} - E_{1\vec{k}}},
\]

(4.142)

where the symbols \(I'_{ab}\) in the integrands of equations 4.140 - 4.142 actually stand for the integrands of equations 4.137 - 4.139. From Figure 4.18, there is a large variation at small \(n_{mesh}\) that is not present in any of the previous figures. (Note that the vertical axis of Figure 4.18 is logarithmic!) Whereas the ratio settles down for \(n_{mesh} \approx 40\), it is not clear such variation won’t occur at larger \(n_{mesh}\). Furthermore, this huge change occurs only when the term \(E_{3\vec{k}+\vec{q}} - E_{1\vec{k}}\) is present in the denominator.

If we can fix this anomaly, then all parts of the matrix elements behave properly, and we can be fairly certain that it is "just" a matter of using a large enough mesh to achieve convergence. We can see why the \(E_{3\vec{k}+\vec{q}} - E_{1\vec{k}}\) term is problematic by noting that the Kronecker delta \(\delta_{\vec{k}',\vec{k}+\vec{q}}\) we have been writing is actually \(\delta_{\vec{k}',\vec{k}+\vec{q}+\vec{Q}}\), where \(\vec{Q}\) is a reciprocal lattice vector. Thus, if \(\vec{k} + \vec{q}\) strays outside the first Brillouin zone, we use a reciprocal lattice vector to bring it back. Physically, this amounts to including Umklapp scattering.

In Figure 4.19(a) we plot the band \(E_{3\vec{k}}\) along the \(\Gamma X\) direction in the Brillouin zone. (\(\Gamma\) is the zone center and \(X\) is the zone boundary along the x-axis.) In Figure 4.19(b) we plot the same band shifted by \(\vec{q} = 0.5\vec{x}\), i.e. we plot \(E_{3\vec{k}+\vec{q}}\). Note that the shifted band has a sharp (non-analytic) point at the value of \(k_x\) where \(k_x + 0.5 = 1\). Such a sharp peak can wreak havoc with the matrix
Figure 4.18:
Ratios of the functions \( (I_{\lambda\lambda}'/I_{\sigma\lambda}') \) (solid line) and \( (I_{\ast\lambda}'/I_{ss}') \) (dash-dot line) as a function of the mesh parameter, \( n_{\text{mesh}} \). This figure is a check of the contribution of the shifted energy \( E_{3\xi-\xi} \) as a function of mesh size. The large variation at small \( n_{\text{mesh}} \) points to a problem with these shifted energies.
elements. This follows from the simple fact that for one mesh size the matrix elements may be evaluated near to the peak of $E_{3k+\mathbf{q}}$, while for a small change in mesh, because of the large gradient of the band energy near the peak, the matrix elements may experience a large change in size.

This sharp peak is artificial, since we know that in reality the itinerant electrons will experience a periodic lattice potential (call it $U$) that will cause a quadratic downturn in the bands near the zone boundary\[22\]. (See Figure 4.19(c). We also remind the reader of the discussion in Chapter 2 about effects of the lattice potential.) Finally, Figure 4.19(d) shows that such a simple addition of a quadratic downturn as a function of $k_x$ to the band $E_{3k}$ smooths over the peak in $E_{3k+\mathbf{q}}$. We used a potential of $U = 0.3 \text{ eV}$ for this calculation.

Figure 4.20 shows the results for the ratios $(I_{ss}^{\nu}/I_{s\lambda}^{\nu})$ and $(I_{s\lambda}^{\nu}/I_{ss}^{\nu})$, as plotted before in Figure 4.18. The huge variations at small $n_{\text{mesh}}$ have vanished, and the plot looks similar to Figures 4.16 and 4.17. Thus the smoothing of the peak in $E_{3k+\mathbf{q}}$ means that the full matrix elements $M_{ss}$, $M_{s\lambda}$, and $M_{\lambda\lambda}$ are well behaved. Of course, because we assume the matrix elements are constant inside a tetrahedron, the remaining question is how large of a mesh parameter, $n_{\text{mesh}}$, is needed for the convergence of the Bosonic Green functions. Unfortunately, there is no obvious answer to that question.

In the final part of this chapter, we return to the functions $I_{s\lambda\Gamma\nu}(\mathbf{q})$, $I_{\lambda\lambda\Gamma\nu}(\mathbf{q})$, and $I_{\lambda\lambda\Gamma\nu}(\mathbf{q})$. At the end of section 4.2, we discussed how to sum these expression properly over $\Gamma$ and $\Gamma'$. We define the quantities

$$I_{ss}(\mathbf{q}) = \sum_{\Gamma\Gamma'} \frac{I_{s\lambda\Gamma\nu}(\mathbf{q})}{\sqrt{N_\Gamma} \sqrt{N_{\Gamma'}}},$$  \hspace{1cm} (4.143)

$$I_{s\lambda}(\mathbf{q}) = \sum_{\Gamma\Gamma'} \left( \frac{I_{s\lambda\Gamma\nu}(\mathbf{q})}{\sqrt{N_\Gamma}} + \frac{I_{s\lambda\lambda\Gamma\nu}(\mathbf{q})}{\sqrt{N_{\Gamma'}}} \right).$$  \hspace{1cm} (4.144)
Figure 4.19:

(a). The energy band $E_{3\hat{z}}$ along the $\Gamma X$ direction. (b). The shifted band $E_{3\hat{z}+\vec{q}}$ for $\vec{q} = 0.5\hat{x}$ shows the sharp peak at $k_x = 0.5$, which leads to problems for the matrix elements evaluated near the peak. (c). A lattice potential of strength $U = 0.3eV$ pulls the band energies down near the $X$ point. (d). The shifted band now has a rounded peak at $k_x = 0.5$, which is sufficient to have well behaved matrix elements.
Figure 4.20:

Ratios of the integrals $(I''_{\lambda})/I''_{s\lambda}$ and $(I''_{s\lambda})/I''_{s\eta}$ in the presence of a lattice potential of strength $U = 0.3eV$. Note the ratios are well behaved at small $n$.

and

$$I_{\lambda\lambda}(\vec{q}) = \sum_{\Gamma'} I_{\lambda\Gamma'\Gamma'}(\vec{q}),$$

which are plotted as a function of the mesh parameter, $n_{\text{mesh}}$, in Figures 4.21 - 4.23 for parameter set (b) and in Figures 4.24- 4.26. (Note that in these six figures, we chose $\vec{q} = 0.5\hat{z}$.) It is clear that these integrals have not converged well at about $n_{\text{mesh}} \approx 50$. It is also clear that if we need convergence of the Green functions to several decimal places, it would require much more than $n_{\text{mesh}} = 50$. Empirically, we believe $n_{\text{mesh}} > 100$ would be necessary to achieve such convergence. In background, a calculation for $n_{\text{mesh}} = 40$ takes about one hour on a DEC 5100. (It takes longer on a DEC 3100.) Since the computing time goes as $n_{\text{mesh}}^3$, it is clear that a run with $n_{\text{mesh}} = 100$ would require a very long time indeed. We attempted to vectorize our code so as to take advantage of the local CRAY Y-MP supercomputer, but we discovered that the unwieldy logic statements required for the integration over a tetrahedron (See Table 4.1.)
hindered vectorization. That is, the many cases in Table 4.1 that arise to handle special limits of equation 4.113 require a plethora of logic statements in the computer code, which hinders vectorization. Actually, this numerical integration is parallel in nature. Each of the $n_{\text{mesh}}^3$ subcubes could, in principle, be integrated independently of the others, and at the end the net result would be the sum of the results from each subcube. This is the kind of problem a parallel machine should be able to handle well.

It is also interesting to note that calculations of the susceptibility or dielectric constant based on electronic structure data, generally are not performed for $n_{\text{mesh}}$ greater than about 30 [23]. The complicated nature of our matrix elements have forced us to push the procedure to very large values (by anyone's standards) of $n_{\text{mesh}}$.

Since we did not have easy access to a parallel machine, we proceeded in the following manner. As discussed in detail in the next chapter, we calculated the Fermi-surface averaged quasiparticle interactions for many different (self-energy) mesh parameters, in order to see if there was a strong dependence of the averaged interactions on the mesh size. After all, why work ourselves to death to calculate the Green functions to $x$ decimal places if the averaged interactions are only sensitive to $x-1$ places? The next chapter gives the results of this last stage of the calculation.
Figure 4.21:
Numerically evaluated function $I_{ss}(q)$ as a function of the mesh parameter, $n_{mesh}$ for mean-field parameter set (b). Here we used $\bar{q} = 0.5\bar{z}$. The variations near $n_{mesh} \approx 10$ is due to the spline fit to the data points.
Figure 4.22:
Numerically evaluated function $I_{s\lambda}(\bar{q})$ as a function of the mesh parameter, $n_{\text{mesh}}$ for mean-field parameter set (b). Here we used $\bar{q} = 0.5\bar{z}$. 
Numerically evaluated function $I_{\lambda}(\bar{q})$ as a function of the mesh parameter, $n_{\text{mesh}}$ for mean-field parameter set (b). Here we used $\bar{q} = 0.5\hat{q}$. 
Figure 4.24:
Numerically evaluated function $I_{ss}(q)$ as a function of the mesh parameter, $n_{\text{mesh}}$ for mean-field parameter set (a). Here we used $\bar{q} = 0.5\bar{\varepsilon}$. 
Figure 4.25:

Numerically evaluated function $I_{\lambda}(\tilde{q})$ as a function of the mesh parameter, $n_{\text{mesh}}$, for mean-field parameter set (a). Here we used $\tilde{q} = 0.5\tilde{z}$. 
Figure 4.26:
Numerically evaluated function $I_{\lambda\lambda}(\bar{q})$ as a function of the mesh parameter, $n_{\text{mesh}}$, for mean-field parameter set (a). Here we used $\bar{q} = 0.5\bar{z}$. 
Chapter IV  REFERENCES


7. see, e.g., F. M. Mueller, in ref[6].

8. see, e.g., J. F. Janak, in ref[6].


17. I am grateful to M. Alouani for this suggestion.


20. see, e.g., D. L. Cox, Ph. D. Thesis (Cornell University, 1985) unpublished.


22. see, e.g., ref[18], p. 151.

23. M. Steiner, private communication.
5.1 Introduction

As has been emphasized throughout this thesis, our ultimate goal is to look for a superconducting instability within the Anderson lattice in the presence of a large crystal field splitting on the 4f sites. (Large here means the crystal field splitting of the $J = 5/2$ multiplet, $\Delta_{CEF}$, is much larger than the Kondo temperature of the low lying $\Gamma_7$ doublet, $T_{o7}$.) We have pursued this goal by assuming there is an infinite Coulomb repulsion for double occupation of the 4f sites and by using a slave-Boson operator in the hybridization term—rather than a cumbersome projection operator. We also introduced a Lagrange multiplier, $\lambda$, at each site to require that the number of Fermions and Bosons be unity. In Chapter 3, we calculated the action of our model within a mean-field approximation, in which the slave Boson and Lagrange multiplier were assumed spatially and temporally uniform. This gave us the quasiparticle states $|Q_{n\xi\sigma}\rangle$ and energies, $E_{n\xi}$, where $n$ is the band index and $\sigma$ is the pseudo-spin index. In Chapter 4, we saw that
fluctuations (away from mean-field) of the slave Boson and Lagrange multiplier could be dressed by particle-hole excitations of the coupled conduction and 4f electron systems. We also briefly discussed the quasiparticle/Boson vertices, which can give rise to interactions between quasiparticles.

It is the last statement of the previous paragraph that introduces the focal point of this chapter. Using the dressed Bosonic Green functions and the quasiparticle/Boson vertices, we can construct the quasiparticle scattering amplitude, $\Gamma_{QP}(\vec{k}, \vec{k}')$. Note the subscript "QP". This was included to minimize confusion with the (matrix) vertex functions for the Bosons, $\hat{\Gamma}_\sigma$ and $\hat{\Gamma}_\Gamma$, which were derived in the previous chapter. We shall see that, after projecting $\Gamma_{QP}(\vec{k}, \vec{k}')$ onto states of cubic symmetry, $\Phi_\eta(\vec{k})$, the so-called cubic harmonics, and averaging over the Fermi surface, a superconducting instability of symmetry $\eta$ will be signaled by the average $\langle \Gamma_{QP} \rangle_\eta$ being negative. The word "average" here means:

$$\langle \Gamma_{QP} \rangle_\eta = \int \frac{d\vec{k}}{4\pi} \int \frac{d\vec{k}'}{4\pi} \Phi^*_\eta(\vec{k}') \Gamma_{QP}(\vec{k}, \vec{k}') \Phi_\eta(\vec{k}). \quad (5.1)$$

In practice, the strong anisotropy of the dressed Boson Green function, $\hat{D}(\vec{q})$, throughout the Brillouin zone makes it slow to converge as a function of mesh size. Since $\hat{D}_\Gamma(\vec{q}) = [\hat{\Gamma}_\Gamma(\vec{q})]^{-1}$ is fed into the scattering amplitude, representing an exchanged density fluctuation, this in turn renders conclusions about the possible pairing instabilities difficult to draw. We shall present our results as a function of the Bosonic propagator mesh size for mean field parameter seta (a), which was introduced in the previous chapter.

In chapter 4, we saw that the functions $I_{\sigma\Gamma'}(\vec{q})$, $I_{\lambda\Gamma'}(\vec{q})$, and $I_{\lambda\Gamma'}(\vec{q})$, which are the contributions to the Bosonic self-energy that are of order $\tilde{V}^4$, are the reasons why $\hat{D}_\Gamma$ is slow to converge. (Recall, we had a mesh parameter $n_{\text{mesh}}$, such that $8 \times n_{\text{mesh}}^3$ was the total number of tetrahedra throughout the
Brillouin zone.) In this chapter, we shall present results for the Fermi-surface averaged scattering amplitude, \( \langle \Gamma_{QP} \rangle_n \), as a function of the mesh parameter \( n_{\text{mesh}} \). Because of the complicated matrix elements discussed in chapter 4, we find that there can be large variations in \( \langle \Gamma_{QP} \rangle_n \) even for \( n_{\text{mesh}} \) of the order of 40. The only cure for these fluctuations is, as far as we are aware, to use a very fine mesh (probably \( n_{\text{mesh}} \approx 70 \)), which in turn requires a great deal of computer time. We shall present our results for as many values of \( n_{\text{mesh}} \) as we have been able to run. The consequences of these results for a superconducting instability in the Anderson lattice will be discussed at the end of the chapter.

We have found it useful to study the properties of the scattering amplitude in two steps. First, by setting the functions \( I_{\text{soft}}(\vec{q}) \), \( I_{\text{hard}}(\vec{q}) \), and \( I_{\text{int}}(\vec{q}) \) to zero, we simplify the problem considerably to that of two quasiparticles scattering via exchange of a momentum independent Boson. In real space, this corresponds to a local interaction between the quasiparticles. Note that we do not call this a hard-core interaction, since "hard-core" strictly means a contact interaction, which is possible only between two particles with zero relative angular momentum. In our case, the word "local" signifies an interaction between two particles in the same unit cell. Within the unit cell, the anisotropic, crystal field split, 4f wavefunctions allow for interactions between states of non-zero relative angular momentum.

We find these local interactions, when averaged over the Fermi surface, are substantially different from those calculated for the case of spherical symmetry by Zhang and T. K. Lee[1]. As we shall discuss, the averaged local interactions in the \( E_g \) symmetry channel are actually attractive; Zhang and Lee found that interactions in \( s, d, \) and \( g \)-wave pairing states were all repulsive.
As an aside, we would like to mention that one might find it useful to think (in general terms) of Zhang and Lee’s calculation as follows. Consider a regular array of “impurity” atoms, each with one 4f electron (prior to hybridization) embedded in a positive, uniform (jellium) background. This ensures that the underlying symmetry of the “host” is spherical. The local 4f wavefunctions at an arbitrary “impurity” site are of course anisotropic, and therefore the hybridization with the plane wave conduction states is also anisotropic. Furthermore, in spherical symmetry, the states in the 4f multiplets must be eigenstates of the (z-component) of the total angular momentum operator (in the presence of spin-orbit coupling). There can be no crystal field splitting of the multiplets. Thus one has anisotropic hybridization in the presence of over-all spherical symmetry.

In the case of cubic symmetry, inclusion of the functions \( I_{ss\Gamma'}(\mathbf{q}) \), \( I_{s\lambda\Gamma'}(\mathbf{q}) \), and \( I_{\lambda\lambda\Gamma'}(\mathbf{q}) \) is the computationally intensive part of this calculation. If there are strong local repulsive interactions, then the only way to get \( \langle \Gamma_{QP} \rangle_{\eta} < 0 \) for a given channel \( \eta \), is to have the \( I_{ss\Gamma'} \), \( I_{s\lambda\Gamma'} \), and \( I_{\lambda\lambda\Gamma'} \), which represent the effect of non-local interactions, overcome the repulsion. Zhang and Lee discovered that in spherical symmetry these q-dependent contributions are too weak to overcome the local repulsions in the s, d, and g-wave states. Although our averaged scattering amplitude is slow to converge, we can see that in cubic symmetry (with crystal-field splitting) the local interactions give hopeful signs for an \( E_g, T_{1g}, \) or \( T_{2g} \) pairing instability.
5.2 Motivation

5.2.1 CeCu$_2$Si$_2$

Although there has been a large amount of formalism in the last two chapters, we have always had a very specific heavy Fermion superconductor in mind, CeCu$_2$Si$_2$. In essence, we are asking: does the Anderson lattice have a superconducting instability for parameters realistically representing CeCu$_2$Si$_2$? The cubic symmetry and crystal field splitting were added to the Anderson lattice so as to agree with experimental properties of the material, such as: the temperature dependence of the specific heat for $T \geq 100$ K[2]; the isotropy of the slope of the upper critical field ($B'_c$) near $T_c$ for magnetic fields in the plane or perpendicular to the plane of the tetragonal unit cell[3]; and the isotropic effective mass as measured by de Hass-van Alphen experiments[4]. We also have chosen mean-field parameters that give a Kondo temperature of about 10 K, as deduced from the quasielastic linewidth of neutron scattering data[5].

When we calculate the quasiparticle scattering amplitude, we shall focus only on the even-parity, spin singlet case. Even parity pairing in CeCu$_2$Si$_2$ seems likely from the following experimental evidence (discussed in Chapter 1): strong Pauli limiting, as seen in the low temperature dependence of $B_{c2}$[6],[7]; and a relatively strong temperature dependence of the Knight shift below $T_c$[8].

Figure 5.1 shows the scattering amplitude, $\Gamma_{\sigma_1,\sigma_2,\sigma_3,\sigma_4}(\vec{k}, \vec{k}')$, including the exchange term, for a quasiparticle of momentum and pseudo-spin $\vec{k}, \sigma_1$ interacting (via Boson exchange) with another particle described by $-\vec{k}, \sigma_2$. The scattered particles are labeled by $\vec{k}', \sigma_4$ and $-\vec{k}', \sigma_3$. The wavy lines in the figure represent any one of the three components, $ss$, $s\lambda$, or $\lambda\lambda$, of the dressed Bose Green function. The vertices $\gamma_{mix}(\vec{k}, \vec{k}')$ and $\gamma_{ff}(\vec{k}, \vec{k}')$ were also introduced in the previous
Figure 5.1:
Quasiparticle scattering amplitude for incoming particles (solid lines) of momenta $\vec{k}$ and $-\vec{k}$. The wavy lines are dressed Boson propagators, and the vertices $\gamma_i$ ($i =$ f or mix) were introduced in the previous chapter.

Chapter, but for convenience we present them again below:

$$\gamma_{fi}(\vec{k}, \vec{k}') = \frac{A_n(\vec{k})A_{n'}(\vec{k}')}{(\epsilon_i - E_n\vec{k})(\epsilon_i - E_{n'}\vec{k}')} \tilde{s}_{fi} \tilde{V}_{i\alpha\sigma'}(\vec{k}') \tilde{V}_{i\alpha\sigma}(\vec{k}),$$  \hspace{1cm} (5.2)

$$\gamma_{mix}(\vec{k}, \vec{k}') = -\frac{A_n(\vec{k})A_{n'}(\vec{k}')}{(\epsilon_i - E_{n'}\vec{k}') \epsilon_i - E_n\vec{k}'} \tilde{s}_{gil} \tilde{V}_{i\alpha\sigma'}(\vec{k}') \tilde{V}_{i\alpha\sigma}(\vec{k}),$$ \hspace{1cm} (5.3)

where $A_n(\vec{k})$ is the quasiparticle normalization function for band $n$.

5.2.2 Ladder Series for Repeated Quasiparticle Scattering.

Before calculating $\Gamma_{\sigma_1\sigma_2\sigma_3\sigma_4}(\vec{k}, \vec{k}')$ explicitly, it is instructive to look at the ladder series of diagrams produced by repetition of the scattering depicted in Figure 5.1. It is clear that we have a Dysonesque equation for the dressed scattering amplitude, $\bar{\Gamma}_{\sigma_1\sigma_2\sigma_3\sigma_4}(\vec{k}, \vec{k}')$, as seen in Figure 5.2. Mathematically, $\bar{\Gamma}$ obeys the Bethe-Salpeter equation[13],
\[ \bar{\Gamma}(\vec{k}, \vec{k}') = \Gamma(\vec{k}, \vec{k}') - \frac{1}{2\beta N_s} \sum \Gamma(\vec{k}, \vec{k}'')G_{QP}(\vec{k}'', i\omega'')G_{QP}(-\vec{k}'', -i\omega'')\bar{\Gamma}(\vec{k}'', \vec{k}'), \]

(5.4)

where we have assumed that the bare and dressed amplitudes are static, and where (for simplicity) we have dropped all the subscripts on \( \Gamma \) and \( \bar{\Gamma} \). We shall discuss later the physical implications of such an approximation. The quasiparticle propagators come directly from the mean-field Hamiltonian (equation 4.32), written in the quasiparticle basis,

\[ G_{QP}(\vec{k}'', i\omega'') = \frac{1}{i\omega'' - E_{\vec{k}''}}. \]

(5.5)

There is no band subscript on the energy \( E_{\vec{k}''} \) because we know that only the quasiparticles near the Fermi energy (in the lowest band) can participate in the scattering. Summing over the Matsubara frequencies, \( i\omega'' \) in equation 5.4 gives

\[ \frac{1}{\beta} \sum_{\omega''} \frac{1}{i\omega'' - E_{\vec{k}''}} \frac{1}{-i\omega'' - E_{\vec{k}''}} = \frac{1}{2E_{\vec{k}''}} \tanh \left( \frac{\beta E_{\vec{k}''}}{2} \right). \]

(5.6)

Next, we project equation 5.4 onto states of cubic symmetry, the so-called cubic harmonics [11]. This statement requires some explanation. When we say cubic symmetry here, we are formally referring to the octahedral group, including inversions, \( O_h \)[12]. Knowing all the operations (rotations, reflections through mirror planes, etc.) that leave an octahedron unchanged, and using standard group theoretical arguments, it is possible to find the irreducible representations of the group, which are listed in Table 6.1. (See Appendix D of reference[10] for a detailed discussion.) We can construct functions that transform like the irreducible representations of the group, which in the case of octahedral symmetry, are called cubic harmonics. Altmann and Cracknell[11] have published extensive
Figure 5.2:
Ladder series for the dressed quasiparticle scattering amplitude $\Gamma_{\sigma_1\sigma_2\sigma_3\sigma_4}(k, k')$, in terms of the bare scattering amplitude, $\Gamma_{\sigma_1\sigma_2\sigma_3\sigma_4}(\bar{k}, \bar{k}')$, which is given in figure 5.1. The solid lines are quasiparticle propagators, and the wavy lines represent exchanged Bosons.
Table 5.1:
Irreducible representations of the octahedral group, $O$. To get the group $O_h$, we add inversions to the allowed symmetry operations, the result of which is that all representations pick up a subscript, $g$ (for even parity) or $u$ (for odd parity).

<table>
<thead>
<tr>
<th>Representation</th>
<th>Dimensionality</th>
<th>Transforms like</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>1</td>
<td>$x^2 + y^2 + z^2$</td>
</tr>
<tr>
<td>$A_2$</td>
<td>1</td>
<td>$(x^2 - y^2)(z^2 - x^2)(y^2 - z^2)$</td>
</tr>
<tr>
<td>$E$</td>
<td>2</td>
<td>$x^2 - y^2, 3z^2 - r^2$</td>
</tr>
<tr>
<td>$T_1$</td>
<td>3</td>
<td>$x, y, z$</td>
</tr>
<tr>
<td>$T_2$</td>
<td>3</td>
<td>$xy, yz, zx$</td>
</tr>
</tbody>
</table>

tables of cubic harmonics constructed as linear combinations of the more common spherical harmonics. We shall denote a cubic harmonic by $\Phi_\eta(\hat{k})$, where $\eta$ labels the representation. (For the group $O_h$, $\eta$ can stand for $A_{1g}, A_{2g}, E_g, T_{1g},$ or $T_{2g}$.) For example, for the representation $A_{1g}(\hat{k})$, we use the following function:

$$
\Phi_{A_{1g}}(\hat{k}) = \frac{1}{\sqrt{2}} \left( Y_{00} + 0.76376262 Y_{40}(\hat{k}) + 0.4564355 \left[ Y_{44}(\hat{k}) + Y_{4-4}(\hat{k}) \right] \right). \quad (5.7)
$$

There can be more terms in the expression for $\Phi_{A_{1g}}$, but they will all have spherical harmonics with $l$ greater than four. On physical grounds, we do not worry much about higher order contributions, since they would correspond to a wavefunction that is varying a great deal throughout the Brillouin zone and hence would represent a high energy component of the pairing state. In general, for each cubic harmonic, we have taken the lowest order contribution from the spherical harmonics that have $l > 0$. See Table 5.2 for a list of the cubic harmonics used in this calculation.

We now return to our equation for the dressed amplitude, $\Gamma(\vec{k}, \vec{k}')$ (equa-
Table 5.2:
Realizations of the cubic harmonics, $\Phi_\eta$, as linear combinations of the spherical harmonics $Y_{lm}$. For each representation, $\eta$, of cubic symmetry, the expansion was cut off after the lowest set of spherical harmonics with $l > 0$.

<table>
<thead>
<tr>
<th>$\eta$</th>
<th>$\Phi_\eta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_{1g}$</td>
<td>$\frac{1}{\sqrt{2}} (Y_{00} + 0.76376261 Y_{40} + 0.4564355 (Y_{44} + Y_{4-4}))$</td>
</tr>
<tr>
<td>$A_{2g}$</td>
<td>0.82915619 $Y_{62}^c - 0.3952847 (Y_{66} + Y_{6-6})$</td>
</tr>
<tr>
<td>$E_g$</td>
<td>$Y_{20}$</td>
</tr>
<tr>
<td>$E_g$</td>
<td>$\frac{1}{\sqrt{2}} (Y_{22} + Y_{2-2})$</td>
</tr>
<tr>
<td>$T_{1g}$</td>
<td>$(-0.93541435 i (Y_{41} - Y_{4-1}) - \frac{0.353553391 i}{\sqrt{2}} (Y_{43} - Y_{4-3}))$</td>
</tr>
<tr>
<td>$T_{1g}$</td>
<td>$(0.93541435 (Y_{41} + Y_{4-1}) - \frac{0.353553391 i}{\sqrt{2}} (Y_{43} + Y_{4-3}))$</td>
</tr>
<tr>
<td>$T_{1g}$</td>
<td>$\frac{i}{\sqrt{2}} (Y_{44} - Y_{4-4})$</td>
</tr>
<tr>
<td>$T_{2g}$</td>
<td>$\frac{i}{\sqrt{2}} (Y_{21} - Y_{2-1})$</td>
</tr>
<tr>
<td>$T_{2g}$</td>
<td>$\frac{1}{\sqrt{2}} (Y_{21} + Y_{2-1})$</td>
</tr>
<tr>
<td>$T_{2g}$</td>
<td>$\frac{i}{\sqrt{2}} (Y_{22} - Y_{2-2})$</td>
</tr>
</tbody>
</table>
tion 5.4). To project onto states of cubic symmetry, we multiply both sides of
the equation by the cubic harmonics $\Phi_\eta(\hat{k})\Phi_\eta(\hat{k}')$. The next steps follow the
ideas of Patton and Zaringhalam[13], whose work was first applied to the superfluid transition in $^3$He -- $^4$He mixtures. For temperatures below the Kondo temperature, $T_{o7}$, our version of the Anderson model behaves like a Fermi liquid. So the same basic ideas of Patton and Zaringhalam should apply in our case, as long as we assume the temperature is less than the Kondo temperature.

To solve the Bethe-Saltpeter equation, several approximations are made. We
know that the Fermi energy lies in a flat region of the lowest energy band, $E_1\hat{k}$,
where the energy is only weakly dependent on the magnitude of the momentum,
$|\hat{k}|$. Similarly, we assume that the scattering amplitudes $\Gamma(\hat{k}, \hat{k}')$ and $\Gamma(\hat{k}, \hat{k}')$,
have a stronger dependence on the angles made by $\hat{k}$ and $\hat{k}'$ than on the magni-
tudes $|\hat{k}|$ and $|\hat{k}'|$ (at least near the Fermi surface). This means the approximate
Bethe-Saltpeter equation becomes

$$\tilde{\Gamma}_\eta = \Gamma_\eta - \frac{1}{2} \int_{\mu - T_{o7}}^{\mu + T_{o7}} dE \tilde{N}(E) \frac{\tanh\left(\frac{\beta E}{2}\right)}{2E} \Gamma_\eta \tilde{\Gamma}_\eta,$$

(5.8)

where

$$\Gamma_\eta = \int \frac{d\hat{k}}{4\pi} \int \frac{d\hat{k}'}{4\pi} \Phi_\eta^*(\hat{k}) \Gamma_{QP}(\hat{k}, \hat{k}') \Phi_\eta(\hat{k}')$$

(5.9)

is the double average over a spherical surface of constant energy, and where $\mu$ is the quasiparticle chemical potential. Note that since the scattering amplitude has cubic symmetry, it is diagonal in the representation index $\eta$. The energy integral is over a shell of width $2T_{o7}$ around the Fermi surface. As we did in the solution of the mean-field equations, we assume a spherical Fermi surface.

The famous energy integral can be calculated if we assume the quasiparticle
density of states, $\tilde{N}(E)$ is constant throughout the domain of integration. Then
we find

\[ \tilde{N}(0) \int_{-T_{\sigma \tau}}^{T_{\sigma \tau}} dE \frac{\tanh(\frac{\theta E}{2})}{2E} = 2\tilde{N}(0) \ln \left| \frac{1.13T_{\sigma \tau}}{T} \right|, \]  

(5.10)

where \( \tilde{N}(0) \) is the density of states at the Fermi surface. Substituting this equation into equation 5.8 and solving for the dressed scattering amplitude gives

\[ \bar{\Gamma}_\eta = \frac{\Gamma_\eta}{1 + \tilde{N}(0)\Gamma_\eta \ln(\frac{1.13T_{\sigma \tau}}{T})}. \]  

(5.11)

A superconducting instability in the \( \eta \)-th pairing channel is signaled by the divergence of \( \bar{\Gamma}_\eta \), which in turn follows from the vanishing of the denominator on the right side. We are interested in temperatures less than \( T_{\sigma \tau} \). Thus the logarithm in the denominator will always be positive. An instability thus require \( \Gamma_\eta < 0 \), otherwise the denominator can not vanish at a finite \( T_c \). If, for a given \( \eta \), \( \Gamma_\eta \) is indeed negative, then we are assured of an instability at the transition temperature given by

\[ T_c = -1.13T_{\sigma \tau} e^{1/\tilde{N}(0)\Gamma_\eta}. \]  

(5.12)

This gives us a physical motivation to focus our attention on determining if \( \langle \Gamma \rangle < 0 \) for any of the irreducible representations of cubic symmetry. In the next section, we derive the bare scattering amplitude in the presence of cubic symmetry and crystal fields.

5.3 Derivation of the Bare Scattering Amplitude

5.3.1 Formalities

In this section, we give a detailed derivation of the quasiparticle scattering amplitude in the even-parity, spin-singlet pairing channel, which we call \( \Gamma_{QP}(\vec{k}, \vec{k}') \). Readers interested in knowing the result straightway, should see equation 5.39.
Figure 5.1 shows the diagrams we need to evaluate. Substituting in terms of
the components of the dressed (matrix) Bose propagator \((ss, s\lambda, \lambda\lambda)\) and also
for the vertices \((\gamma_{f\Gamma}, \gamma_{m_{\text{mix}}\Gamma})\), we have the following expression:

\[
\Gamma_{\sigma_1\sigma_2\sigma_3\sigma_4}(\vec{k}, \vec{k}') = \sum_{\Gamma \Gamma'} \left[ (\hat{\gamma}_{\Gamma}^{\sigma_1\sigma_4}(\vec{k}, \vec{k}'))^{Tr} \hat{D}_{\Gamma\Gamma'}(\vec{k} - \vec{k}') \hat{\gamma}_{\Gamma'}^{\sigma_2\sigma_3}(\vec{k}, \vec{k}') \right. \\
\left. - (\hat{\gamma}_{\Gamma}^{\sigma_1\sigma_4}(\vec{k}, -\vec{k}'))^{Tr} \hat{D}_{\Gamma\Gamma'}(-\vec{k} - \vec{k}') \hat{\gamma}_{\Gamma'}^{\sigma_2\sigma_3}(-\vec{k}, \vec{k}') \right],
\]  
(5.13)

where the 2x2 matrix \(\hat{D}_{\Gamma\Gamma'}\) is given by

\[
\hat{D}_{\Gamma\Gamma'}(\vec{q}) \equiv \begin{pmatrix} D_{ss\Gamma\Gamma'}(\vec{q}) & D_{s\lambda\Gamma\Gamma'}(\vec{q}) \\ D_{s\lambda\Gamma\Gamma'}(\vec{q}) & D_{\lambda\lambda\Gamma\Gamma'}(\vec{q}) \end{pmatrix},
\]  
(5.14)

and where the column vector \(\hat{\gamma}_{\Gamma}^{\sigma_1\sigma_4}(\vec{k}, \vec{k}')\) is

\[
\hat{\gamma}_{\Gamma}^{\sigma_1\sigma_4}(\vec{k}, \vec{k}') \equiv \begin{pmatrix} \gamma_{m_{\text{mix}}\Gamma}(\vec{k}, \vec{k}') \\ \gamma_{f_{\Gamma}}(\vec{k}, \vec{k}') \end{pmatrix}.
\]  
(5.15)

Note, also, that the superscript \(Tr\) on the \(\hat{\gamma}\) means the transpose of the vector
in equation 5.15 is to be taken.

In the previous chapter, we calculated the Green functions

\[
D_{ss}(\vec{q}, \tau) = \langle T_\tau \delta s_{-\vec{q}}(\tau) \delta s_{\vec{q}}(0) \rangle,
\]  
(5.16)

\[
D_{s\lambda}(\vec{q}, \tau) = \langle T_\tau \delta s_{-\vec{q}}(\tau) \delta \lambda_{\vec{q}}(0) \rangle,
\]  
(5.17)

\[
D_{\lambda\lambda}(\vec{q}, \tau) = \langle T_\tau \delta \lambda_{-\vec{q}}(\tau) \delta \lambda_{\vec{q}}(\tau) \rangle,
\]  
(5.18)

From these expressions, we can calculate the multiplet dependent Boson Green
functions. For simplicity, we do not show the explicit imaginary time (or the
frequency) dependence of the propagators.

\[
D_{ss\Gamma\Gamma'}(\vec{q}) = \langle \delta s_{-\vec{q}_{\Gamma}} \delta s_{\vec{q}_{\Gamma'}} \rangle = \frac{D_{ss}(\vec{q})}{\sqrt{N_{\Gamma}N_{\Gamma'}}},
\]  
(5.19)
\[ D_{\lambda \lambda}(\hat{q}) = \langle \delta S_{-\hat{q}} \delta \lambda \xi \rangle = \frac{D_{\lambda \lambda}(\hat{q})}{\sqrt{N_{\Gamma}}}. \]  

(5.20)

Note that \( D_{\lambda \lambda}(\hat{q}) \) has no factors of \( N_{\Gamma} \) with which we must be concerned.

The vertices \( \gamma_{\Gamma \Gamma} \) and \( \gamma_{\text{mix}} \) above can be written in terms of \( +\hat{k} \) and \( +\hat{k}' \) as opposed to \( -\hat{k} \) and \( -\hat{k}' \). To do this, we need to know if they are eigenfunctions of the parity operator. We know from equations 5.2 and 5.3 that the vertices are functions of the band energies, \( E_{n\xi} \), the normalization function, \( A_{n}(\hat{k}) \), and the product of hybridization matrix elements

\[ \tilde{V}_{\Gamma \alpha \sigma}(\hat{k}) \tilde{V}_{\sigma \Gamma \alpha}(\hat{k}'). \]

From the secular equation constructed from the mean field Hamiltonian (equation 3.60), it is easy to see that \( E_{-\xi} = E_{\xi} \), for any of the three hybridizing bands.

The normalization function has the form

\[ A_{n}(\hat{k}) = \left[ 1 + \sum_{\Gamma \alpha} \frac{\xi_{\alpha}}{\epsilon_{\Gamma} - E_{n\xi}} \right]^{-1/2}, \]  

(5.21)

which is also manifestly of even parity. Next, we look at the matrix element

\[ \tilde{V}_{\Gamma \alpha \sigma}(\hat{k}) = \sqrt{N_{\Gamma}} \sum_{m} c_{\Gamma \alpha m} V_{m \sigma}(\hat{k}), \]  

(5.22)

where \( c_{\Gamma \alpha m} \) are the coefficients relating the crystal field states \( |\Gamma \alpha \rangle \) to the \( J = 5/2 \) states \( |m \rangle \). (See equations 2.62-2.67.) The spin-orbit coupled multiplet, \( J = 5/2 \), is composed of an orbital angular momentum \( l = 3 \) and a spin \( s = 1/2 \). So all the matrix elements \( V_{m \sigma}(\hat{k}) \) depend on \( \hat{k} \) through a spherical harmonic \( Y_{3,m-\frac{2}{3}}(\hat{k}) \), which in turn is odd under parity. Thus

\[ V_{m \sigma}(\hat{k}) = -V_{m \sigma}(\hat{k}), \]

which results in the odd-parity properties for the hybridization in the presence of crystal fields,

\[ \tilde{V}_{\Gamma \alpha \sigma}(\hat{k}) = -\tilde{V}_{\Gamma \alpha \sigma}(\hat{k}), \]  

(5.23)
and also
\[ \gamma(-\vec{k}, -\vec{k'}) = \gamma(\vec{k}, \vec{k'}) \]  
(5.24)
\[ \gamma(-\vec{k}, \vec{k'}) = -\gamma(\vec{k}, \vec{k'}) = \gamma(\vec{k}, -\vec{k'}) \]  
(5.25)
where the lack of subscript in equations 5.24 and 5.25 means the result is applicable to either \( \gamma_f \) or \( \gamma_{mix} \).

As the next step on the path to deriving \( \Gamma_Q(\vec{k}, \vec{k'}) \), we use the bare amplitude \( \Gamma_{\sigma_1 \sigma_2 \sigma_3 \sigma_4}(\vec{k}, \vec{k'}) \) to construct a function of even parity in \( \vec{k'} \),

\[ \frac{1}{2} \left[ \Gamma_{\sigma_1 \sigma_2 \sigma_3 \sigma_4}(\vec{k}, \vec{k'}) + \Gamma_{\sigma_1 \sigma_2 \sigma_3 \sigma_4}(\vec{k}, -\vec{k'}) \right]. \]  
(5.26)
This new function is composed of a total of sixteen terms, the first eight of which are just equation 5.13; the second eight terms can be derived from equation 5.13 by letting \( \vec{k'} \rightarrow -\vec{k'} \). For simplicity, let us focus on all contributions to this new even parity function which come from \( ss \) components of the Bose propagator:

\[ \frac{1}{2} \sum_{\Gamma \Gamma'} \left[ \gamma_{mix}^{s\sigma_4}(\vec{k}, \vec{k'}) \gamma_{mix}^{s\sigma_2}(\vec{k}, \vec{k'}) - \gamma_{mix}^{s\sigma_4}(\vec{k}, \vec{k'}) \gamma_{mix}^{s\sigma_2}(\vec{k}, \vec{k'}) \right] \times \left[ D_{ss\Gamma \Gamma'}(\vec{k'} - \vec{k}) + D_{ss\Gamma \Gamma'}(-\vec{k'} - \vec{k}) \right], \]  
(5.27)
where the parity properties of equations 5.24 and 5.25 were used.

Now things get a little messy, but we wish to show the details for the \( D_{ss\Gamma \Gamma'} \) terms; the results for the \( D_{ss\Gamma} \) and \( D_{ss\Gamma} \) terms will then be given without derivation. We substitute for the vertices \( \gamma_{mix} \) and \( \gamma_{mix} \) from equation 5.3 into equation 5.27 to get

\[ \frac{1}{2} \sum_{\Gamma \Gamma'} \frac{A_2^2(\vec{k}) A_2^2(\vec{k'})}{(\epsilon - E_{\Gamma \vec{k}})(\epsilon' - E_{\Gamma' \vec{k'}})} \left[ \tilde{V}_{\Gamma \Gamma', \alpha'}(\vec{k'}) \tilde{V}_{\Gamma \Gamma', \alpha'}(\vec{k'}) \tilde{V}_{\Gamma \Gamma', \alpha'}(\vec{k'}) \tilde{V}_{\Gamma \Gamma', \alpha'}(\vec{k'}) \right] \times \left[ D_{ss\Gamma \Gamma'}(\vec{k'} - \vec{k}) + D_{ss\Gamma \Gamma'}(-\vec{k'} - \vec{k}) \right]. \]  
(5.28)
As discussed previously, we have focused on pseudospin-singlet pairing because we believe experimental evidence for CeCu$_2$Si$_2$ points in that direction. Generally speaking, triplet pairing should be investigated as well. It may be that the strongest average pairing interactions are actually in the triplet channel. One can not know for sure until both triplet and singlet pairing channels are studied. For this thesis, however, we have focused on the case of singlet pairing.

To describe (pseudo)spin-singlet pairing, we set $\sigma_2 = -\sigma_1$ and $\sigma_3 = -\sigma_4$. With this substitution, the first product of four hybridization matrix elements in equation 5.28 becomes

$$\sum_{\alpha\alpha'} \hat{V}_{\Gamma'\alpha\sigma_4}(\vec{k}') \hat{V}_{\sigma_1\Gamma\alpha}(-\vec{k}) \hat{V}_{\Gamma'\alpha'\sigma_4}(-\vec{k}') \hat{V}_{-\sigma_1\Gamma\alpha'}(\vec{k}).$$

(5.29)

Next, we use the following property of the matrix elements in spherical symmetry:

$$V_{m-\sigma}(\vec{k}) = (-1)^{m+\frac{\sigma}{2}} V_{-m\sigma}^*(\vec{k}),$$

(5.30)

which follows from the expression

$$V_{m\sigma}(\vec{k}) = -V_{0k} \sqrt{\frac{4\pi}{3}} (-i)^{2\sigma} \sqrt{\frac{7-2m\sigma}{14}} Y_{3,m-\frac{\sigma}{2}}^*(\vec{k}),$$

where $V_{0k}$ denotes the dependence on the radial component of the momentum.

For our matrix elements in the presence of crystal fields, equation 5.30 becomes

$$\hat{V}_{-\sigma\Gamma\alpha}(\vec{k}) = \sqrt{N_{\Gamma}} \sum_m (-1)^{m+\frac{\sigma}{2}} c_{\Gamma\alpha m} V_{-m\sigma}^*(\vec{k}).$$

(5.31)

This means we must rewrite equation 5.29 as

$$N_{\Gamma} N_{\Gamma'} \sum_{m_1 m_2 m_3 m_4 \alpha \alpha'} c_{\Gamma_1 m_1} c_{\Gamma_2 m_2} c_{\Gamma'\alpha' m_3} c_{\Gamma'\alpha' m_4} (-1)^{m_1 + m_2 + \frac{\alpha_1}{2} + \frac{\alpha_2}{2}}$$

$$\times V_{m_1 \sigma_4}^*(\vec{k}') \hat{V}_{\sigma_1 m_2}(\vec{k}) \hat{V}_{-m_4 \sigma_1}(\vec{k}) V_{\sigma_4 - m_3}(\vec{k}').$$
We shall skip a few steps in the formal derivation here, since it is just algebra. It turns out that equation 5.29 can be written as

\[ N_{\Gamma} N_{\Gamma'} \sum_{m_1 m_2 m_3 m_4 \alpha \alpha'} c_{\Gamma \alpha m_1} c_{\Gamma' \alpha' m_3} c_{\Gamma' \alpha' m_4} (-1)^{-m_3 - m_4 - (\sigma_1 + \sigma_4)/2} \times V_{m_1 \sigma_4}^*(\vec{k}') V_{\sigma_1 m_2}^*(\vec{k}) V_{m_4 \sigma_1}^*(\vec{k}) V_{\sigma_4 m_3}^*(\vec{k}'). \]

We can push this expression even further. Consider the product \( c_{\Gamma' \alpha' m_3} c_{\Gamma' \alpha' m_4} \).

It is useful to ask about the possible choices for \( m_3 \) and \( m_4 \) for particular crystal field quantum numbers \( \Gamma', \alpha' \). Happily, for \textit{any} of the six possible choices of \( \Gamma', \alpha' \), the equality

\[ (-1)^{-m_3 - m_4} = -1 \]

is always true. So now we have

\[ N_{\Gamma} N_{\Gamma'} (-1)^{-(\sigma + \sigma')/2} \sum_{m_1 m_2 m_3 m_4 \alpha \alpha'} c_{\Gamma \alpha m_1} c_{\Gamma \alpha m_2} c_{\Gamma' \alpha' m_3} c_{\Gamma' \alpha' m_4} \times V_{m_1 \sigma_4}^*(\vec{k}') V_{\sigma_1 m_2}^*(\vec{k}) V_{m_4 \sigma_1}^*(\vec{k}) V_{\sigma_4 m_3}^*(\vec{k}), \]

where we have made the substitution \( \sigma' = \sigma_4 \) and \( \sigma = \sigma_1 \). Summing over the \( m_i \) (\( i=1,2,3,4 \)) gives

\[ (-1)^{(\sigma + \sigma')/2} \sum_{\alpha \alpha'} \tilde{V}_{\Gamma \alpha \sigma_4}*(\vec{k}') \tilde{V}_{\alpha' \Gamma' \sigma_1}*(\vec{k}') \tilde{V}_{\Gamma' \alpha' \sigma_1}*(\vec{k}) \tilde{V}_{\alpha \Gamma \sigma}(\vec{k}). \quad (5.32) \]

Without showing the proof here, we state that the second product of four hybridization matrix elements in equation 5.28 can be manipulated to give a result identical to that of equation 5.32 with one difference: \( \sigma' \rightarrow -\sigma' \). Such a difference in signs was foreseeable. The only difference between the two sets of matrix elements in equation 5.28 is an interchange of the spin variables \( \sigma_3 \) and \( \sigma_4 \). From the facts that we set \( \sigma_3 = -\sigma_4 \) and \( \sigma_4 = \sigma' \), the source of the \( -\sigma' \) above is clear.
By time reversal symmetry, it can’t matter whether we have $\sigma'$ or $-\sigma'$. That means we can combine all the matrix elements together into one big term and pick up a prefactor of 2 along the way. Then equation 5.28 finally becomes

$$(-1)^{(\sigma+\sigma')/2} \sum_{\Gamma_\alpha'\Gamma_\alpha} \frac{A_{\sigma'}^2(\vec{k})A_{\sigma}^2(\vec{k}')\tilde{s}_{\sigma'}\tilde{s}_{\sigma}}{(\epsilon_{\Gamma'} - E_{1k})(\epsilon_{\Gamma'} - E_{1k'})} \tilde{V}_{\Gamma_\alpha'\sigma'}(\vec{k})\tilde{V}_{\Gamma_\alpha\sigma}(\vec{k}')\tilde{V}_{\Gamma_\alpha'\sigma'}(\vec{k}')\tilde{V}_{\Gamma_\alpha\sigma}(\vec{k})$$

$$\times \left[ D_{\sigma\Gamma'}(\vec{k} - \vec{k}) + D_{\sigma\Gamma'}(-\vec{k'} - \vec{k}) \right]. \tag{5.33}$$

This is the contribution from the $D_{\sigma\Gamma'}$ components of the Bose propagator.

From the off-diagonal $(s\lambda)$ components of the propagator, we have the result:

$$i(-1)^{(\sigma+\sigma')/2} \sum_{\Gamma_\alpha'\Gamma_\alpha} \frac{A_{\sigma'}^2(\vec{k})A_{\sigma}^2(\vec{k}')\tilde{s}_{\sigma'}\tilde{s}_{\sigma}}{(\epsilon_{\Gamma'} - E_{1k})(\epsilon_{\Gamma'} - E_{1k'})} \tilde{V}_{\Gamma_\alpha'\sigma'}(\vec{k})\tilde{V}_{\Gamma_\alpha\sigma}(\vec{k}')\tilde{V}_{\Gamma_\alpha'\sigma'}(\vec{k}')\tilde{V}_{\Gamma_\alpha\sigma}(\vec{k})$$

$$\times \left[ \frac{\tilde{s}_{\sigma}}{\epsilon_{\Gamma'} - E_{1k'}} \left( D_{s\lambda\Gamma'}(\vec{k} - \vec{k}) + D_{s\lambda\Gamma'}(-\vec{k'} - \vec{k}) \right) ight.$$ \n
$$+ \frac{\tilde{s}_{\sigma}}{\epsilon_{\Gamma'} - E_{1k'}} \left( D_{s\lambda\Gamma}(\vec{k} - \vec{k}) + D_{s\lambda\Gamma}(-\vec{k'} - \vec{k}) \right) \right]; \tag{5.34}$$

and from the $\lambda\lambda$ component comes:

$$(-1)^{(\sigma+\sigma')/2} \sum_{\Gamma_\alpha'\Gamma_\alpha} \frac{A_{\sigma'}^2(\vec{k})A_{\sigma}^2(\vec{k}')\tilde{s}_{\sigma'}\tilde{s}_{\sigma}}{(\epsilon_{\Gamma'} - E_{1k})(\epsilon_{\Gamma'} - E_{1k'})} \tilde{V}_{\Gamma_\alpha'\sigma'}(\vec{k})\tilde{V}_{\Gamma_\alpha\sigma}(\vec{k}')\tilde{V}_{\Gamma_\alpha'\sigma'}(\vec{k}')\tilde{V}_{\Gamma_\alpha\sigma}(\vec{k})$$

$$\times \left[ D_{\lambda\lambda}(\vec{k} - \vec{k}) + D_{\lambda\lambda}(-\vec{k'} - \vec{k}) \right]. \tag{5.35}$$

We now combine equations 5.33- 5.35 as follows:

$$\Gamma_{\text{even},\sigma-\sigma'-\sigma'}(\vec{k}, \vec{k}') = (-1)(-1)^{(\sigma+\sigma')/2} \Gamma_{\text{even}}(\vec{k}, \vec{k}'), \tag{5.36}$$

where

$$\Gamma_{\text{even}}(\vec{k}, \vec{k}') \equiv \sum_{\Gamma_\alpha'\Gamma_\alpha} \frac{A_{\sigma'}^2(\vec{k})A_{\sigma}^2(\vec{k}')\tilde{s}_{\sigma'}\tilde{s}_{\sigma}}{(\epsilon_{\Gamma'} - E_{1k})(\epsilon_{\Gamma'} - E_{1k'})} \tilde{V}_{\Gamma_\alpha'\sigma'}(\vec{k})\tilde{V}_{\Gamma_\alpha\sigma}(\vec{k}')\tilde{V}_{\Gamma_\alpha'\sigma'}(\vec{k}')\tilde{V}_{\Gamma_\alpha\sigma}(\vec{k})$$

$$\times \left[ D_{s\sigma\Gamma'}(\vec{k} - \vec{k}) + D_{s\sigma\Gamma'}(-\vec{k'} - \vec{k}) - i\frac{\tilde{s}_{\sigma}}{\epsilon_{\Gamma'} - E_{1k'}} \left( D_{s\lambda\Gamma'}(\vec{k} - \vec{k}) + D_{s\lambda\Gamma'}(-\vec{k'} - \vec{k}) \right) \right].$$
\[-i \frac{\tilde{s}_\omega \Gamma'}{\epsilon_{\Gamma'} - E_{1k'}} \left( D_{\ast \lambda \Gamma'}(\vec{k}' - \vec{k}) + D_{\ast \lambda \Gamma'}(-\vec{k}' - \vec{k}) \right) \]
\[-\frac{\tilde{s}_\omega \Gamma' \tilde{\tilde{s}}_{\omega \Gamma'}}{(\epsilon_{\Gamma'} - E_{1k'})(\epsilon_{\Gamma'} - E_{1k'})} \left( D_{\lambda \lambda}(\vec{k}' - \vec{k}) + D_{\lambda \lambda}(-\vec{k}' - \vec{k}) \right) \right]. \quad (5.37)

The final step in the derivation is to construct a spin-singlet function. This is done by taking linear combinations of the even-parity function \( \Gamma_{\text{even},\sigma' - \sigma' \sigma} \) defined above,

\[ \Gamma_{QP} = \frac{1}{4} \left[ \Gamma_{\text{even},++-} - \Gamma_{\text{even},-+-} - \Gamma_{\text{even},+--} + \Gamma_{\text{even},---} \right], \quad (5.38) \]

where for convenience we have not explicitly shown the momentum dependences.

Note that we have shown the spin indices as "+" or "-"; the choice of signs in the linear combination ensures that we pick up a minus sign upon the interchange of two spins. Note that for the four possible values of \( \sigma \) and \( \sigma' \), the factor \((-1)^{(\sigma + \sigma')}\) in equation 5.36 has just the right behavior to give the correct signs in equation 5.38. This means we can write

\[ \Gamma_{QP}(\vec{k}, \vec{k}') = \frac{1}{4} \sum_{\sigma \sigma'} \Gamma_{\text{even}}(\vec{k}, \vec{k}') \]

\[ = \frac{1}{4} \sum_{\Gamma' \alpha' \sigma' \sigma} \frac{A_1^2(\vec{k}) A_2^2(\vec{k}') \tilde{s}_{\omega \Gamma'} \tilde{\tilde{s}}_{\omega \Gamma'} \tilde{\tilde{V}}_{\Gamma' \alpha' \sigma'}(\vec{k}') \tilde{\tilde{V}}_{\Gamma' \alpha' \sigma'}(\vec{k}) \tilde{\tilde{V}}_{\Gamma \alpha \sigma}(\vec{k}) \tilde{\tilde{V}}_{\Gamma \alpha \sigma}(\vec{k})}{(\epsilon_{\Gamma'} - E_{1k'})(\epsilon_{\Gamma'} - E_{1k'})} \]
\[ \times \left[ D_{\ast \lambda \Gamma'}(\vec{k}' - \vec{k}) + D_{\ast \lambda \Gamma'}(-\vec{k}' - \vec{k}) - i \frac{\tilde{s}_{\omega \Gamma'}}{\epsilon_{\Gamma'} - E_{1k'}} \left( D_{\ast \lambda \Gamma'}(\vec{k}' - \vec{k}) + D_{\ast \lambda \Gamma'}(-\vec{k}' - \vec{k}) \right) \right] \]
\[ \left. - i \frac{\tilde{s}_{\omega \Gamma'} \tilde{\tilde{s}}_{\omega \Gamma'}}{(\epsilon_{\Gamma'} - E_{1k'})(\epsilon_{\Gamma'} - E_{1k'})} \left( D_{\lambda \lambda}(\vec{k}' - \vec{k}) + D_{\lambda \lambda}(-\vec{k}' - \vec{k}) \right) \right], \quad (5.39) \]

where the symbols mean the following:

- \( \tilde{\tilde{V}}_{\Gamma \alpha \sigma}(\vec{k}) = \sqrt{N_{\Gamma}} V_{\sigma \Gamma} \) is the hybridization matrix element between a plane wave conduction state of momentum \( \vec{k} \) and spin \( \sigma \) and a crystal field state in the \( \Gamma \)
multiplet; $\alpha$ labels the degenerate crystal field states within the $\Gamma$ multiplet. $N_{\Gamma}$ labels the degeneracy of the $\Gamma$ multiplet.

- $\tilde{s}_{\alpha \Gamma} = s_{\alpha} / \sqrt{N_{\Gamma}}$ is the mean field hybridization renormalization coefficient. At mean field, the bare hybridization is renormalized (due to the constraint of only allowing hopping onto an empty $4f$ site) to the value $\tilde{s}_{\alpha \Gamma} \tilde{V}_{\sigma \Gamma \alpha}$.
- $\epsilon_{\Gamma}$ is the self-consistent mean field energy of the $\Gamma$ multiplet.
- $E_{1\vec{k}}$ is the quasiparticle energy for the lowest, or first, band as a function of momentum.

- $A_{\Gamma}^2(\vec{k})$ is the quasiparticle normalization function defined by

$$A_{\Gamma}^2(\vec{k}) \equiv \left[ 1 + \sum_{\Gamma' \alpha} \frac{\tilde{s}_{\alpha \Gamma}^2 |\tilde{V}_{\Gamma' \alpha \sigma}(\vec{k})|^2}{(\epsilon_{\Gamma' \alpha} - E_{1\vec{k}})^2} \right]^{-1}$$

and which is very strongly peaked at the six points where the Brillouin zone axes intersect the spherical Fermi surface.

- The components of the Bosonic Green function are:

$$D_{s\sigma \Gamma' \tau}(\vec{q}) \equiv \langle \delta \tilde{s}_{-\vec{q} \sigma} \delta \tilde{s}_{\vec{q} \Gamma'} \rangle;$$

$$D_{s\lambda \Gamma}(\vec{q}) \equiv \langle \delta \tilde{s}_{-\vec{q} \sigma} \delta \lambda_{\vec{q}} \rangle;$$

$$D_{\lambda\lambda}(\vec{q}) \equiv \langle \delta \lambda_{-\vec{q}} \delta \lambda_{\vec{q}} \rangle.$$

Note that we are not concerned with the time dependence of these Green functions. Also, the variables $\delta \tilde{s}$ and $\delta \lambda$ signify fluctuations of these fields away from their self-consistent mean field values.

As seen in equation 5.8 we are limiting ourselves to a Fermi surface average of the scattering amplitude, that is, a weak-coupling calculation. It became clear to us that including the frequency dependence of the boson Green function was impossible, given the difficult numerical integrals encountered in the static
limit. Within this approximation, the band energies $E_{1\mathbf{k}}$ and $E_{1\mathbf{k}'}$ are set equal to the quasiparticle chemical potential, $\mu$. Thus a term like $\epsilon_{\Gamma} - E_{1\mathbf{k}}$, where $\epsilon_{\Gamma}$ is the mean field shifted energy of the $\Gamma$ multiplet. When evaluated at the Fermi surface, this energy difference becomes

$$\epsilon_{\Gamma} - \mu = T_{0\Gamma},$$

(5.40)

which we have defined to be the Kondo temperature of the $\Gamma$ multiplet. Our physical motivation for such a definition is that in spherical symmetry this energy is equal to the expression for the impurity Kondo temperature[27], namely,

$$\epsilon - \mu = e^{-|E_{f}|/(N N(0)^{1/2})},$$

(5.41)

which is valid for any integral value of the multiplet degeneracy, $N$; $|E_{f}|$ is the unshifted $4f$ multiplet energy, which is about $2.0 \text{ eV}$ below the Fermi surface. For the case of CeCu$_{2}$Si$_{2}$, the Kondo temperature of the $\Gamma_7$ doublet is approximately 10 K (The bare mean field parameters were chosen to give a Kondo temperature of approximately 10 K.), while for the $\Gamma_8$ quartet,

$$T_{08} = T_{07} + \Delta_{CEF} = 370K$$

(5.42)

is dominated by the crystal field splitting. This explains how to treat all the energy denominators in equation 5.39.

There is one last, helpful manipulation to make. Substituting for the elements of the Bosonic Green function, $\hat{D}$, from equations 4.5-4.10, we write the expression for the scattering amplitude in terms of a defined function, $F(\vec{q})$, that carries all the momentum dependence of the dressed, Bosonic propagator. This is done so that we can easily extract the local contribution—that due to
the quasiparticle exchange of momentum independent slave Bosons to \( \Gamma_{QP} \). We find the following result:

\[
\Gamma_{QP}(\vec{k}, \vec{k}') = \frac{1}{4} \sum_{\alpha \alpha'} \frac{A_\alpha^2(\vec{k}) A_{\alpha'}^2(\vec{k}') \tilde{s}_{\alpha \Gamma} \tilde{s}_{\alpha' \Gamma'} \tilde{V}_{\alpha \alpha' \gamma}(\vec{k}) \tilde{V}_{\alpha' \gamma \alpha}(\vec{k}') \tilde{V}_{\gamma \alpha \alpha'}(\vec{k}) \tilde{V}_{\gamma \alpha' \alpha}(\vec{k})}{T_{\alpha \Gamma} T_{\alpha' \Gamma'}} \\
\times \left[ \frac{\tilde{s}_{\alpha \Gamma}}{\sqrt{N_{\gamma} T_{\alpha \Gamma} \Gamma_{\alpha \gamma}}} + \frac{\tilde{s}_{\alpha' \Gamma'}}{\sqrt{N_{\gamma'} T_{\alpha' \Gamma'} \Gamma_{\alpha' \gamma'}}} - \frac{\Gamma_{\alpha \alpha'}}{\sqrt{N_{\gamma} N_{\gamma'} T_{\alpha \Gamma} T_{\alpha' \Gamma'}}} \right] \left[ \frac{1}{1 + F(\vec{k}' - \vec{k})} + \frac{1}{1 + F(\vec{k} - \vec{k})} \right],
\]

where

\[
\Gamma_{\alpha \gamma} \equiv \sum_{\Gamma} \left( \frac{1}{2} N_{\gamma} \tilde{s}_{\alpha \Gamma} + \frac{x_{\gamma}}{\tilde{s}_{\alpha \Gamma}} \right),
\]

\[
\Gamma_{\alpha \alpha'} \equiv \sum_{\Gamma} \frac{y_{\gamma}}{T_{\gamma \Gamma}},
\]

\[
F(\vec{q}) = \frac{1 + A(\vec{q})}{1 - B(\vec{q})} - 1.
\]

\( \Gamma_{\alpha \gamma} \) and \( \Gamma_{\alpha \alpha'} \) represent the momentum independent terms in the bosonic vertex function, \( \hat{\Gamma} \), which is (in turn) the negative inverse of the bosonic Green function. The expressions \( x_{\gamma}/\tilde{s}_{\alpha \Gamma} \) and \( y_{\gamma}/T_{\gamma \Gamma} \) come from evaluating the contributions to the bosonic vertex function (or self-energy) which are dependent on the square of the hybridization matrix element, \( \tilde{V}_{\gamma \alpha}^2 \). We evaluated these expressions in Chapter 4 (equation 4.43 gives the \( x_{\gamma}/\tilde{s}_{\alpha \Gamma} \) term and equation 4.53 gives the \( y_{\gamma}/T_{\gamma \Gamma} \) term) and found numerical values for \( x_{\gamma} \) and \( y_{\gamma} \) for both mean field parameter sets (a) and (b). Table 5.3 reviews the meaning and value of the mean field parameters themselves, and Table 5.4 lists the numbers \( x_{\gamma} \) and \( y_{\gamma} \) for both mean field parameter sets. The functions \( A \) and \( B \) appearing in the definition of the momentum dependent function \( F(\vec{q}) \) are given by:

\[
A \equiv \frac{I_{\alpha \alpha}}{\Gamma_{\alpha \alpha}} \left( 1 + \frac{I_{\alpha \alpha}}{\Gamma_{\alpha \alpha}} \right) - \frac{2I_{\gamma \gamma}}{\Gamma_{\gamma \gamma}^2} \left( \Gamma_{\alpha \alpha} + \frac{I_{\alpha \alpha}^2}{2} \right),
\]

\[
B \equiv \frac{I_{\alpha \alpha}}{2\sqrt{N_{\gamma} N_{\gamma'} \Gamma_{\alpha \alpha}^2}} + \frac{I_{\alpha \alpha}}{\Gamma_{\alpha \alpha}^2} \left( \frac{\tilde{s}_{\alpha \Gamma}}{T_{\gamma \Gamma} \sqrt{N_{\gamma}}} + \frac{\tilde{s}_{\alpha' \Gamma'}}{T_{\gamma' \Gamma} \sqrt{N_{\gamma'}}} \right) + \frac{2\tilde{s}_{\alpha \Gamma} \tilde{s}_{\alpha' \Gamma'} I_{\gamma \gamma}}{T_{\gamma \Gamma} T_{\gamma' \Gamma} \Gamma_{\alpha \alpha}^2},
\]
where

\[ I_{ss}(\vec{q}) = \sum_{\Gamma \Gamma'} \frac{I_{ss\Gamma\Gamma'}(\vec{q})}{\sqrt{N_\Gamma N_{\Gamma'}}}, \]

\[ I_{s\lambda}(\vec{q}) = \sum_{\Gamma \Gamma'} \frac{I_{s\lambda\Gamma\Gamma'}(\vec{q})}{\sqrt{N_\Gamma}}, \]

\[ I_{\lambda\lambda}(\vec{q}) = \sum_{\Gamma \Gamma'} I_{\lambda\lambda\Gamma\Gamma'}(\vec{q}). \]

For convenience, the momentum dependence of the \( I_{ss}(\vec{q}) \), \( I_{s\lambda}(\vec{q}) \), and \( I_{\lambda\lambda}(\vec{q}) \) has not been explicitly shown in the definitions of \( A \) and \( B \). The functions \( I_{ss}(\vec{q}) \), \( I_{s\lambda}(\vec{q}) \), and \( I_{\lambda\lambda}(\vec{q}) \) originate from the terms of order of the fourth power of the hybridization matrix element, and in the limit where these functions are set to zero, \( F(\vec{q}) \) also goes to zero. As a result, equation 5.43 reduces to

\[ \Gamma_{local}(\vec{k}, \vec{k}') = \frac{1}{4} \sum_{\Gamma_0 \Gamma' \alpha' \sigma} \frac{A_1^2(\vec{k}) A_1^2(\vec{k}') \delta_{\sigma \Gamma} \delta_{\sigma' \Gamma'} \hat{V}_{\sigma' \alpha}(\vec{k}') \hat{V}_{\sigma' \alpha'}(\vec{k}) \hat{V}_{\sigma \alpha}(\vec{k})}{(E_{1k} - E_{1k})(E_{1\Gamma} - E_{1\Gamma'})} \]

\[ \times 2 \left[ \frac{\delta_{\sigma \Gamma}}{\sqrt{N_{\Gamma} T_{\Gamma} T_{\Gamma'}}} + \frac{\delta_{\sigma \Gamma'}}{\sqrt{N_{\Gamma} T_{\Gamma} T_{\Gamma'}}} - \frac{\Gamma_{\alpha \lambda}}{\sqrt{N_{\Gamma} N_{\Gamma'} \Gamma_{\alpha \lambda}}}. \right] \] (5.47)

The combination of normalization functions, \( A_1^2(\vec{k}) A_1^2(\vec{k}') \), and the product of four hybridization matrix elements is due to the anisotropic vertices \( \gamma_{mix}(\vec{k}, \vec{k}') \) and \( \gamma_{\Gamma}(\vec{k}, \vec{k}') \). The contribution from the Bose Green function is that which remains inside the square brackets in equation 5.47. We see that in this limit, the quasiparticles interact by exchanging a momentum-independent Boson. In real space, this translates into a local interaction. Note, as mentioned at the beginning of this chapter, we do not call this a hard-core interaction. Strictly speaking, "local" here means within a unit cell. That is, the quasiparticles find themselves within the same volume (of order \( a^3 \)), but because of the complicated spatial dependence of the quasiparticle wavefunctions near the 4f sites, their interactions can be anisotropic in k-space.
The local scattering amplitude of equation 5.47 is much simpler to deal with than the full expression of equation 5.43 (or equation 5.39). The local amplitude can also be helpful in guiding us through the complicated physics of quasiparticle interactions. Roughly, the function $F(q)$, which represents non-local interactions, can be thought of as renormalizing the local interactions. It is not a priori clear how strong the non-local interactions are in comparison to the local ones, but it seems reasonable to calculate $\Gamma_{\text{local}}$ first and then include the non-local physics through the function $F(q)$. This is how we shall proceed.

5.3.2 Simplifications in the Presence of Spherical Symmetry.

Before discussing our results, we want to study our expression for the scattering amplitude in the limit of spherical symmetry. We start from equation 5.39 and make the following changes:

- The scaled fields, $\tilde{s}_\sigma \Gamma$ become $\tilde{s}_\sigma = s_\sigma / \sqrt{N}$, where $N$ is the full degeneracy of the $J=5/2$ multiplet.
- The Kondo temperature $T_\sigma \Gamma$ becomes $T_\sigma$, the Kondo temperature of the full $J=5/2$ multiplet.
- The hybridization matrix elements, $V_{\Gamma \sigma}(k)$ become $V_{m\sigma}(\vec{k})$, where $m$ is the $z$-component of the total angular momentum, $J_z (-\frac{5}{2} \leq m \leq \frac{5}{2})$. We follow Zhang and Lee[1] and separate the angular dependence of the matrix element from the radial dependence by writing

$$V_{m\sigma}(\vec{k}) = V_{\eta k} \beta_{m\sigma} (\hat{k}),$$

where the angular dependence is in the function

$$\beta_{m\sigma}(\hat{k}) \equiv -\sqrt{\frac{4\pi}{3}} (-i)^3 \sigma \sqrt{\frac{7 - 2m\sigma}{14}} Y_{3,m-\frac{5}{2}}(\hat{k}). \quad (5.48)$$
\( V_{0k} \) contains the dependence of the hybridization upon the magnitude of the momentum. Since all matrix elements are to be evaluated on the Fermi surface, the momentum dependence of \( V_{0k} \) may be ignored. That is, \( V_{0k} \) depends on \(|k|\) only near the zone center (\(|k| \rightarrow 0\)). Thus, we write \( V_{0k} \rightarrow V_0 \), where \( V_0 \) is the bare hybridization strength.

The crystal field dependent Bosonic Green functions are replaced with the appropriate expressions for spherical symmetry: \( D_{ss}^{(\text{sphere,local})} \), \( D_{s\lambda}^{(\text{sphere,local})} \); and \( D_{\lambda\lambda}^{(\text{sphere,local})} \). For simplicity, we look at only the momentum independent contribution, which amounts to taking the local limit. Using the results of Zhang and Lee [1], we take

\[
\begin{align*}
D_{ss}^{(\text{sphere,local})} &= -\frac{s_0^2}{T_o}, \\
D_{s\lambda}^{(\text{sphere,local})} &= i\tilde{s}_o, \\
D_{\lambda\lambda}^{(\text{sphere,local})} &= 0.
\end{align*}
\]

The normalization function, \( A_1^2(\vec{k}) \), becomes spherically symmetric

\[
\left(A_1^{(\text{sphere})(k_F)}\right)^2 = \frac{1}{1 + \frac{s_0^2 V_0^2}{T_o^2}} \approx \frac{T_o^2}{s_0^2 V_0^2} \ll 1,
\]

where \( k_F \) is the magnitude of the Fermi wavevector.

Making all the substitutions for these quantities into equation 5.39 will give us a local limit of the scattering amplitude in spherical symmetry. Note that the product of the normalization functions will give a contribution \((T_0/s_0 V_0)^4\). The combination of Bose Green functions inside the square brackets becomes

\[
2\left[ D_{ss}^{(\text{sphere,local})} - 2i \frac{s_0^2}{T_o} D_{s\lambda}^{(\text{sphere,local})} - \frac{s_0^2}{T_o^2} D_{\lambda\lambda}^{(\text{sphere,local})} \right],
\]

when all quasiparticle energies are evaluated at the Fermi surface. Substituting for the Bose Green functions in spherical symmetry reduces equation 5.49 to the
simple expression $2(z_o^2/T_o)$. Finally, equation 5.39 becomes

$$\Gamma_{(\text{sphere, local})} = \frac{1}{4} \sum_{mm'\sigma\sigma'} V_o^4 z_o^2 \beta_{m\sigma}(\hat{k})\beta_{m'\sigma'}(\hat{k}')\beta_{m'\sigma'}(\hat{k}') \beta_{m\sigma}(\hat{k}') \left( \frac{T_o}{s_o V_o} \right)^2 T_o^2 \{2z_o^2 \right. \}

(5.50)

For ease of writing, we define a function which contains all the angular dependence due to the hybridization matrix elements,

$$B(\mathbf{k} \cdot \mathbf{k}') = \sum_{mm'\sigma\sigma'} \beta_{m\sigma}^*(\mathbf{k})\beta_{m'\sigma}^*(\mathbf{k})\beta_{m'\sigma'}(\mathbf{k}')\beta_{m\sigma}(\mathbf{k}'). \quad (5.51)$$

Then equation 5.50 reduces to

$$\Gamma_{(\text{sphere, local})} = \frac{1}{2} B(\mathbf{k} \cdot \mathbf{k}') T_o. \quad (5.52)$$

This result agrees exactly with the result of Zhang and Lee[1] in the local limit and thereby gives us a reasonable check of our expression for the scattering amplitude. The full scattering amplitude, including the momentum dependence of the Boson Green functions, is

$$\Gamma_{(\text{sphere})}(\mathbf{k}, \mathbf{k}') = \frac{1}{2} B(\mathbf{k} \cdot \mathbf{k}') \left[ \frac{1}{1 + F_{\text{sphere}}(\mathbf{k} \cdot \mathbf{k}')} + \frac{1}{1 + F_{\text{sphere}}(\mathbf{k} + \mathbf{k}')} \right], \quad (5.53)$$

where the function $F_{\text{sphere}}(\mathbf{q})$ is the analog of equation 5.46 for spherical symmetry.

The sums in equation 5.51 can be done exactly (see Appendix C) to give

$$B(\mathbf{k} \cdot \mathbf{k}') = \frac{2}{3} P_0(\mathbf{k} \cdot \mathbf{k}') + \frac{16}{21} P_2(\mathbf{k} \cdot \mathbf{k}') + \frac{2}{7} P_4(\mathbf{k} \cdot \mathbf{k}'). \quad (5.54)$$

Physically, equation 5.54 says that the local interactions for s-wave ($l = 0$), d-wave ($l = 2$), and g-wave ($l = 4$) pairings are all repulsive (and approximately the same size). This tells us that the only way a superconducting instability can appear in this model is if the non-local interactions due to $F_{\text{sphere}}$ are attractive.
and strong enough to overcome the local repulsion so that, when averaged over the Fermi surface, the scattering amplitude is negative. Zhang and Lee claim that in spherical symmetry the non-local interactions are not strong enough to overcome the local repulsion. They see no evidence of a pairing instability.

We also mention here the work of Lavagna, Millis, and P. A. Lee[14]. Their calculation can be thought of as the limit of Zhang and Lee's work in which the hybridization matrix element is entirely isotropic in k-space (i.e. $V_{m\sigma}(\vec{k}) \rightarrow V$). They also assumed that, if $N$ is the degeneracy of states on the 4f sites, the conduction states are also N-fold degenerate. This is just the SU(N) model discussed briefly in chapter 2. Lavagna, Millis, and P. A. Lee found that the local repulsive interactions exist only in the s-wave pairing channel. There are no local interactions in pairing states of higher angular momentum. With no repulsion to overcome, the inclusion of non-local physics leads to a d-wave instability. They found that

$$\Gamma_{d\text{-wave}} \approx \frac{-0.01T_o}{N},$$

(5.55)

which, although very weak, is nevertheless a signal of an instability toward d-wave pairing. We note here in passing, that such a small value for the scattering amplitude would be (numerically) very difficult to verify. Said another way, if one is calculating $\Gamma/T_o$ numerically, one must be certain all numerical integrals have properly converged, such that fluctuations in the Fermi surface averaged amplitude (as a function of mesh size) are considerably smaller than 0.01/N; this is a tall order to fill.

The principal shortcoming of Lavagna, Millis, and Lee's work, insofar as its application to heavy Fermion superconductors, is the simplifying assumption of an isotropic hybridization matrix element, V. Although their result is interesting,
the calculation of Zhang and T. K. Lee, with an anisotropic matrix element, seems more realistic for heavy Fermion systems. Thus, the null result of Zhang and Lee's work seems to be bad news for those searching for an electronic pairing mechanism from a microscopic model (such as the Anderson Hamiltonian). We wish to emphasize, however, that the driving motivation of this thesis project, has been to push Zhang and Lee's calculation one step further by including the crystal field splitting of the \( J = 5/2 \) multiplet. We now return to our expression for the scattering amplitude and see what interesting physics we can extract from it.

5.3.3 A few more Ideas Before the Results

The first question we shall pose is this: how do the local interactions in cubic symmetry qualitatively compare to those in the case of spherical symmetry? This leads us back to equation 5.47. To get a preliminary feeling for what to expect, let us simplify the expression in order to study the relative size of the contributions to the scattering amplitude from the \( \Gamma_7 \) and \( \Gamma_8 \) multiplets.

- To do this, we approximate the quasiparticle normalization as follows:

\[
A_i^2 \approx \left( \frac{T_{07}}{s_0 V_0} \right)^4.
\] (5.56)

- Furthermore, from equations 5.44 and 5.45, and from the values of the parameters \( x_\Gamma \) and \( y_\Gamma \) in Table 5.4, we see that, to a very good approximation, the momentum independent vertices \( \Gamma_{o\lambda\lambda} \) and \( \Gamma_{o\lambda\lambda} \) can be written as

\[
\Gamma_{o\lambda\lambda} = \frac{2}{s_0 t},
\]

\[
\Gamma_{o\lambda\lambda} = \frac{1}{T_{07}},
\]
where \( \hat{s}_{o\gamma} = s_o / \sqrt{2} \), and where the values for \( s_o \) are in Table 5.3.

In analogy with the spherically symmetric limit, we break the hybridization matrix element into radial and angular pieces via the expression

\[
\tilde{V}_{\Gamma\alpha\sigma}(\hat{k}) = \tilde{V}_{ok\Gamma} \beta_{\Gamma\alpha\sigma}(\hat{k}),
\]

(5.57)

where \( \tilde{V}_{ok\Gamma} = \sqrt{N_{\Gamma}} V_{ok} \) is the factor dependent on the magnitude of the momentum, and where

\[
\beta_{\Gamma\alpha\sigma}(\hat{k}) = \sum_m c_{\Gamma\alpha m} \beta_{m\sigma}(\hat{k})
\]

(5.58)

contains the angular dependence of the hybridization matrix elements. The coefficients \( c_{\Gamma\alpha m} \) tell us which angular momentum states \(|m\rangle\) in spherical symmetry contribute to a given crystal field state \(|\Gamma\alpha\rangle\). See equations 2.62-2.67 for all possible values of the \( c_{\Gamma\alpha m} \) in the case of the splitting of the \( J=5/2 \) multiplet in cubic symmetry. The functions \( \beta_{m\sigma}(\hat{k}) \) are defined in equation 5.48.

Also like we did for spherical symmetry, we define a function to contain all the angular dependence of the hybridization matrix elements

\[
B_{\Gamma\Gamma'}(\hat{k}, \hat{k}') = \sum_{\alpha\sigma\alpha'\sigma'} \beta_{\Gamma\alpha\sigma}(\hat{k}) \beta_{\Gamma'\alpha'\sigma'}(\hat{k}) \beta_{\Gamma\alpha\sigma}(\hat{k}') \beta_{\Gamma'\alpha'\sigma'}(\hat{k}').
\]

(5.59)

Evaluating equation 5.47 at the Fermi surface means that terms like \((\epsilon_{\Gamma} - E_{1\hat{k}})(\epsilon_{\Gamma'} - E_{1\hat{k}'})\) become \((\epsilon_{\Gamma} - \mu)(\epsilon_{\Gamma'} - \mu) = T_{\sigma\Gamma} T_{\sigma'\Gamma'}\). Using all the notation defined above (as marked by the •), equation 5.47 for the scattering amplitude in the local limit becomes

\[
\Gamma_{\text{local}}(\hat{k}, \hat{k}') = \frac{1}{4} \sum_{\Gamma\Gamma'} \tilde{V}_{\Gamma\alpha}(\hat{k}) \tilde{V}_{\Gamma'\alpha'}(\hat{k}') \left( \frac{T_{\sigma\Gamma} \hat{s}_{o\gamma}}{s_o V_o} \right)^4 \hat{s}_{o\gamma} \hat{s}_{o\gamma'} \frac{T_{\sigma'\Gamma'} \hat{s}_{o\gamma'}}{T_{\sigma'\Gamma'}},
\]

\[
\times 2 \left[ \frac{\hat{s}_{o\gamma} \hat{s}_{o\gamma}}{2\sqrt{N_{\Gamma} T_{\sigma\Gamma}}} + \frac{\hat{s}_{o\gamma} \hat{s}_{o\gamma'}}{2\sqrt{N_{\Gamma} T_{\sigma'\Gamma'}}} - \frac{\hat{s}_{o\gamma}^2}{4\sqrt{N_{\Gamma} N_{\Gamma'} T_{\sigma\Gamma} T_{\sigma'\Gamma'}}} \right],
\]

(5.60)
where we have ignored the dependence of the hybridization matrix element on the radial component of the momentum. We can look at equation 5.60 in three cases: \( \Gamma = \Gamma' = \Gamma_7; \Gamma = \Gamma_7, \Gamma' = \Gamma_8 \) (or \( \Gamma = \Gamma_8, \Gamma' = \Gamma_7 \)); and \( \Gamma = \Gamma' = \Gamma_8 \). Since it is just a matter of algebra, we merely quite the resultant contributions to \( \Gamma_{\text{local}} \) for each of these three cases,

\[
\Gamma_{\text{local},77} = \left( \frac{B_{77}}{2} \right) \left( \frac{T_{07}}{2} \right) \left( \sqrt{2} - \frac{1}{4} \right),
\]

(5.61)

\[
\Gamma_{\text{local},78} = \left( \frac{B_{78}}{2} \right) \left( \frac{T_{07}}{2} \right) \left( \frac{T_{07}}{\sqrt{2}T_{08}} \right) \left( 1 - \frac{\sqrt{2}}{4} + \frac{T_{07}}{T_{08}} \right),
\]

(5.62)

\[
\Gamma_{\text{local},88} = \left( \frac{B_{88}}{2} \right) \left( \frac{T_{07}}{2} \right) \left( \frac{T_{07}}{T_{08}} \right)^2 \left( \frac{1}{4} - \frac{\sqrt{2}T_{07}}{T_{08}} \right).
\]

(5.63)

Noting that \( \frac{T_{07}}{T_{08}} \approx 0.025 \), and assuming that \( B_{77} \approx B_{78} \approx B_{88} \) for a k-point not on a Brillouin zone axis (something special happens at these points), we see that

\[
\left| \frac{\Gamma_{78}}{\Gamma_{77}} \right| \approx \frac{T_{07}}{T_{08}},
\]

(5.64)

and

\[
\left| \frac{\Gamma_{88}}{\Gamma_{77}} \right| \approx 0.2 \left( \frac{T_{07}}{T_{08}} \right)^2,
\]

(5.65)

where the 0.2 prefactor comes from the fact that

\[
\frac{1}{4} - \frac{\sqrt{2}T_{07}}{T_{08}} \approx 0.2.
\]

Within these approximations, we see that the contribution to the local interactions from the \( \Gamma_7, \Gamma_7 \) term should dominate over the \( \Gamma_7, \Gamma_8 \) and \( \Gamma_8, \Gamma_8 \) terms. We can push this idea a bit further. As mentioned in the previous chapter, we can calculate the functions \( B_{\Gamma \Gamma'} \), exactly. For \( \Gamma = \Gamma_7 \) and \( \Gamma' = \Gamma_7 \), we have

\[
B_{77}(\hat{k}, \hat{k}') = \frac{8\pi}{18} \left[ Y_{00}^*(\hat{k}) - \frac{1}{3} Y_{40}^*(\hat{k}) - \frac{1}{3} \sqrt{\frac{5}{14}} (Y_{44}^*(\hat{k}) + Y_{4-4}^*(\hat{k})) \right]
\]
Now, recall from equation 5.7 that the cubic harmonic for the representation $A_{1g}$ is given by

$$\Phi_{A_{1g}}(\hat{k}) = \frac{1}{\sqrt{2}} \left[ Y_{00}(\hat{k}) + 0.76376261 Y_{40}(\hat{k}) + 0.4564355 \left( Y_{44}(\hat{k}) + Y_{4-4}(\hat{k}) \right) \right].$$

(5.67)

When we evaluate the double average over the spherical Fermi surface, we find

$$\int_{FS} \frac{d\hat{k}}{4\pi} \int_{FS} \frac{d\hat{k}'}{4\pi} \Phi_{A_{1g}}^*(\hat{k}') B_{77}(\hat{k}, \hat{k}') \Phi_{A_{1g}}(\hat{k}) = 0.44346. \quad (5.68)$$

Interestingly, when we try other possible cubic harmonics, $\Phi_\eta \ (\eta = E_g, T_{1g}, T_{2g})$ in equation 5.68, they vanish upon averaging. There is a non-zero overlap of $B_{77}$ only with a cubic harmonic of $A_{1g}$ symmetry. We can thus write

$$B_{77}(\hat{k}, \hat{k}') = 0.44346 \Phi_{A_{1g}}^*(\hat{k}) \Phi_{A_{1g}}(\hat{k}').$$

(5.69)

Equation 5.69 tells us that, if the only contribution to the local quasiparticle interactions came from the $\Gamma_7$ doublet, then only the $A_{1g}$ pairing state would experience a local repulsion. There would be (rigorously) zero local interactions in all other pairing states of cubic symmetry. Of course, in actuality, equations 5.64 and 5.65 tell us that the $\Gamma_8$ quartet has a non-zero contribution to the interactions, and so we expect that there will be nonzero contributions to pairing states other than just $A_{1g}$. In a rough way, we would expect

$$\sum_{\Gamma} B_{\Gamma \Gamma'}(\hat{k}, \hat{k}') = 0.4436 \left[ \Phi_{A_{1g}}^*(\hat{k}) \Phi_{A_{1g}}(\hat{k}') + \sum_{\eta \neq A_{1g}} a_\eta \Phi_\eta^*(\hat{k}) \Phi_\eta(\hat{k}') \right], \quad (5.70)$$

where the coefficient $a_\eta \ll 1$. Physically, the $\Gamma_7$ states are most important as far as the local interactions are concerned.
Since our simplified picture yields a dominant multiplet with the same degeneracy as that of the conduction states, the problem has (in a broad sense) reduced to that of the SU(N) (with N=2) calculation of Lavagna, Millis, and P. A. Lee. As we mentioned in the previous subsection, LML found a non-zero local interaction only in the s-wave pairing state. They also found that the inclusion of non-local interactions was sufficient to yield a (very weak) d-wave instability. Of course, in our calculation, this is the 64 million dollar question. If there is an appreciable local repulsion only in the $A_{1g}$ channel, can inclusion of non-local interactions yield an instability of $E_g$, $T_{1g}$, or $T_{2g}$ symmetry?

5.4 Results for Local Quasiparticle Interactions

5.4.1 The Strong Anisotropy of the Quasiparticle Normalization Function

In this section we shall discuss the numerical evaluation of the integrals

$$\int_{FS} \frac{d\hat{k}}{4\pi} \int_{FS} \frac{d\hat{k}'}{4\pi} \Phi^*(\hat{k}') \Gamma_{local}(\hat{k}, \hat{k}') \Phi(\hat{k}),$$

(5.71)

where $\Gamma_{local}(\hat{k}, \hat{k}')$ is given by equation 5.60, where $\Phi$ are the cubic harmonics, (See Table 5.2 for the functional form of the cubic harmonics we have used) and where no simplifying approximations about the normalization functions, $A^2(\hat{k}) A^2(\hat{k}')$ inside $\Gamma_{local}(\hat{k}, \hat{k}')$ have been made. In fact, we wish to focus on the $A^2(\hat{k})$, which were derived and Chapter 3. It has the functional form

$$A^2(\hat{k}) = \left[ 1 + \frac{1}{2} \sum_{\Gamma, \alpha} \frac{s^2_{1\Gamma} |\hat{V}_{\Gamma, \alpha}(\hat{k})|^2}{(\epsilon_{\Gamma} - E_{1\Gamma})^2} \right]^{-1},$$

(5.72)

where we have used time-reversal symmetry to introduce a sum over the pseudospin variable, $\sigma$. We shall study equation 5.72 in detail. By summing over $\Gamma, \alpha$,
and $\sigma$ (see Table 4.2), we can write for the inverse of equation 5.72

$$1 + \frac{2\sqrt{\pi}}{3} \frac{s_o^2 V_o^2}{T_{o7}^2} \left[ Y_{00} - \frac{1}{3} Y_{40} - \frac{1}{3} \sqrt{\frac{5}{14}} \left( Y_{44} + Y_{4-4} \right) \right]$$

$$+ \frac{2\sqrt{\pi}}{3} \frac{s_o^2 V_o^2}{T_{o8}^2} \left[ 2 Y_{00} + \frac{1}{3} Y_{40} + \frac{1}{3} \sqrt{\frac{5}{14}} \left( Y_{44} + Y_{4-4} \right) \right],$$

where the quasiparticle energy $E_{k\mathbf{k}}$ has been evaluated at the Fermi surface, and where we have used the fact that $s_o^2 \tilde{V}_{0i} = s_o^2 V_o^2$. These factors can be combined to give

$$1 + \frac{1}{3} s_o^2 V_o^2 \left[ \frac{1}{T_{o7}^2} + \frac{2}{T_{o8}^2} \right] + \frac{2\sqrt{\pi}}{9} s_o^2 V_o^2 \left[ Y_{40} + \sqrt{\frac{5}{14}} \left( Y_{44} + Y_{4-4} \right) \right] \left[ \frac{1}{T_{o8}^2} - \frac{1}{T_{o7}^2} \right]. \quad (5.73)$$

Note that

$$\frac{1}{3} s_o^2 V_o^2 \left( \frac{1}{T_{o7}^2} + \frac{2}{T_{o8}^2} \right) \gg 1,$$

and so the 1 will be dropped.

Next we use this expression to evaluate equation 5.72 at a point along one of the axes of the Brillouin zone. We saw in Chapter 3, that at these points the hybridization matrix elements of $\Gamma_7$ symmetry vanish. The normalization then becomes (for $T_{o8} < s_o V_o$)

$$A_1^2(\mathbf{k}_{axis}) = \left( \frac{T_{o8}}{s_o V_o} \right)^2.$$

At a general point in the zone, we have

$$A_1^2 = \frac{\left( \frac{T_{o7}}{s_o V_o} \right)^2}{\frac{1}{3} + \frac{2}{3} \left( \frac{T_{o7}}{T_{o8}} \right)^2 - \frac{2\sqrt{\pi}}{9} \left[ 1 - \left( \frac{T_{o7}}{T_{o8}} \right)^2 \right] \left[ Y_{40} + \sqrt{\frac{5}{14}} \left( Y_{44} + Y_{4-4} \right) \right]}. \quad (5.74)$$

Figure 5.3 shows a plot of equation 5.74 along the equator of our spherical Fermi surface, with $\phi$ denoting the azimuthal angle measured with respect to a
Figure 5.3:
A plot of the normalization function $A_{k}^{2}(\vec{k})$ along the equator of a sphere as a function of azimuthal angle, $\phi$. The sharp spikes occur at the intersections of the equator with the coordinate axes. At these points the $\Gamma_7$ hybridization matrix elements vanish exactly, and the width of these peaks is set completely by the ratio of the two Kondo temperatures $T_{\Gamma 7}/T_{08} \approx T_{\Gamma 7}/\Delta_{CEF}$. The behavior for a fixed azimuthal angle ($\phi=0$) as a function of the polar angle, $\theta$, is identical to this.

coordinate axis. Note the extremely sharp variations near the axes, representing the vanishing of $\Gamma_7$ matrix elements. The figure emphasizes the fact that if we must average the scattering amplitude over a spherical surface, we have basically three choices: (1) use a non-uniform mesh on the surface such that there is a high density of mesh points near the axes; (2) be (apparently) more naive and use a uniform (but dense) mesh all over the surface, thus guaranteeing adequate sampling near the axes (and oversampling everywhere else); or (3), use the fact that in the very small angular regions where the normalization is rapidly varying, every other factor in equation 5.60 is not varying much at all. We opted for the third choice for reasons that are discussed in Appendix E.

To treat the strongly anisotropic normalization adequately, we used the fact
that it varies rapidly only in a small solid angle, $\Delta \Omega$, near a coordinate axis. Thus, near the six points where the axes intersect the surface of our sphere, we integrate $A^2$ exactly, treating all other factors in the local scattering amplitude as constant. See Appendix E for all the details of this integration. This procedure requires only a relatively modest mesh over the Fermi surface (of the order of 100 mesh points). Note, however, that equation 5.60 actually requires a double surface average, and so there are two identical meshes. We also remind the reader at this juncture that these meshes for the surface averages are separate from the mesh for the Brillouin zone integrations used to calculate the dressed Bosonic Green functions. (See the second half of the previous chapter.)

As discussed in Appendix E, the mesh used for the averages has 102 points distributed in a configuration of cubic symmetry. That is, if we perform an operation of cubic symmetry to the averaging mesh, it remains unchanged. This is merely the common sense notion that when integrating functions of cubic symmetry, it is expedient to use a mesh also of cubic symmetry.

5.4.2 Contributions from the Hot-Spots

It is difficult not to notice the large values of the normalization at the six points where the Brillouin zone axes intersect the Fermi surface. We shall call these points "hot-spots". The width of these peaks is set by the ratio of the two Kondo temperatures, $T_{07}/T_{08} = T_{07}/(T_{07} + \Delta_{CEF}) \approx T_{07}/\Delta_{CEF}$. This can be seen by expanding the spherical harmonics in the denominator of equation 5.74 about one of the hot-spots on the Fermi surface. For concreteness, we expand about
\[ \theta = \pi/2 \text{ and } \phi = 0 \text{ to find} \]
\[ A_1^2 \approx \frac{\left( \frac{T_{77}}{V_0} \right)^2}{\frac{1}{3} + \frac{2}{3} t^2 - \frac{1}{3}(1 - t^2)(1 - 5\delta \theta^2 - 5\phi^2)}, \]
(5.75)

where \( t^2 \equiv (T_{77}/T_{68})^2 = 0.0251 \) for CeCu₂Si₂, and where \( \delta \theta \equiv \theta - (\pi/2) \). First, we note that the \( \theta \) and \( \phi \) dependences are identical. This means, that if we were to set \( \delta \theta = 0 \) and study \( A_1^2 \) as a function of small \( \phi \), we would get the same behavior as if we had set \( \phi = 0 \) and were studying the behavior of \( A_1^2 \) with small \( \delta \theta \).

This tells us that the normalization function has a spike at the hot-spots. It could be informative, then, to replace the normalization functions in the expressions for the local scattering amplitude (equation 5.60) with delta functions at the six hot-spots. Each delta function would have a weight equal to the area under the spikes of figure 5.3[28],

\[ A_1^2(\vec{k}) = \sum_{\{\vec{k}^*\}} A_1^2 \delta(\vec{k} - \vec{k}^*). \]
(5.76)

The set of six \( \vec{k}^* \) label the hot spots on the Fermi surface, and \( A_1^2 \) is the integrated weight for each delta function. The procedure for calculating \( A_1^2 \) is given in Appendix E.

Within this approximation, we have the following simplifications of the local scattering amplitude:

- The hybridization of the conduction states with crystal field states of \( \Gamma_7 \) symmetry vanishes exactly. (i.e. all \( V_{7\sigma\sigma}(\vec{k}) = 0 \) when \( \vec{k} \) is on an axis of the Brillouin zone) Only the matrix elements \( V_{\sigma\sigma}(\vec{k}) \) are non-zero.

- The combination of four hybridization matrix elements defined as \( B_{88}(\hat{k}, \hat{k}') \) (see equation 5.59) equals unity when evaluated at a hot-spot. This is the only non-zero combination.
Thus the local scattering amplitude becomes

\[ \Gamma_{\text{local,hot}}(\vec{k}, \vec{k}') = \frac{1}{4} A_1^* \delta(\vec{k} - \vec{k}^*) \delta(\vec{k}' - \vec{k}'^*) \left( \frac{\tilde{s}_{08}^2 \tilde{V}_{08}^4}{T_{08}^2} \right) \times \left[ \frac{\tilde{s}_{08}}{T_{08} \Gamma_{\text{os}}} - \frac{\Gamma_{o\lambda\lambda}}{4 \Gamma_{o\lambda}^2} \right]. \tag{5.77} \]

Using the mean field values of parameter set (a) (see Table 5.3) and equations 5.44 and 5.45, we can numerically evaluate the vertices \( \Gamma_{\text{os}} \) and \( \Gamma_{o\lambda\lambda} \):

\[ \Gamma_{\text{os}} = \sum_{\Gamma} \left( \frac{1}{2} N_{\Gamma} \tilde{s}_{0\Gamma} + \frac{x_{\Gamma}}{\tilde{s}_{0\Gamma}} \right) = 29.235, \tag{5.78} \]

\[ \Gamma_{o\lambda\lambda} = \sum_{\Gamma} \frac{y_{\Gamma}}{T_{0\Gamma}} = 1035.686 \text{ (eV)}^{-1}. \tag{5.79} \]

Furthermore, from mean field parameter set (a), we have

\[ \frac{\tilde{s}_{08}}{T_{08} \Gamma_{\text{os}}} = 0.043294 \text{ (eV)}^{-1}, \]

\[ \frac{\Gamma_{o\lambda\lambda}}{4 \Gamma_{o\lambda}^2} = 0.3029 \text{ (eV)}^{-1}, \]

\[ \frac{\tilde{s}_{08}^2 \tilde{V}_{08}^4}{T_{08}^2} = 13.989 \text{ (eV)}^2. \]

Substituting all these numbers into equation 5.77 and combining, we find

\[ \Gamma_{\text{local,hot}} = (-0.908 \text{ eV}) A_1^* \delta(\vec{k} - \vec{k}^*) \delta(\vec{k}' - \vec{k}'^*), \tag{5.80} \]

where \( A_1 \) is the integrated weight of the spikes shown in figure 5.3. The important point here is the sign of this expression. When \( \Gamma_{\text{local,hot}} \) is averaged over a spherical Fermi surface, this will give the contribution of the hot-spots to the full average of equation 5.60.

Because the cubic harmonics of \( T_{1g} \) and \( T_{2g} \) vanish on the Brillouin zone axes (see Table 5.2), the averages \( \langle \Gamma_{\text{local,hot}} \rangle_{T_{1g}} \) and \( \langle \Gamma_{\text{local,hot}} \rangle_{T_{2g}} \) will be identically
zero. The cubic harmonics of $A_{1g}$ and $E_g$ symmetry do not vanish at the hotspots, and so their Fermi surface averages need not vanish. Table 5.5 shows the values of the averages $\langle \Gamma_{local, hot} \rangle_{A_{1g}}$ and $\langle \Gamma_{local, hot} \rangle_{E_g}$. The negative (attractive) value in the $E_g$ channel,

$$\frac{\langle \Gamma_{local, hot} \rangle_{E_g}}{T_{07}} = -0.0696,$$

(5.81)

is informative. Since states of $E_g$ symmetry have their maximum values at the hot spots (see Table 5.2), the average $\langle \Gamma_{local} \rangle_{E_g}$ should be highly susceptible to what happens at these points. The negative sign in equation 5.80 thus is evidence that the hot spots are the source of the overall attraction in the full Fermi surface average. Note in Table 5.5, that the full surface average in the $E_g$ channel is

$$\frac{\langle \Gamma_{local} \rangle}{T_{07}} = -0.0275,$$

while equation 5.81 gives a value of -0.0696. Thus we see that the contribution from the hot-spots is reduced by positive (repulsive) local interactions at other points on the Fermi surface, but the hot-spots still dominate the result.

Furthermore, from equation 5.77, we can see why no similar negative signs appear in the average local interactions in spherical symmetry. The combination of terms

$$\frac{\tilde{\delta}_{o8}}{T_{o8}\Gamma_{o8\lambda}} - \frac{\Gamma_{o\lambda\lambda}}{4\Gamma_{o\lambda\lambda}^2} = -0.25965 \ (eV)^{-1}$$

should not be negative in spherical symmetry, since in the denominator of the first term, the temperature $T_{o8}$ would be replaced by a much smaller Kondo temperature which would be of the order of $T_{07}$ ($T_{07} \ll T_{o8}$). As a simple check of this idea, if we assume the related quantity

$$\frac{\tilde{\delta}_{o7}}{T_{o7}\Gamma_{o\lambda\lambda}} - \frac{\Gamma_{o\lambda\lambda}}{4\Gamma_{o\lambda\lambda}^2} = 2.14 \ (eV)^{-1},$$


is more indicative of the case of *spherical* symmetry, we see that the contribution to the local scattering amplitude would be *positive*. Thus, the presence of the second energy scale, $T_{o8} = T_{o7} + \Delta_{CEF}$, coupled with the fact that $T_{o7}/T_{o8} \ll 1$, yields the negative value for the scattering amplitude in the $E_g$ channel.

It is surprising that the contribution from the hot-spots in the $A_{1g}$ channel is attractive

$$\frac{\langle \Gamma_{local, hot} \rangle A_{1g}}{T_{o7}} = -0.215,$$

(see Table 5.5), while the overall average is still large and repulsion,

$$\frac{\langle \Gamma_{local} \rangle A_{1g}}{T_{o7}} = 3.54.$$

Clearly, the contribution to the overall average in the $A_{1g}$ channel is not dominated by the hot-spots. That this is the case for $A_{1g}$ but not $E_g$ probably stems from the following facts:

• As mentioned above, the cubic harmonics of $E_g$ symmetry are most sensitive to what happens at the hot-spots, since their maxima occur at these points. Only the $Y_{00}$ spherical harmonic survives when the $A_{1g}$ cubic harmonic is evaluated at a hot spot. So $A_{1g}$ states do not place any special emphasis on the hot spots.

• Although figure 5.3 shows us that the normalization function is very strongly peaked at the hot-spots, equation 5.77 shows that part of this large numerator is canceled out in the local scattering amplitude by the presence of two factors of the $\Gamma_8$ Kondo temperature, $T_{o8}$, in the denominator of that expression. Since any contribution to $\Gamma_{local}$ from crystal field states of $\Gamma_7$ symmetry would contribute factors of $T_{o7}$ in the denominator, and since $T_{o7}/T_{o8} \ll 1$, we see that the enhancement of the hot-spots, relative to a general point on the Fermi surface, is diminished.
Thus, since the $E_g$ cubic harmonics themselves peak up at the hot-spots, the average in the $E_g$ channel is most susceptible to the hot-spots, with the average in the $A_{1g}$ channel less sensitive.

At the end of this subsection, we offer a few words about the robustness of the "hot-spots". They arise because of the following circumstances. First, the lowering of the symmetry below spherical means that the spherical harmonic sum rules are not valid. In spherical symmetry, the sum rules give an overall combination of matrix elements that is isotropic. In non-spherical symmetry, this simplification is not allowed; the combinations of hybridization matrix elements are perforce anisotropic. Then, for any symmetry of the lattice, there will most likely be points in the Brillouin zone where some matrix elements vanish, giving rise to a "hot-spot" at that point. Thus, we expect the appearance of these "hot-spots" to be a general consequence of a symmetry lower than spherical. It should not be a phenomenon peculiar only to cubic lattices.

5.4.3 Full Fermi-Surface Average

We are now ready to present our results for full Fermi surface averaged (local) interactions, $\langle \Gamma_{\text{local}} \rangle_{\eta}$, where $\eta = A_{1g}$, $E_g$, $T_{1g}$, or $T_{2g}$. We have not included the $A_{2g}$ representation for two reasons: (1) the lowest order spherical harmonic present in $\Phi_{A_{2g}}$ is $Y_6^m[11]$ and would thus require an even finer averaging mesh; and (2) the relatively rapid variation throughout the Brillouin zone would correspond to a pairing state with a high energy and hence should be less important than the states labeled by the other representations.

Table 5.5 gives the ratio $\langle \Gamma_{\text{local}} \rangle_{\eta}/T_{\text{K}}$ for both mean-field parameter sets (a) and (b). Both parameter sets have Kondo temperatures of about 10 K. We see
that our physical intuition of the previous subsection was correct. Namely, the 
\(A_{1g}\) state has (by-far) the largest (repulsive) local interaction. In comparison, the 
remaining states have very small interactions. We also have found the following:

- In the \(E_g\) channel, the anisotropy due to cubic symmetry, especially the strong 
anisotropy of the normalization function, gives rise to an *attractive* local inter-
action. In fact, the attractive local interaction here is dominated by the contribu-
ptions from the hot-spots. We note from Table 5.2 that a pairing state of \(E_g\) 
symmetry is like a \(d_{x^2-y^2}\) or \(d_{3z^2-r^2}\) state.

- The repulsive (local) interaction in the \(A_{ig}\) channel is quite large, about two 
or three times larger than the Kondo temperature of the \(\Gamma_7\) doublet, \(T_{07}\), but is 
not dominated by the hot-spots.

As mentioned in the previous subsection, that a \(d_{x^2-y^2}\) or \(d_{3z^2-r^2}\) state is so 
susceptible to the normalization function is not surprising if we think in terms 
of a simple atomic-orbital picture. These orbitals have their largest values along 
the axes. But along the axes is where the normalization is also *strongly* peaked. 
Thus the states of \(x^2 - y^2\) or \(3z^2 - r^2\) symmetry are greatly affected by \(A_{ig}(\vec{k})\). 
The \(A_{1g}\) function, is also affected by the normalization, but not as much as the 
\(E_g\) states. And the \(T_{1g}\) and \(T_{2g}\) states all vanish along the axes and so are only 
weakly affected by the normalization.

In Table 5.6, we present the values of \(\langle \Gamma \rangle / T_o\) from Zhang and Lee’s[1] cal-
culation. Since they assumed spherical symmetry, the pairing states can be 
represented by Legendre polynomials, \(P_\eta\). States with \(\eta=0\) are s-wave; \(\eta=2\) 
corresponds to d-wave; and \(\eta=4\) is g-wave. Zhang and Lee find all non-zero 
interactions are repulsive and of about the same strength. As we have said, 
they found the inclusion of non-local interactions, which represents the effects
Table 5.3:

Self-consistent mean field parameter sets, labeled as (a) and (b). At mean field there are three coupled integral equations, which are solved self-consistently. The input parameters are: the bare hybridization strength, \( V_0 \); the lower edge of the conduction electron band in the absence of hybridization, \( -D \); the total number of electrons, \( n_{\text{total}} = n_{\text{cond}} + n_f \), per unit cell; the bare, or unshifted, energy of the \( \Gamma_7 (E_7) \) and the \( \Gamma_8 (E_8 = E_7 + \Delta_{CEF}) \) multiplets; and the fixed crystal field splitting, \( \Delta_{CEF} = 360 \text{ K} \). The self-consistent parameters which solve the equations are: the hybridization renormalization coefficient, \( s_0 \), where the mean field renormalized hybridization is \( s_0 V_0 \); the shifted \( \Gamma_7 (\epsilon_7) \) and \( \Gamma_8 (\epsilon_8 = \epsilon_7 + \Delta_{CEF}) \) multiplet energies; the quasiparticle chemical potential, \( \mu \); and the Kondo temperature \( T_{\alpha 7} \equiv \epsilon_7 - \mu \) of the \( \Gamma_7 \) doublet. In both parameter sets (a) and (b), the total number of particles was fixed at \( n_{\text{total}} = 1.5 \). And the input parameters were chosen to give approximate Kondo temperatures of 10 K, i.e. \( T_{\alpha 7} \approx 10 \text{ K} \). All energies are measured relative the chemical potential in the absence of hybridization. In both parameter sets, \( \Delta_{CEF}=360 \text{ K} \), and the unshifted \( \Gamma_7 \) energy is \( E_7 = -2.0 \text{ eV} \).

<table>
<thead>
<tr>
<th>parameter set</th>
<th>( V_0 ) (eV)</th>
<th>( s_0 ) (eV)</th>
<th>( \epsilon_7 ) (eV)</th>
<th>( \mu ) (eV)</th>
<th>( T_{\alpha 7} ) (K)</th>
<th>( D ) (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>0.8595</td>
<td>0.093472</td>
<td>0.0217648</td>
<td>0.0208399</td>
<td>9.25</td>
<td>2.4405</td>
</tr>
<tr>
<td>b</td>
<td>0.650</td>
<td>0.142409</td>
<td>-0.8437021</td>
<td>-0.844999</td>
<td>13.0</td>
<td>3.33856</td>
</tr>
</tbody>
</table>

of the functions \( F(\vec{k}' - \vec{k}) \) and \( F(\vec{k}' + \vec{k}) \), was not sufficient to overcome the local repulsions. The final topic to be addressed in this chapter now arises: in the presence of cubic symmetry and crystal field splitting, does the inclusion of non-local interactions lead to a pairing instability (with \( \langle \Gamma \rangle_\eta < 0 \))?
Table 5.4:
Contributions to the Bosonic vertex functions, $\Gamma_{o\sigma\lambda}$, $\Gamma_{e\lambda\lambda}$ which are momentum independent and which begin as terms of the order of the square of the hybridization matrix element, $\tilde{V}_{\Gamma o\sigma}^2$. The $s - \lambda$ and $\lambda - \lambda$ contributions are

$$\Gamma_{o\sigma\lambda} = \sum_{\Gamma} \left( \frac{1}{2} N_{\Gamma} \tilde{s}_{o\Gamma} + \frac{x_{\Gamma}}{\tilde{s}_{o\Gamma}} \right), \quad \Gamma_{o\lambda\lambda} = \sum_{\Gamma} \frac{y_{\Gamma}}{T_{o\Gamma}}.$$ 

The parameters $x_{\Gamma}$ and $y_{\Gamma}$ are given for both mean field parameter sets described in Table 5.3.

<table>
<thead>
<tr>
<th>Parameter set</th>
<th>$x_7$</th>
<th>$x_8$</th>
<th>$y_7$</th>
<th>$y_8$</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>1.820</td>
<td>0.0717</td>
<td>0.975</td>
<td>0.04029</td>
</tr>
<tr>
<td>b</td>
<td>1.729</td>
<td>0.0949</td>
<td>0.925</td>
<td>0.0498</td>
</tr>
</tbody>
</table>

5.5 Results in the Presence of Non-local Quasiparticle Interactions

This section discusses our results for the full Fermi surface average of the quasiparticle scattering amplitude, $\Gamma_{QP}(\tilde{k}, \tilde{k}')$, as given in equation 5.43. The function $F(\q)$, which is dependent upon the functions $I_{s\sigma\Gamma}(\q)$, $I_{s\lambda\Gamma}(\q)$, and $I_{\lambda\lambda\Gamma}(\q)$ (see equations 4.8-4.10), contains the physics of the screened (by density fluctuations of the coupled conduction-4f electrons) slave Bosons. The momentum dependence of $F(\q)$ represents the contribution of non-local quasiparticles interactions in real space.

Although Zhang and Lee[1] found that in spherical symmetry the non-local interactions were too weak to overcome the local repulsions, we can not be sure a priori that the non-local interactions will be as weak in the presence of crystal fields. In section 2.3, where we discussed the mean field results of the Anderson impurity model, we said that the Kondo temperature for the lowest crystal field-split multiplet can be reduced significantly in comparison to the
Table 5.5:
The local ("hard-core") quasiparticle scattering amplitude in the presence of crystal electric fields, $\Gamma_{QP}$, averaged over a spherical Fermi surface. Results for both mean field parameter sets (a) and (b) are given. See table 5.3 for a discussion of the mean field parameters themselves. The first column gives the representations, labeled by $\eta$, of the group $O_h$. The second and third columns are the averaged local scattering amplitudes (divided by the $\Gamma_7$ Kondo temperature, $T_{07}$) for the parameter sets (a) and (b), respectively. The fourth column lists (for parameter set (a)) the contribution to the average from the so-called hot-spots, where the Brillouin zone axes intersect the Fermi surface. In column four, in the $E_g$ channel, the attractive interaction seems to be due to these hot-spots; but in the $A_{1g}$ channel the hot-spots do not dominate, since the full Fermi surface average is large and positive. The average in the $E_g$ should be most sensitive to the hot-spots, since that is where the $E_g$ cubic harmonics have their maximum value. In the $T_{1g}$ and $T_{2g}$ channels there is rigorously zero contribution from the hot-spots because the $T_{1g}$ and $T_{2g}$ cubic harmonics vanish at those points.

<table>
<thead>
<tr>
<th>(a) Cubic Symmetry</th>
<th>$\langle \Gamma_{local,\eta} \rangle_{T_{07}} / T_{07}$ set (a)</th>
<th>$\langle \Gamma_{local,\eta} \rangle_{T_{07}} / T_{07}$ set (b)</th>
<th>$\langle \Gamma_{local,\text{hot}} \rangle_{T_{07}} / T_{07}$ set (a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_{1g}(s-wave)$</td>
<td>3.54</td>
<td>3.53</td>
<td>-0.215</td>
</tr>
<tr>
<td>$E_g(d_{x^2-y^2},d_{3z^2-r^2})$</td>
<td>-0.0275</td>
<td>-0.0453</td>
<td>-0.0696</td>
</tr>
<tr>
<td>$T_{1g}$</td>
<td>0.0478</td>
<td>0.0695</td>
<td>0.0</td>
</tr>
<tr>
<td>$T_{2g}(d_{xy},d_{yz},d_{xz})$</td>
<td>0.0487</td>
<td>0.0709</td>
<td>0.0</td>
</tr>
</tbody>
</table>
Table 5.6:

The local ("hard-core") quasiparticle scattering amplitude in the presence of spherical symmetry and an anisotropic, Coqblin-Schrieffer hybridization matrix element. This is from the work of Zhang and Lee[1]. When divided by the Kondo temperature and averaged over the spherical Fermi surface, these results are universal. There are no other parameters involved. In spherical symmetry, the pairing states are labeled by their relative angular momentum, \(l\), with \(l=0\) corresponding the s-wave; \(l=2\), d-wave; and \(l=4\), g-wave. It is meaningful to compare Zhang and Lee's results with ours, because in the limit of spherical symmetry, where all the Bosonic propagators in equation 5.37 are replaced with their values in spherical symmetry, and where the normalization functions, \(A_k^\eta(\vec{k})\) and \(A_{k'}^\eta(\vec{k'})\), are replaced by their isotropic values in spherical symmetry, our expression for \(\Gamma_{QP}\) (equation 5.73) gives exactly the same local interactions as Zhang and Lee. Note that all local interactions are repulsive in spherical symmetry.

<table>
<thead>
<tr>
<th>Spherical Symmetry</th>
<th>(\langle \Gamma_{local} \rangle_\eta / T_o)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\eta=0) (s-wave)</td>
<td>(1/3)</td>
</tr>
<tr>
<td>(\eta=2) (d-wave)</td>
<td>(8/21)</td>
</tr>
<tr>
<td>(\eta=4) (g-wave)</td>
<td>(2/7)</td>
</tr>
</tbody>
</table>
Kondo temperature in spherical symmetry[15]. We presented the result

\[ T_K = T_K^0 \left( \frac{T_K^0}{\Delta_{CEF}} \right)^{N_2 \over N_1}, \]  

(5.82)

where \( T_K^0 \) is the Kondo temperature in spherical symmetry, \( \Delta_{CEF} \) is the crystal field splitting, and where \( N_1(N_2) \) is the degeneracy of the ground(excited) crystal field-split multiplet. If \( T_K^0 \gg \Delta_{CEF} \), we see that \( T_K \ll T_K^0 \). When appearing in the denominator of the expressions for the Bosonic self-energy, this reduced Kondo temperature could increase the size of the self-energy contribution to the scattering amplitude (relative to the case of spherical symmetry). This discussion points us back to equation 5.43. We first say a few words about the numerics of averaging \( \Gamma_{QP}(\vec{k}, \vec{k'}) \) over the Fermi surface.

Unlike in the local approximation, \( \Gamma_{QP}(\vec{k}, \vec{k'}) \) is not separable into two simple functions of momenta, \( \vec{k} \) and \( \vec{k'} \). Thus the average

\[ \langle \Gamma \rangle_n = \int_{FS} \frac{d\vec{k}}{4\pi} \int_{FS} \frac{d\vec{k'}}{4\pi} \Phi^*(\vec{k'}) \Gamma_{QP}(\vec{k}, \vec{k'}) \Phi_n(\vec{k}) \]  

(5.83)

truly is a double integral over \( \vec{k} \) and \( \vec{k'} \). From equation 5.43, we see that we must evaluate the function \( F(\vec{k} \pm \vec{k'}) \) for all unique combinations of \( \vec{k} \pm \vec{k'} \). This we do separately from the actual averaging process. We store the necessary values for \( F(\vec{k} \pm \vec{k'}) \) in a look-up table. The creation of this table is the most time-consuming part of the entire process.

We discussed the general convergence properties of the functions \( I_{ss}(\vec{q}), I_{s\lambda}(\vec{q}) \), and \( I_{\lambda\lambda}(\vec{q}) \) in Chapter 4. By way of a review, we remind the reader that the functions can be written as principal value integrals over the cubic Brillouin zone,

\[ I_{ab}(\vec{q}) = P \int d^3 k f(E_{1\vec{k}}) \frac{M_{ab}(\vec{k}, \vec{k} + \vec{q})}{E_{1\vec{k} + \vec{q}} - E_{1\vec{k}}}, \quad (a, b = s, \lambda) \]  

(5.84)
where $E_{1\bar{k}}$ is the quasiparticle dispersion of the lowest band, and where $M_{ab}(\bar{k}, \bar{k} + \bar{q})$ is an effective matrix element, which is a highly anisotropic function of the momenta $\bar{k}$ and $\bar{q}$. See equations 4.122-4.128 for the full expressions for the matrix elements.

Figure 4.21-4.26 show that for both mean field parameter sets, the integrals $I_{ab}(\bar{q})$ for a given $\bar{q}$ are very slow to converge as a function of the Brillouin zone mesh size. Our integration procedure requires that we break up the Brillouin zone into a large number of small tetrahedra. We define a mesh parameter, $n_{\text{mesh}}$, such that $8n_{\text{mesh}}^3$ gives the total number of tetrahedra in the zone. Thus, when there are still fluctuations in the values of the integral $I_{ab}(\bar{q})$ for $n_{\text{mesh}} \approx 80$, this is not good news. These fluctuations are clearly a result of the matrix elements, $M_{ab}$, since the related integral without the matrix elements, $\int d^3k \frac{f(E_{1\bar{k}})}{E_{1\bar{k}+\bar{q}} - E_{1\bar{k}}}$, converges quickly. (See figure 4.15.)

The slow convergence of the $I_{ab}(\bar{q})$ prompted us to try the following line of attack. We have averaged the scattering amplitude (equations 5.39 or 5.43) over the Fermi surface with a fixed averaging mesh. (See Appendix F for details.) We vary, however, the mesh for calculating the Bosonic Green function, as characterized by $n_{\text{mesh}}$, and study the average interactions as a function of $n_{\text{mesh}}$.

As we studied the variation of $\langle \Gamma \rangle_\eta$ as a function of $n_{\text{mesh}}$, it became clear that $n_{\text{mesh}} \approx 50$ is a practical limit of the mesh size. Creating the look-up table for the Bosonic self-energies would require well over a week of runtime on a DEC5100 for anything bigger. Thus, it is important to ask if we can make any conclusions about possible pairing instabilities for $n_{\text{mesh}} \leq 50$. Unfortunately,
Figure 5.4:
A planar projection of the spherical surface averaging mesh used to average the quasiparticle interactions. The mesh is viewed from along an axis of the cubic Brillouin zone. Because of the symmetry of the mesh, the bottom and top halves of the mesh lie on top of each other in the projected figure. The mesh is invariant under operations of cubic symmetry.

the answer to such a question is not a resounding yes.

There is one last detail of the numerics left to discuss. As we said, the averaging mesh was chosen to have cubic symmetry. As viewed from along an axis of the cubic Brillouin zone, the mesh has the structure depicted in figure 5.4. There is a series of rings, and each ring has an increasing number of mesh points as we move from a pole to an equator on the spherical Fermi surface. Since the integrals in equation 5.83 are written in terms of spherical coordinates, however, cubic symmetry overall is not respected. As we all know, in spherical coordinates a special, polar, axis is chosen against which the polar angle is measured. This choice of a special direction, which breaks the spherical symmetry, does not matter in the limit of infinitesimals present in a true integral over the spherical
coordinates. But in a numerical evaluation of an integral, in some sense this symmetry remains broken. Of course, we only need cubic, as opposed to spherical, symmetry for our averaging. Nevertheless, the choice of a particular polar direction still breaks the cubic symmetry. We overcome this problem in a very straightforward manner. We perform three Fermi surface averages (over both $\vec{k}$ and $\vec{k}'$): one average has $\hat{z}$ as the polar axis; one has $\hat{x}$; uses $\hat{y}$ as the polar axis. We then average the three values, for a given representation $\eta$, to get a result respecting cubic symmetry.

Since the scattering amplitude, $\Gamma_{QF}(\vec{k}, \vec{k}')$, has cubic symmetry, and since the rotations necessary for the three different averages are all operations of cubic symmetry, only the cubic harmonics, $\Phi_\eta(\vec{k})$ and $\Phi_\eta(\vec{k}')$, are changed by the rotations. The results of a test run of this procedure are presented in Table 5.7 for the representations $\eta = A_{1g}, E_g, T_{1g},$ and $T_{2g}$ of the octahedral group. The columns marked as $\hat{x}$, $\hat{y}$, or $\hat{z}$ signify the three averages with different polar axes. The final column gives the average of these three values. We see that the averaged results respect cubic symmetry in that all numbers within a given representation (of dimension of greater than one) are degenerate. It is these averages for a given representation which we shall now discuss.

5.5.1 Contributions from the Hot-Spots

First, let's look at the contribution to the average $\langle \Gamma \rangle_{\eta}/T_{07}$ from our so-called hot spots. To proceed, we merely multiply the expression for the local scattering amplitude, equation 5.77, by the following factor:

$$\left[ \frac{1}{1 + F(\vec{k} + \vec{k}')} + \frac{1}{1 + F(\vec{k}' - \vec{k})} \right], \quad (5.85)$$
Table 5.7:

Averages of the quasiparticle scattering amplitude for mean field parameter set (a). (See Table 5.3.) All results are divided by $T_{o7}$. The averaging mesh is composed of 102 points distributed over the surface of the sphere in a configuration of cubic symmetry. The mesh parameter for the *Bosonic* propagator was fixed at $n_{mesh}=39$. This means that $8\times39^3$ tetrahedra were used to calculate the Bosonic Green functions. The columns labeled by $\hat{a}$ ($a=x,y,z$) denote the polar axis used in the averaging. The fifth column is the average of these three results. Note the degeneracies for $\eta=E_g, T_{1g}$, and $T_{2g}$ are respected by the averaged values. The word “Average” in the last column means $(\langle \Gamma \rangle_x + \langle \Gamma \rangle_y + \langle \Gamma \rangle_z)/3$, where the subscript here denotes the polar axis.

<table>
<thead>
<tr>
<th>Rep. ($\eta$)</th>
<th>$\hat{x}$</th>
<th>$\hat{y}$</th>
<th>$\hat{z}$</th>
<th>Average/$T_{o7}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_{1g}$</td>
<td>2.71</td>
<td>2.71</td>
<td>2.71</td>
<td>2.71</td>
</tr>
<tr>
<td>$E_g$</td>
<td>-0.708</td>
<td>-0.739</td>
<td>-0.739</td>
<td>-0.729</td>
</tr>
<tr>
<td></td>
<td>-0.750</td>
<td>-0.719</td>
<td>-0.719</td>
<td>-0.730</td>
</tr>
<tr>
<td>$T_{1g}$</td>
<td>-0.221</td>
<td>-0.211</td>
<td>-0.221</td>
<td>-0.217</td>
</tr>
<tr>
<td></td>
<td>-0.221</td>
<td>-0.221</td>
<td>-0.221</td>
<td>-0.217</td>
</tr>
<tr>
<td></td>
<td>-0.211</td>
<td>-0.221</td>
<td>-0.221</td>
<td>-0.217</td>
</tr>
<tr>
<td>$T_{2g}$</td>
<td>0.189</td>
<td>0.292</td>
<td>0.189</td>
<td>0.224</td>
</tr>
<tr>
<td></td>
<td>0.189</td>
<td>0.189</td>
<td>0.292</td>
<td>0.224</td>
</tr>
<tr>
<td></td>
<td>0.292</td>
<td>0.189</td>
<td>0.189</td>
<td>0.224</td>
</tr>
</tbody>
</table>
where the function $F(q)$ is defined in equation 5.46. $F(q)$ contains all the momentum dependence of the Bosonic propagator and is constructed from our old friends, the functions $I_{ss}(q)$, $I_{s\lambda}(q)$, and $I_{\lambda\lambda}(q)$. Since we have limited ourselves to the hot-spots here, there are only three unique combinations of the vectors $\vec{k}' - \vec{k}$, and evaluating the Fermi surface average is relatively easy to do. In figures 5.5 and 5.6, we plot the results for the $A_{1g}$ and $E_g$ channels as a function of $n_{\text{mesh}}$ for parameter set (a). For comparison, we also plot the full Fermi surface average in both channels.

- In the $A_{1g}$ channel, we see that the hot-spots contribute about 1/10 of the full average (except for the sudden fluctuation at $n_{\text{mesh}}=51$). We might have expected a larger contribution from the hot-spots, but as we mentioned previously, the presence of the factors of $T_{o8}$ in the denominator, knocks some of the punch out of the large normalization functions, $A_1^2$, in the numerator. (See equation 5.77.)

- In the $E_g$ channel, something very interesting happens. Even though the local interaction due to the hot-spots is attractive (see Table 5.4), when we include the non-local interactions as well, the total contribution from the hot-spots becomes repulsive. Nevertheless, for many values of $n_{\text{mesh}}$, the full average over the entire Fermi surface is still attractive. (See figure 5.8.) This means that there must be some delicate cancellations occurring as we average over the full Fermi surface in order to arrive at a final result that overpowers the repulsion due to the hot-spots. Furthermore, if these cancellations come from a series of terms of the same size but opposite signs, then we would expect the sign of $(\Gamma)_{E_g}/T_{o7}$ to be rather unstable as a function of $n_{\text{mesh}}$. This, indeed, appears to be the case, as the final results show.
Figure 5.5:
Comparison, in the $A_{1g}$ channel, between the full Fermi surface average of the scattering amplitude and the contribution from just the hot-spots, which are the points where the axes of the Brillouin zone intersect the spherical Fermi surface. The hot-spots contribute only about 1/10 the full value. This is due to the fact that, while the quasiparticle normalization function is strongly peaked at the hot-spots, the scattering amplitude has two factors of the $T_s$ Kondo temperature ($T_{os}$) in the denominator. Since $T_{os}$ is a large number in this calculation, some of the effect of the large normalization function is canceled by the large denominator.
Comparison, in the $E_g$ channel, between the full Fermi surface average of the scattering amplitude and the contribution from just the hot-spots, which are the points where the axes of the Brillouin zone intersect the spherical Fermi surface. For $n_{mesh} < 40$, the contribution from the hot-spots is of the same size as the full average, however, the full average is negative (attractive) and the hot-spots contribution is repulsive. This says there is a very interesting and delicate combination of positive and negative quantities as the scattering amplitude is averaged over the entire Fermi surface. This combinations of terms of the same size could also explain why there are more fluctuations in sign (note what happens at $n_{mesh}=17$) in the $E_g$ channel than in the $A_{1g}$ channel.
5.5.2 The Full Fermi Surface Average

The values of \( \langle \Gamma \rangle_{\eta}/T_{\eta} \) for \( \eta = A_{1g} \) and \( \eta = T_{2g} \) are plotted as a function of \( n_{\text{mesh}} \) in figure 5.7 for parameter set (a) and in figure 5.9 for parameter set (b). Also on the plots, the local value for the average are marked by horizontal lines for each representation (except \( A_{1g} \)). The results show the following:

- In the \( A_{1g} \) channel, the interactions are clearly repulsive. The non-local interactions, however, are attractive, since the average local repulsion is of the size \( \langle \Gamma_{\text{local}} \rangle_{A_{1g}}/T_{\eta} \sim 3.54 \), and the inclusion of \( F(\vec{k} \pm \vec{k}') \) gives \( \langle \Gamma \rangle_{A_{1g}}/T_{\eta} \approx 1.2 \). Thus the non-local contribution has reduced the local repulsion by about a factor of two.

- In the \( T_{2g} \) channel, but for a glitch at \( n_{\text{mesh}} = 23 \), the interactions are repulsive for parameter set (a), with \( \langle \Gamma \rangle_{T_{2g}}/T_{\eta} \approx 0.20 \). For parameter set (b) (figure 5.9), however, it is less clear if the average interaction is attractive or repulsive—at least for the mesh sizes run so far.

The values of \( \langle \Gamma \rangle_{\eta}/T_{\eta} \) for \( \eta = E_{g} \) and \( \eta = T_{1g} \) are plotted in figure 5.8 for parameter set (a) and in figure 5.10 for parameter set (b).

- Although certainly not converged, the results for \( T_{1g} \) show attractive interactions, with an average value \( \langle \Gamma \rangle_{T_{1g}}/T_{\eta} = -0.212 \pm 0.025 \) for parameter set (a), and \( = -0.226 \pm 0.049 \) for parameter set (b).

- The interactions in the \( E_{g} \) channel are less well behaved, but are attractive for \( 25 \leq n_{\text{mesh}} \leq 47 \), where the upper limit on the mesh size represents our most recent run to-date. These numbers point to a possible superconducting instability of \( E_{g} \) symmetry, but the results have not converged enough for us to be sure. As a rough guide, using the numbers for \( 25 \leq n_{\text{mesh}} \leq 47 \) would give \( \langle \Gamma \rangle_{E_{g}}/T_{\eta} \approx -0.163 \pm 0.054 \). The values for parameter set (b) have a surpris-
ingly large fluctuation at \( n_{\text{mesh}} = 31 \), which makes it very difficult to make any conclusion for \( n_{\text{mesh}} \leq 35 \).

It is clear from the results gathered so far, that the \( T_{1g} \) pairing state is the most likely candidate for a pairing instability in cubic symmetry. So the reader can actually see some of the numbers, all the results for mean field parameter set (a) are presented in Table 5.7. The look-up table for a run with \( n_{\text{mesh}} = 49 \) requires about a week of run time (in background and at an appropriate niceness level) on a DEC5100.

5.6 Discussion

As we have said, \( n_{\text{mesh}} = 50 \) is most likely a practical limit on the size of the Bosonic self-energy mesh that we could run on a local machine. We have been able to run up to \( n_{\text{mesh}} = 47 \), so far. It is admittedly disappointing that we can not come to a definite conclusion about pairing instabilities for all the symmetry channels of cubic symmetry, but it is not surprising. After all, we know that there are clear fluctuations in the functions \( I_{ss}, I_{s\lambda}, \) and \( I_{\lambda\lambda} \) for \( n_{\text{mesh}} \approx 80 \). As we discussed, such variations are due to the anisotropic matrix elements in the principal value integrals over the Brillouin zone. The zone is divided into a large number of tetrahedra \( (8 \times (n_{\text{mesh}})^3 \) to be exact), and the matrix elements are assumed constant inside a given tetrahedron. If the matrix elements are sharply peaked in some region of the Brillouin zone, then it is easy to see how fluctuations can occur. If the mesh is constructed so that the matrix elements are evaluated very near the peak, then only a small shift in the mesh is required before the matrix elements will be evaluated at a point far down on the sides of the peak. Thus a small change in mesh size could result in a large change in
Figure 5.7:

Fermi surface averages in the $A_{1g}$ and $T_{2g}$ pairing channels of the scattering amplitude, $\langle \Gamma \rangle / T_{07}$, as a function of the Boson mesh parameter $n_{\text{mesh}}$. $8n_{\text{mesh}}^2$ equals the number of tetrahedra used in the Brillouin zone integrals for the Bosonic Green functions. These data are for mean field parameter set (a). (See Table 5.3.)

- The horizontal line marked by $T_{2g,\text{local}}$ denotes the size of the local contribution to the average in the $T_{2g}$ channel. The corresponding local ("hard-core") contribution for the $A_{1g}$ channel is 3.54 and would be just above the top of the graph. We see that the nonlocal contribution in the $T_{2g}$ channel is of the same size as the local contribution. Even with the fluctuation at $n_{\text{mesh}}=23$, it seems unlikely there is a pairing instability of $T_{2g}$ symmetry.

- In the $A_{1g}$ channel, even with the large fluctuation for $n_{\text{mesh}}=39$, there is clearly no pairing instability.
Figure 5.8:
Fermi surface averages in the $E_{1g}$ and $T_{1g}$ pairing channels of the scattering amplitude, $(\Gamma)/T_{07}$, as a function of the Boson mesh parameter $n_{\text{mesh}}$. These data are for mean field parameter set (a). The solid (dashed) horizontal line denotes the local ("hard-core") contribution to the average in the $E_g$ ($T_{1g}$) channel.

- Although not yet converged, the averages in the $T_{1g}$ channel point to the possibility of a pairing instability. Averaging the values of $(\Gamma)_{T_{1g}}/T_{07}$ for all the values of $n_{\text{mesh}}$ used here yields

$$\frac{(\Gamma)_{T_{1g}}}{T_{07}} = -0.212 \pm 0.025.$$

- In the $E_g$ channel, there is a large fluctuation at $n_{\text{mesh}}=39$. Therefore, we are nervous at saying there is a superconducting instability here. However, it is clear that the average interactions in this channel are attractive for a relatively wide range of mesh sizes: $25 \leq n_{\text{mesh}} \leq 47$. 
Figure 5.9:

Fermi surface averages in the $A_{1g}$ and $T_{2g}$ pairing channels of the scattering amplitude, $(\Gamma')/T_{\sigma\tau}$, as a function of the Boson mesh parameter $n_{\text{mesh}}$. $(8n_{\text{mesh}}^3$ equals the number of tetrahedra used in the Brillouin zone integrals for the Bosonic Green functions.) These data are for mean field parameter set (b).

- In the $T_{2g}$ channel, the horizontal, dashed line denotes the local contribution to the average. The fluctuations in the full average are at least a factor of two larger than the local part and are also varying about zero. Thus it is not possible to say, from the present data, if there is a $T_{2g}$ instability or not. Using the results from parameter set (a), however, it still seems unlikely that there is an instability in this channel.
- In the $A_{1g}$ channel, it is easy to see that there average interactions are repulsive and strong. There is no instability in this channel.
Figure 5.10:
Fermi surface averages in the $E_{1g}$ and $T_{1g}$ pairing channels of the scattering amplitude, $(\Gamma)/T_{07}$, as a function of the Boson mesh parameter $n_{\text{mesh}}$. These data are for mean field parameter set (b).

- In the $E_g$ channel, the horizontal line denotes the contribution to the average in the local limit. For the full average, up to $n_{\text{mesh}}=31$, the average value is fluctuating evenly about the local value. The surprisingly large fluctuation at $n_{\text{mesh}}=31$, however, makes it impossible to tell if there is an instability in this channel.

- In the $T_{1g}$ channel, the full average, although fluctuating, remains negative for $21 \leq n_{\text{mesh}} \leq 41$. Averaging these values gives a result of

$$\frac{(\Gamma)_{T_{1g}}}{T_{07}} = -0.226 \pm 0.049.$$
Table 5.8:

Values of $\langle \Gamma \rangle_{\eta}/T_{\eta}$ as a function of self-energy mesh parameter, $n_{mesh}$, for mean field parameter set (a). These data were used to produce figures 5.7 and 5.8.

<table>
<thead>
<tr>
<th>$n_{mesh}$</th>
<th>$A_{1g}$</th>
<th>$E_g$</th>
<th>$T_{1g}$</th>
<th>$T_{2g}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>17</td>
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<td>0.170</td>
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<td>-0.240</td>
<td>-0.484</td>
</tr>
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<td>-0.030</td>
<td>-0.119</td>
<td>0.095</td>
</tr>
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<td>-0.112</td>
<td>-0.311</td>
<td>0.214</td>
</tr>
<tr>
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<td>1.23</td>
<td>-0.034</td>
<td>-0.086</td>
<td>0.145</td>
</tr>
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<td>-0.146</td>
<td>-0.138</td>
<td>0.134</td>
</tr>
<tr>
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<td>-0.049</td>
<td>-0.187</td>
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<td>0.200</td>
</tr>
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<td>37</td>
<td>1.23</td>
<td>-0.149</td>
<td>-0.237</td>
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<td>-0.729</td>
<td>-0.217</td>
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<td>41</td>
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</tr>
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</tr>
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<td>45</td>
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<td>1.41</td>
<td>-0.130</td>
<td>-0.251</td>
<td>0.236</td>
</tr>
</tbody>
</table>
the evaluated matrix elements. A similar problem can arise in finite size lattice problems, where large variations in results can persist up to very large system sizes[16]. The solution for that particular problem is an average over boundary conditions. Our problem, unfortunately, has no such cure, and we must live with reasonable conclusions from the data we are able to gather.

To reiterate, we have been able to draw the following conclusions, based on self-energy meshes of the size $n_{mesh} = 47$:

- Quasiparticle interactions are strong and repulsive in the $A_{1g}$ ("s-wave") pairing channel.
- A pairing instability of $T_{2g}$ ($d_{xy}, d_{xz}, d_{yz}$) symmetry also appears highly unlikely.
- The best candidate for an instability appears to be in the state in which the quasiparticles pair up in a state of $T_{1g}$ symmetry, with $\langle \Gamma \rangle_{T_{1g}}/T_{07} = 0.212 \pm 0.025$.
- The $E_g$ channel ($d_{z^2-r^2}, d_{3z^2-r^2}$) also shows signs (albeit weak) of an instability, with $\langle \Gamma \rangle_{E_g}/T_{07} = -0.163 \pm 0.054$. The evidence here is weaker than in the $T_{1g}$ case.

Using equation 5.12 for the superconducting transition temperature within a given representation, $\eta$, we find

$$T_c(\eta = T_{1g}) = 1.13T_{07}e^{T_{07}/(\langle \Gamma \rangle_{T_{1g}})} \approx 0.09 \ K,$$

which is almost an order of magnitude too small for CeCu$_2$Si$_2$. Note, however, that our average interaction,

$$\frac{\langle \Gamma \rangle_{T_{1g}}}{T_{07}} = -0.212,$$

is considerably larger than the result of Lavagna, Millis, and P. Lee[14] for the
SU(N) model,

\[
\frac{\langle \Gamma \rangle_{d\text{-wave}}}{T_0} \approx \frac{-0.01}{N} = -1.67 \times 10^{-3}. \tag{5.88}
\]

The last number in the equality results from taking \( N = 6 \).

Another issue which we would like to address in this discussion is that of strong versus weak coupling calculations. In the case of heavy Fermions, the effective Fermi temperature is of the order of the Kondo temperature, which is also the energy scale of importance for the superconducting glue. That is, on physical grounds there is no reason to believe that only a very thin energy shell about the Fermi surface is of importance for superconductivity. Thus, a calculation including the energy dependence of the scattering amplitude should be done, as opposed to just an average over the Fermi surface. Given the complexity of the static problem, however, putting the dynamics of the slave Bosons into the problem is not feasible. This does not necessarily mean that the pairing instabilities found in the static problem have no meaning. We shall discuss, generally, why this is so.

It is conventional wisdom[17], that near the Fermi surface the quasiparticle self-energy for heavy Fermions is strongly frequency dependent but only weakly dependent on the magnitude of the momentum, \(|\vec{k}|\). This can be understood intuitively as follows. The characteristic energy scale for the quasiparticles is the Kondo temperature, \( T_{o7} \), which is about 10K. A typical degeneracy temperature for a metal is \( T_F \approx 10,000 \text{K} \). The characteristic momentum, however, is set by the Fermi wavevector, \( k_F \), which for CeCu$_2$Si$_2$ is the size of a typical metal. Thus, broadly speaking, we expect the quasiparticle self-energy, \( \Sigma \), to behave (near the Fermi surface) as

\[
\frac{\partial \Sigma}{\partial \omega} \approx \mathcal{O}\left(\frac{\Sigma}{T_{o7}}\right),
\]
\[ \frac{\partial \Sigma}{\partial \xi_k} \approx \mathcal{O}\left(\frac{\Sigma}{D}\right), \]

where \( D \) is the bandwidth of the conduction band. Then, since

\[ \frac{\partial \Sigma}{\partial \omega} \gg \frac{\partial \Sigma}{\partial \xi_k}, \]

it seems reasonable to ignore the momentum dependence of the self-energy. This intuitive result was reinforced by Millis and Lee\cite{29}, who found (in the SU\((N)\) model) that the momentum dependence of the imaginary part of the conduction electron self-energy (at order \(1/N\)) is very weak (going as \(1/N^2\)), while the frequency dependence depends inversely on the Kondo scale.

If one accepts the dominance of the frequency dependence in the quasiparticle self-energy, then it seems reasonable to assume that including such dependence in a strong coupling calculation (ala McMillan\cite{25}) would serve only to reduce the transition temperature, \( T_c \). We do not believe, furthermore, that the sign of the average scattering amplitude, \( \Gamma_\eta \), would be affected by such frequency dependence. Thus, our conclusions about which pairing channels, \( \eta \), show a superconducting instability should not be changed as the result of a strong coupling calculation.

Please note that we are not saying that the reduction of the transition temperature due to the frequency dependence of the residual quasiparticle interactions would be identical in structure to the case of electron-phonon coupling\cite{25}. We can only say now that we expect \( T_c \) to be reduced; we can not give an estimate of how large the reduction would be.

The superconducting instabilities themselves appear to be based heavily on the underlying symmetry of the problem, which does not care if one performs a strong or weak coupling calculation. The fact that our estimated (weak-coupling)
transition temperature for the $T_{1g}$ pairing instability is smaller than the measured value for CeCu$_2$Si$_2$, is not a terrible surprise. The major purpose of this calculation has not been to give a precise numerical recipe for calculating the $T_c$ of heavy Fermion systems. We wished to study the importance of local, or "multiplet", physics upon quasiparticle interactions. Thus the author feels that a weak coupling calculation has been sufficient.
Chapter V REFERENCES


28. I thank John Wilkins for suggesting this calculation.

CHAPTER VI

Conclusions and Directions for Future Work

6.1 Summary

In this thesis, we have calculated quasiparticle interactions within the infinite-U Anderson lattice, looking specifically for signs of a superconducting instability. The 4f sites in this model were chosen to reflect the splitting of a $J=5/2$ spin-orbit coupled multiplet in the presence of crystal electric fields of cubic symmetry. The result is a $\Gamma_7$ doublet and a $\Gamma_8$ quartet at each 4f site, and we have chosen the $\Gamma_7$ doublet having the lower energy. The crystal field splitting was fixed at $\Delta_{CEF}=360$ K, to be indicative of the splitting seen by inelastic neutron scattering in CeCu$_2$Si$_2$ [1].

We used slave-Bosons to represent the 4f$^0$ configuration and calculated the necessary Green functions within the functional integral formalism. We summarize our work as follows:

• At the mean field level, we require that the free energy be a minimum with respect to the magnitude and phase of the slave-Boson fields. This produces a
set of coupled integral equations, which we solved numerically as a function of
the following parameters: the bare hybridization strength, $V_0$; the unshifted $\Gamma_7$
($\Gamma_8$) multiplet energy, $E_7$ ($E_8$); the crystal field splitting, $\Delta_{CEF} = E_8 - E_7$; and
the lower edge for the conduction band in the absence of hybridization, $-D$. The
self-consistent solutions give the following new parameters: the quasiparticle
chemical potential, $\mu$; the shifted $\Gamma_7$ ($\Gamma_8$) multiplet energy, $\epsilon_7$ ($\epsilon_8$); and the
hybridization renormalization coefficient, $s_0$. We solved the mean field equations
for two different sets of initial parameters, both sets yielding (approximately)
Kondo temperatures of about 10 K. These mean field results are summarized in
Table 6.1. See sections 3.73 and 3.74 for details.

- We calculated the slave-Boson Green function, including self-energy contributions from particle-hole bubbles composed of conduction and $4f$ electron Green functions. The resulting expressions for the dressed Boson Green functions contain principal value integrals that must be evaluated over the cubic Brillouin zone. These integrals contain effective matrix elements in the numerator, which are anisotropic functions and can vary in complicated ways throughout the zone. We used the so-called analytic tetrahedron method to handle the principal value nature of the integral and discovered that, because of the anisotropic matrix elements, the integrals are extremely slow to converge, requiring of the order of $8 \times 80^3$ tetrahedra. See sections 4.3.3 and 4.3.4.

- We found that the normalization function, $A^2(k)$, for quasiparticle states is
  highly anisotropic in k-space. This is the first time (to our knowledge) that such
  an anisotropic function has been used in the calculation of quasiparticle inter-
  actions in the Anderson lattice. Any calculation assuming spherical symmetry
Table 6.1:
Self-consistent mean field parameter sets, labeled as (a) and (b). At mean field there are three coupled integral equations, which are solved self-consistently. The input parameters are: the bare hybridization strength, $V_0$; the lower edge of the conduction electron band in the absence of hybridization, -D; the total number of electrons, $n_{\text{total}} = n_{\text{cond}} + n_f$, per unit cell; the bare, or unshifted, energy of the $\Gamma_7$ ($E_7$) and the $\Gamma_8$ ($E_8 = E_7 + \Delta_{\text{CEF}}$) multiplets; and the fixed crystal field splitting, $\Delta_{\text{CEF}} = 360$ K. The self-consistent parameters which solve the equations are: the hybridization renormalization coefficient, $s_0$, where the mean field renormalized hybridization is $s_0 V_0$; the shifted $\Gamma_7$ ($\epsilon_7$) and $\Gamma_8$ ($\epsilon_8 = \epsilon_7 + \Delta_{\text{CEF}}$) multiplet energies; the quasiparticle chemical potential, $\mu$; and the Kondo temperature $T_{\text{K}} \equiv \epsilon_7 - \mu$ of the $\Gamma_7$ doublet. In both parameters sets the total number of particles was fixed at $n_{\text{total}}=1.5$. And the input parameters were chosen to give approximate Kondo temperatures of 10 K, i.e. $T_{\text{K}} \approx 10$ K. All energies are measured relative the chemical potential in the absence of hybridization. In both parameter sets, $\Delta_{\text{CEF}}=360$ K, and the unshifted $\Gamma_7$ energy is $E_7=-2.0$ eV.

<table>
<thead>
<tr>
<th>parameter set</th>
<th>$V_0$ (eV)</th>
<th>$s_0$</th>
<th>$\epsilon_7$ (eV)</th>
<th>$\mu$ (eV)</th>
<th>$T_{\text{K}}$ (K)</th>
<th>$D$ (eV)</th>
</tr>
</thead>
<tbody>
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<td>a</td>
<td>0.8595</td>
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<td>0.0217648</td>
<td>0.0208399</td>
<td>9.25</td>
<td>2.4405</td>
</tr>
<tr>
<td>b</td>
<td>0.650</td>
<td>0.142409</td>
<td>-0.8437021</td>
<td>-0.844999</td>
<td>13.0</td>
<td>3.33856</td>
</tr>
</tbody>
</table>
at the $4f$ sites would yield an isotropic normalization function. The anisotropy in our problem arises from the lowering of the symmetry from spherical to cubic. The function $A_1^2(\vec{k})$ is strongly peaked at the six points we call hot-spots, where the axes of the cubic Brillouin zone intersect the (assumed) spherical Fermi surface. The width of these peaks is determined completely by the ratio of the Kondo temperatures for the two multiplet $(T_{07}/T_{08}) \approx (T_{07}/\Delta_{CEF})$. We have also determined that these hot-spots are very important in determining the local interactions between two quasiparticle in a state of $E_g$ ($d_{x^2-y^2}, d_{3z^2-r^2}$) symmetry. See section 5.4.1.

- We have calculated the quasiparticle scattering amplitude, $\Gamma_{QP}(\vec{k}, \vec{k}')$, which describes the interaction of two quasiparticles at the Fermi surface via the exchange of a dressed slave Boson. We project $\Gamma_{QP}$ onto the so-called cubic harmonics and average over a spherical Fermi surface. We find it useful to consider two cases: in the first case, we ignore the momentum dependence of the slave Boson Green function (what we call the local limit); and the second case includes the full Boson Green function. In the local limit, we find that the average interactions are (see sections 5.4.2 and 5.4.3):
  - in the $A_{1g}$ limit, repulsive and large;
  - in the $E_g$ limit, due to the anisotropic normalization function (i.e. the hot-spots), attractive and weak;
  - in the $T_{1g}$ and $T_{2g}$ channels, repulsive and weak.

The second case, with the full momentum dependence of the slave Boson Green function, is slow to converge as the number of tetrahedra (used to calculate the Boson Green function) is increased. This slow convergence allows us to make only qualitative conclusions about possible superconducting instabilities in the
model. Here is what we can say:

• in the $A_{1g}$ channel, we found repulsive quasiparticle interactions and hence no chance for a superconducting instability;
• there is weak evidence for a pairing instability of $E_g$ instability;
• the best candidate for a pairing instability is in the $T_{1g}$ channel, where the average interactions have a strength

\[
\frac{\langle \Gamma \rangle_{T_{1g}}}{T_c} = -0.212 \pm 0.025,
\]

which would give a superconducting transition temperature of $T_c = 0.09$ K. This is almost an order of magnitude too small to describe the heavy Fermion superconductor CeCu$_2$Si$_2$, which has a $T_c$ of about 0.6 K. We do not put too much emphasis on an exact calculation of $T_c$ here, since we still have to check the robustness of the results as a function of the number of tetrahedra in the Boson Green function mesh. We have found that large fluctuations can still occur for numbers of tetrahedra of the order of $8 \times 10^3$, and so we are running the code for as many tetrahedra as we are able to use; we will probably be limited to a maximum of about $8 \times 50^3$ tetrahedra. See sections 5.5.1 and 5.5.2.

6.2 Directions for Future Work

This calculation has taught us a great deal about the hidden complexities in a realistic $1/N$ calculation for the Anderson lattice. The anisotropic hybridization matrix elements under cubic symmetry have made the calculation of the static dressed (to order $1/N$) Boson propagator extremely difficult. It is clear that diagrams of order $1/N^2$ are intractable with our present procedure. This is a shame, since the $1/N^2$ diagrams are the first ones were spin fluctuations (RKKY
interactions) start to enter into the picture. Since the competition between magnetic ordering and superconductivity is a major piece of physics in heavy Fermions, it would be nice to have a microscopic calculation of $1/N^2$ diagrams in the presence of an anisotropic hybridization. One possibly tractable calculation could be the extension of Zhang and T. K. Lee's[2] work to order $1/N^2$. Zhang and Lee, let it be recalled, used a Coqblin-Schrieffer hybridization in the presence of spherical symmetry. Thus, if the $1/N^2$ diagrams could be calculated, this would be a more realistic result than that of Houghton, Read, and Won[3], who did the calculation for the completely isotropic SU(N) ("spherical cow") model.

If one is determined to study the effects of crystal fields upon quasiparticle interactions at order $1/N^2$ the author feels (in the absence of very powerful computing capabilities—such as with a CM5) a whole new angle of attack is required.

The calculation (including the crystal fields) for quasiparticles in the odd-parity pairing channel should also be performed. It is possible that an odd-parity state could have an overall stronger attraction than the even-parity states. One never knows until one checks. Of course, we have looked at only the even-parity states in this thesis, because we believe the experimental evidence for CeCu$_2$Si$_2$ points to even-parity pairing. It would be prudent, if one were going to study the odd-parity pairing states, to begin by first performing the calculation without crystal field splitting (but with anisotropic hybridization). This amounts to doing the Zhang and Lee calculation in the odd-parity channel. The knowledge gained from such a calculation could be useful in the crystal field problem.

Along slightly different lines, one could also apply the weak-coupling, $1/N$ calculation to other Ce systems, such as CeAl$_3$, which are not superconducting.
One could then ask, does the underlying symmetry of the system (hexagonal for CeAl₃) result in averaged quasiparticle interactions that show no pairing instabilities? If the averaged interactions do indeed show no instabilities, then it is a nice piece of evidence for the argument that the local, or "multiplet" physics is fundamental to the superconductivity in (at least Ce based) heavy Fermions.
Chapter VI REFERENCES


APPENDIX A: Matsubara sum for the Mean Field Free Energy

In this appendix, we shall sum over the Fermionic Matsubara frequencies, 
\( i\omega_n = i(2n + 1)\pi/\beta \), that arise in the mean field Free energy. (See equation 3.76.) After tracing over the Grassmann fields, we saw in Chapter 3 that the partition function took the form

\[
Z_{MF} = Z_{cond} \int D\mathcal{S} D\lambda 
\times \exp \left[ \text{Tr} \ln G^{-1}_{\Gamma \alpha \Gamma' \alpha'}(\vec{k}, i\omega_n) - \frac{\beta N_s}{2} \sum_{\Gamma} N_{\Gamma} i\lambda_{\alpha} \left( \delta_{\alpha \Gamma}^2 - q_{\alpha \Gamma} \right) \right], \quad (A.1)
\]

where \( Z_{cond} \) is the conduction electron contribution to the partition function, and \( G_{\Gamma \alpha \Gamma' \alpha'} \) is the hybridization dressed 4f Green function. We calculated this dressed propagator from its matrix Dyson's equation and found

\[
G_{\Gamma \alpha \Gamma' \alpha'}(\vec{k}, z) = \frac{1}{z - \epsilon_{\Gamma}} \left[ \delta_{\Gamma \Gamma'} \delta_{\alpha \alpha'} + \frac{1}{z - \epsilon_{\Gamma'}} \left( \frac{(z - \epsilon_{\Gamma})(z - \epsilon_{\Gamma'})}{(z - E_{1k})(z - E_{2k})(z - E_{3k})} \right) \right], \quad (A.2)
\]

where \( E_{n\vec{k}} \) is the quasiparticle energy for the \( n \)-th band. We thus are faced with the following sum to perform:

\[
\sum_{i\omega_n} \ln G^{-1}_{\Gamma \alpha \Gamma' \alpha'}(\vec{k}, i\omega_n), \quad (A.3)
\]
which we do by the standard procedure of calculating a related contour integral. That is, we integrate in the complex plane over the contour C shown in Figure A.1

\[ \text{Tr} \oint \frac{dz}{2\pi i} f(z) \ln G_{\Gamma_0\Gamma'_{\sigma'}}^{-1}(\vec{k}, z), \quad (A.4) \]

where \( f(z) \) is the usual Femi function. Since the trace is invariant under a unitary transformation, we shall work in the quasiparticle basis, in which \( G_{\Gamma_0\Gamma'_{\sigma'}}^{-1} \) is diagonal and is a function only of the band energies, \( E_n(\vec{k}) \). Then we can write

\[ \text{Tr} \ln G_{\Gamma_0\Gamma'_{\sigma'}}^{-1}(\vec{k}, z) \]

as \( \ln \det G_{n\sigma}^{-1}(\vec{k}, z) \), where \( n \) is the band index and \( \sigma \) is the pseudo-spin index. Further, if \( z = E_n(\vec{k}) \), then \( \det G_{n\sigma}^{-1}(\vec{k}, E_n) = 0 \), since

\[ G_{n\sigma}^{-1} = \begin{bmatrix} z - E_{1\vec{k}} & 0 & 0 \\ 0 & z - E_{2\vec{k}} & 0 \\ 0 & 0 & z - E_{3\vec{k}} \end{bmatrix}. \]

(For simplicity, the two-fold pseudo-spin degeneracy is not show in this matrix.)

To integrate the logarithm we take a branch cut along the line defined by

\[ \text{Re} \left[ \det G_{n\sigma}^{-1}(\vec{k}, E_n) \right] \leq 0 \quad \text{and} \quad \text{Im} \left[ \det G_{n\sigma}^{-1}(\vec{k}, E_n) \right] = 0. \quad (A.5) \]

For a given \( n \) and \( \vec{k} \), the point \( z \) on the real axis where \( z = E_n(\vec{k}) \) is the end point of the branch cut. That is, the branch cut is for all real \( z \) so that \( |z| \leq E_n(\vec{k}) \) (see Figure A.1). Across the cut, the argument of the log has a discontinuity of \( 2\pi i \).

Performing the integral

\[ \text{Tr} \oint \frac{dz}{2\pi i} f(z) \ln \det G_{n\sigma}^{-1}(\vec{k}, z) = -\frac{1}{\beta} \text{Tr} \sum_{\omega_n} \ln \det G_{n\sigma}^{-1}(\vec{k}, i\omega) = \]

\[ = \int_{-D}^{E_{n\vec{k}}} \frac{dz}{2\pi i} f(z) \left[ \text{Arg}(z + i\delta) - \text{Arg}(z - i\delta) \right] \]

\[ = \int_{-D}^{E_{n\vec{k}}} dz f(z), \quad (A.6) \]
Figure A.1:
The contour C for performing the Matsubara sum of equation 3.76. The dashed line represents the branch cut of the logarithm.

where we have to put a lower cut-off (−D) in the integral, and where the large semicircular portions of the contour C do not contribute because they are damped out by the Fermi function, f(z). The integral remaining in equation A.6 yields

$$\ln\left(1 + e^{-\beta z}\right)\bigg|_{-D}^{E_n}$$

$$= \ln\left(1 + e^{-\beta E_n}\right) - \ln\left(1 + e^{-\beta D}\right). \quad (A.7)$$

The second term in equation A.7 gives rise to a multiplicative term in the partition function (call it $Z_D$). We can remove $Z_D$ by redefining the original partition function as $Z/Z_D$. Since this just amounts to shifting the zero of the energy scale, it is allowed [1].
APPENDIX A REFERENCES

APPENDIX B: Green Function Identities and the Gaussian Free Energy

B.1 Green Function Identities

This appendix discusses several identities used in Chapter 4 to simplify the expressions for the Bosonic self-energies. In Chapter 3 we found the hybridization dressed conduction Green function was

\[
G_\sigma(\vec{k}, i\omega) = \frac{(i\omega - \epsilon_\gamma)(i\omega - \epsilon_\delta)}{(i\omega - E_1)(i\omega - E_2)(i\omega - E_3)},
\]

(B.1)

where the band energies, \( E_n(\vec{k}) \), are function of \( \vec{k} \). It is useful to think of \( G_\sigma \) as a 2x2 (diagonal) matrix due to the spin degrees of freedom. Then from equation B.1 we can write

\[
G_\sigma^\dagger(\vec{k}, i\omega) = G_\sigma(\vec{k}, -i\omega).
\]

(B.2)

For the f Green function, we have

\[
G_{\Gamma\Gamma'\alpha\alpha'}(\vec{k}, i\omega) = \frac{1}{i\omega - \epsilon_\Gamma} \left[ \delta_{\Gamma\Gamma'}\delta_{\alpha\alpha'} + \frac{1}{i\omega - \epsilon_{\Gamma'}} \frac{(i\omega - \epsilon_\gamma)(i\omega - \epsilon_\delta)\hat{s}_\alpha \hat{s}_{\alpha'} \hat{V}_{\Gamma\alpha\sigma}^* \hat{V}_{\Gamma'\alpha'\sigma'}}{(i\omega - E_1)(i\omega - E_2)(i\omega - E_3)} \right],
\]

(B.3)
which is a $6 \times 6$ matrix due to the crystal field degrees of freedom. Taking the hermitian conjugate of B.3 yields

$$G_{\Gamma \alpha \Gamma' \alpha'}^\dagger(\vec{k}, i\omega) = G_{\Gamma' \alpha' \Gamma \alpha}(\vec{k}, -i\omega).$$

(B.4)

To study the hermitian conjugate of the mixing Green function, we return to the definition

$$G_{\Gamma \alpha \sigma}(\vec{k}, \tau_1 - \tau_2) = -(f_{\vec{k} \Gamma \alpha}(\tau_1) c_{\vec{k} \sigma}^\dagger(\tau_2)),$$

(B.5)

where we assume that $\tau_1 > \tau_2$. Recalling that $[f_{\vec{k} \Gamma \alpha}(\tau_1)]^\dagger = f_{\vec{k} \Gamma \alpha}^\dagger(-\tau_1)$, which is also true for the conduction electron creation operator, we find that

$$G_{\Gamma \alpha \sigma}^\dagger(\vec{k}, \tau_1 - \tau_2) = -(c_{\vec{k} \sigma}(-\tau_2) f_{\vec{k} \Gamma \alpha}^\dagger(-\tau_1))$$

(B.6)

$$= G_{\sigma \Gamma \alpha}(\vec{k}, -\tau_2 + \tau_1).$$

(B.7)

Writing equation B.7 in terms of Matsubara frequencies,

$$\frac{1}{\beta} \sum_n G_{\Gamma \alpha \sigma}^\dagger(\vec{k}, i\omega_n)e^{-i\omega_n(\tau_1 - \tau_2)} = \frac{1}{\beta} \sum_n G_{\sigma \Gamma \alpha}(\vec{k}, i\omega_n)e^{i\omega_n(\tau_1 - \tau_2)}.$$  

(B.8)

Letting $i\omega_n \to -i\omega_n$ on the right side leads to

$$G_{\Gamma \alpha \sigma}^\dagger(\vec{k}, i\omega) = G_{\sigma \Gamma \alpha}(\vec{k}, -i\omega),$$

(B.9)

where $G_{\Gamma \alpha \sigma}$ is a $6 \times 2$ matrix and $G_{\sigma \Gamma \alpha}$ is a $2 \times 6$ matrix.

Next, we remind the reader of the result from Chapter 3 (equation 3.73) for the mixing Green function,

$$G_{\Gamma \alpha \sigma}(\vec{k}, i\omega) = G_{\Gamma \alpha}(i\omega)\tilde{V}_{\Gamma \alpha \sigma}(\vec{k})\tilde{s}_{\sigma \Gamma}G_{\sigma}(\vec{k}, i\omega).$$

(B.10)

Using equations B.9-B.4, we have

$$G_{\Gamma \alpha \sigma}^\dagger(\vec{k}, i\omega) = G_{\sigma \Gamma \alpha}(\vec{k}, -i\omega) = G_{\sigma}(\vec{k}, i\omega)\tilde{s}_{\sigma \Gamma}^\dagger\tilde{V}_{\sigma \Gamma \alpha}(\vec{k})G_{\Gamma \alpha}(i\omega)$$
where \( G_{\Gamma\alpha}(i\omega) = 1/(i\omega - \epsilon_{f}) \).

In Chapter 3, we calculated the Green function \( G_{\Gamma\sigma\alpha} \) by the equation of motion technique. We can do the same to calculate \( G_{\sigma\Gamma\alpha} \). Since the procedure is the same as that already used, we will just give the result:

\[
G_{\sigma\Gamma\alpha}(k, i\omega) = G_{\sigma\alpha}(k, i\omega)\delta_{\sigma\Gamma} V_{\sigma\Gamma\alpha}(k) G_{\Gamma\alpha}(i\omega),
\]

(B.11)

where \( G_{\sigma\alpha} = 1/(i\omega - \xi_{k}) \). There is an implied sum over \( \Gamma' \) and \( \alpha' \). This is sufficient for us to proceed with the evaluation in Chapter 4.

### B.2 Derivation of the Quadratic Action

Starting with equations 4.17, we expand the second logarithm to second order in the Bose fluctuations, \( \delta\tilde{s}_{\pi} \) and \( \delta\lambda_{\pi} \). The result is

\[
\text{Tr} \left[ G_{\Gamma'\alpha'\alpha}(\bar{k} - \bar{q}, i\omega - iv)\delta\tilde{s}_{\pi'}(iv)G_{\Gamma'\alpha'\alpha}(\bar{k}, i\omega)\delta\tilde{s}_{-\pi'}(iv) \right]
\]

\[
+ \frac{1}{2} G_{\Gamma'\alpha'\alpha}(\bar{k} - \bar{q}, i\omega - iv)G_{\Gamma'\alpha'\alpha}(\bar{k}, i\omega)\delta\tilde{s}_{\pi'}(iv) G_{\Gamma'\alpha'\alpha}(\bar{k} - \bar{q}, i\omega - iv)G_{\Gamma'\alpha'\alpha}(\bar{k}, i\omega)
\]

\[
\times G_{\Gamma'\alpha'\alpha}(\bar{k}, i\omega)\delta\tilde{s}_{-\pi'}(iv) \]

\[
+ \frac{1}{2} G_{\Gamma'\alpha'\alpha}(\bar{k} - \bar{q}, i\omega - iv)G_{\Gamma'\alpha'\alpha}(\bar{k}, i\omega)\delta\tilde{s}_{\pi'}(iv) G_{\Gamma'\alpha'\alpha}(\bar{k} - \bar{q}, i\omega - iv)G_{\Gamma'\alpha'\alpha}(\bar{k}, i\omega)
\]

\[
\times G_{\Gamma'\alpha'\alpha}(\bar{k}, i\omega)\delta\tilde{s}_{-\pi'}(iv) \]

\[
+ \frac{1}{2} G_{\Gamma'\alpha'\alpha}(\bar{k} - \bar{q}, i\omega - iv)G_{\Gamma'\alpha'\alpha}(\bar{k}, i\omega)\delta\tilde{s}_{\pi'}(iv) G_{\Gamma'\alpha'\alpha}(\bar{k} - \bar{q}, i\omega - iv)G_{\Gamma'\alpha'\alpha}(\bar{k}, i\omega)
\]

\[
\times G_{\Gamma'\alpha'\alpha}(\bar{k}, i\omega)\delta\tilde{s}_{-\pi'}(iv) \]

\[
+ \frac{1}{2} G_{\Gamma'\alpha'\alpha}(\bar{k} - \bar{q}, i\omega - iv)G_{\Gamma'\alpha'\alpha}(\bar{k}, i\omega)\delta\tilde{s}_{\pi'}(iv) G_{\Gamma'\alpha'\alpha}(\bar{k} - \bar{q}, i\omega - iv)G_{\Gamma'\alpha'\alpha}(\bar{k}, i\omega)
\]

\[
\times G_{\Gamma'\alpha'\alpha}(\bar{k}, i\omega)\delta\tilde{s}_{-\pi'}(iv) \]
\[
\begin{align*}
\times & \mathcal{G}_{\Gamma}^{C,\alpha,\mu,\nu,\sigma}(\vec{k}, i\omega) G_{\Gamma''\alpha,\mu,\nu,\sigma}(\vec{k}, i\omega) \delta s_{-\sigma^T}(-i\nu) \\
+ & \frac{1}{2} G_{\Gamma\alpha,\gamma,\rho}(\vec{k}, i\omega - i\nu) i\delta \lambda (i\nu) G_{\Gamma''\alpha,\gamma,\rho}(\vec{k}, i\omega) G_{\Gamma''\alpha,\gamma,\rho}(\vec{k}, i\omega) \delta s_{-\sigma^T}(-i\nu) \\
+ & \frac{1}{2} G_{\Gamma\alpha,\gamma,\rho}(\vec{k}, i\omega - i\nu) i\delta \lambda (i\nu) G_{\Gamma''\alpha,\gamma,\rho}(\vec{k}, i\omega) \delta s_{-\sigma^T}(-i\nu) G_{\Gamma''\alpha,\gamma,\rho}(\vec{k}, i\omega) \delta \lambda (-i\nu) \\
+ & \frac{1}{2} G_{\Gamma\alpha,\gamma,\rho}(\vec{k}, i\omega - i\nu) \delta s_{-\sigma^T}(-i\nu) G_{\Gamma''\alpha,\gamma,\rho}(\vec{k}, i\omega) \delta \lambda (-i\nu) \\
+ & \frac{1}{2} G_{\Gamma\alpha,\gamma,\rho}(\vec{k}, i\omega - i\nu) i\delta \lambda (i\nu) G_{\Gamma''\alpha,\gamma,\rho}(\vec{k}, i\omega) i\delta \lambda (-i\nu) \bigg].
\end{align*}
\]

For convenience, we present again the definitions of the functions $\mathcal{G}^A$, $\mathcal{G}^B$, and $\mathcal{G}^C$:

\[
\begin{align*}
\mathcal{G}_{\Gamma\alpha,\gamma,\rho}^{A}(\vec{k}, i\omega) \equiv & \sum_{\sigma} \tilde{V}_{\Gamma\alpha,\sigma}^{*}(\vec{k}) G_{\sigma,\alpha}(\vec{k}, i\omega) \tilde{V}_{\sigma,\gamma,\rho}(\vec{k}), \\
\mathcal{G}_{\Gamma\alpha,\gamma,\rho}^{B}(\vec{k}, i\omega) \equiv & \delta_{\sigma,\alpha} \mathcal{G}_{\Gamma\alpha,\gamma,\rho}^{A}(\vec{k}, i\omega), \\
\mathcal{G}_{\Gamma\alpha,\gamma,\rho}^{C}(\vec{k}, i\omega) \equiv & \mathcal{G}_{\Gamma\alpha,\gamma,\rho}^{A}(\vec{k}, i\omega) \delta_{\sigma,\alpha},
\end{align*}
\]

where $G_{\sigma,\alpha}(\vec{k}, i\omega) = 1/(i\omega - \xi_{\vec{k}})$.

We focus, first, on the $\delta s$ fields. We want to simplify the complicated terms above that are quadratic in $\delta s$. This requires the use of equations B.5 and B.12 proved in the first section of this appendix. In the expansion of equation B.13, we focus on the fourth term,

\[
\frac{1}{2} G_{\Gamma\alpha,\gamma,\rho}(\vec{k}, i\omega - i\nu) \delta s_{-\sigma^T}(-i\nu) G_{\Gamma''\alpha,\gamma,\rho,\nu}(\vec{k}, i\omega) G_{\Gamma''\alpha,\gamma,\rho}(\vec{k}, i\omega) \delta s_{-\sigma^T}(-i\nu).
\]

(B.17)

Substituting for $\mathcal{G}^C$ and $\mathcal{G}^B$ from equations B.16 and B.15, and dropping the momentum and frequency variables gives:

\[
\frac{1}{2} G_{\Gamma\alpha,\gamma,\rho} \delta s_{T^T,\sigma} \tilde{V}_{\Gamma\alpha,\sigma}^{*} G_{\sigma,\alpha} \tilde{V}_{\sigma,\gamma,\rho,\nu} \delta_{\sigma,\nu} G_{\Gamma''\alpha,\gamma,\rho,\nu} \delta s_{\sigma,\nu} \tilde{V}_{\Gamma''\alpha,\sigma}^{*} G_{\sigma,\rho} \tilde{V}_{\sigma,\gamma,\rho} \delta s_{\sigma}.
\]

(B.18)
Next, use equation B.12 to write

\[ \frac{1}{2} G_{\Gamma \alpha^\prime \sigma^\prime} \delta \Gamma^\prime \tilde{V}_{\Gamma \alpha^\prime \sigma} G_{\alpha^\prime \sigma^\prime \sigma} \delta \Gamma^\prime \tilde{V}_{\Gamma \sigma^\prime \sigma} G_{\sigma \sigma^\prime} \tilde{V}_{\sigma \Gamma \sigma} \delta \Gamma. \]  \hspace{1cm} (B.19)

In the previous chapter, we defined the 2×2 matrix

\[ \gamma_{\sigma \sigma^\prime} \equiv \delta_{\sigma \sigma^\prime} \tilde{V}_{\sigma \sigma^\prime}, \]  \hspace{1cm} (B.20)

which is diagonal because of time-reversal symmetry. \( \gamma_{\sigma \sigma^\prime} \) should not be confused with the elementary vertices, \( \gamma_f \) and \( \gamma_{\text{mix}} \), already defined in this chapter, as the latter will always have the subscript \( f \) or \( \text{mix} \). From equations B.5 and B.20 we see that

\[ G_{\Gamma \mu^\prime \alpha^\prime \sigma^\prime} \delta \Gamma^\prime \tilde{V}_{\Gamma \mu^\prime \alpha^\prime \sigma^\prime} G_{\alpha^\prime \sigma^\prime \sigma^\prime} \delta \Gamma^\prime \tilde{V}_{\Gamma \sigma^\prime \sigma^\prime} G_{\sigma \sigma^\prime} \delta \Gamma^\prime \tilde{V}_{\sigma \Gamma \sigma^\prime} G_{\sigma \sigma^\prime} \delta \Gamma, \]

\[ = G_{\sigma \sigma^\prime}. \]

Equation B.19 now reduces to

\[ \frac{1}{2} G_{\Gamma \alpha^\prime \sigma^\prime} \delta \Gamma^\prime \tilde{V}_{\Gamma \alpha^\prime \sigma^\prime} G_{\sigma \sigma^\prime} \delta \Gamma^\prime \tilde{V}_{\sigma \Gamma \sigma^\prime} G_{\sigma \sigma^\prime} \delta \Gamma, \]  \hspace{1cm} (B.21)

since \( \gamma_{\sigma \sigma^\prime} \) is diagonal. Note that, by cyclic invariance of the trace, the third term of equation B.13 will give a result identical to equation B.21. Finally, combine the third and fourth terms with the first term of equation B.13 to get

\[ G_{\Gamma \alpha^\prime \sigma^\prime} \delta \Gamma^\prime \tilde{V}_{\Gamma \alpha^\prime \sigma^\prime} G_{\sigma \sigma^\prime} \delta \Gamma^\prime \tilde{V}_{\sigma \Gamma \sigma^\prime} G_{\sigma \sigma^\prime} \delta \Gamma, \]

\[ + G_{\Gamma \alpha^\prime \sigma^\prime} \delta \Gamma^\prime \tilde{V}_{\Gamma \alpha^\prime \sigma^\prime} G_{\sigma \sigma^\prime} \delta \Gamma^\prime \tilde{V}_{\sigma \Gamma \sigma^\prime} G_{\sigma \sigma^\prime} \delta \Gamma, \]

\[ = G_{\Gamma \alpha^\prime \sigma^\prime} \delta \Gamma^\prime \tilde{V}_{\Gamma \alpha^\prime \sigma^\prime} \left[ G_{\sigma \sigma^\prime} + G_{\sigma \sigma^\prime} \right] \tilde{V}_{\sigma \Gamma \sigma^\prime} \delta \Gamma. \]  \hspace{1cm} (B.22)
A diagram contributing to the $\Gamma_{ss,\Gamma'}(\vec{q},i\nu)$ vertex. The wavy line represents $\delta\tilde{s}_{\Gamma}(i\nu)$. All internal variables are summed over. The Fermion Green functions are the same as in figure 4.1.

In Chapter 3 we found that the bare and dressed conduction Green functions are related by

$$G_{\sigma\sigma} = G_{\sigma}(1 - \gamma)_{\sigma\sigma}. \quad (B.23)$$

Substituting equation B.23 into B.22, and writing the momentum and frequency dependence explicitly, yields

$$G_{\Gamma\Gamma'}(\vec{k},\vec{q},i\omega - i\nu)\delta\tilde{s}_{\Gamma}(i\nu)\tilde{V}_{\Gamma\Gamma'}(\vec{k})G_{\sigma}(\vec{k},i\omega)\tilde{V}_{\sigma\Gamma}(\vec{k})\delta\tilde{s}_{-\Gamma'}(-i\nu), \quad (B.24)$$

which is represented diagrammatically in Figure B.1 as a contribution to the s-component of $\Gamma_{ss,\Gamma'}(\vec{q},i\nu)$.

There are still two terms in equation B.13 that are quadratic in $\delta\tilde{s}$, the second and the fifth terms. From the defined functions $G^B$ and $G^C$, equations B.15 and B.16, and using the cyclic invariance of the trace, these two terms will give the same contribution to the action,

$$G_{\Gamma\Gamma'}(\vec{k},\vec{q},i\omega - i\nu)\tilde{s}_{\Gamma}(\vec{k})\tilde{V}_{\Gamma\Gamma'}(\vec{k})G_{\sigma}(\vec{k} - \vec{q},i\omega - i\nu)\tilde{V}_{\sigma\Gamma}(\vec{k} - \vec{q})$$
Figure B.2:

Another contribution to the vertex, $\Gamma_{ss',\Gamma'}(\vec{q}, i\nu)$. The symbols are the same as in figure 4.1. The combination dashed and solid line represents the mixing Green function $G_{\Gamma\sigma}$. Note there is no sum over $\Gamma$ and $\Gamma'$.

$$\times \delta\bar{\sigma}_{\Gamma'}(i\nu) G_{\Gamma^\nu \sigma' \sigma}^\alpha \bar{\sigma}_{\Gamma'}(\vec{k}, \bar{\nu}(i\nu)\delta_{s'}(\vec{k}) G_{\Gamma^\nu \sigma}^\alpha (\vec{k}, \bar{\nu}) V_{\sigma' \Gamma'}(\vec{k}) \delta\bar{\sigma}_{-\Gamma'}(-i\nu).$$

(B.25)

Using equation B.12, we can see that

$$G_{\Gamma\sigma}(\vec{k}, \bar{\nu}(i\nu)\delta_{s'}(\vec{k}) G_{\Gamma^\nu \sigma}^\alpha (\vec{k}, \bar{\nu}) V_{\sigma' \Gamma'}(\vec{k}),$$

(B.26)

where there is an implicit sum over $\Gamma'$ and $\alpha'$. This means B.25 becomes

$$G_{\Gamma\sigma}(\vec{k} - \vec{q}, \bar{\nu}(i\nu)\delta_{s'}(\vec{k}) G_{\Gamma^\nu \sigma}^\alpha (\vec{k}, \bar{\nu}) V_{\sigma' \Gamma'}(\vec{k}),$$

(B.27)

which is represented diagrammatically in Figure B.2. This represents all contributions to the vertex that are quadratic in the $s - s$ fields.
APPENDIX C: Exact Results for the Hybridization Matrix Elements

In this appendix, we will show how to reduce the combination of hybridization matrix elements in equation 5.37 by summing over the spin variables, and over the various angular momentum quantum numbers that are buried in the equation. For a given set of crystal field quantum numbers, $\Gamma, \alpha, \Gamma', \alpha'$, we want to simplify the following expression:

$$
\sum_{\sigma, \sigma'} V_{\Gamma \alpha \sigma}^*(\tilde{k}) V_{\sigma \Gamma' \alpha'}(\tilde{k}) V_{\Gamma' \alpha' \sigma'}(\tilde{k}') V_{\sigma' \Gamma \alpha}(\tilde{k}'),
$$

(C.1)

where

$$
V_{\Gamma \alpha \sigma}(\tilde{k}) = V_{\sigma \Gamma}(k) \beta_{\Gamma \alpha \sigma}(\hat{k}).
$$

(C.2)

We have separated the dependence of the matrix element by the radial and angular components of the momentum. We can relate the $\beta_{\Gamma \alpha \sigma}(\hat{k})$ with the corresponding functions $\beta_{m \sigma}(\hat{k})$ in the case of spherical symmetry, where $m$ is the $z$-component of the total angular momentum, $J = 5/2$, i.e. $-5/2 \leq m \leq 5/2$:

$$
\beta_{\Gamma \alpha \sigma}(\hat{k}) = \sum_{m} c_{\Gamma \alpha m} \beta_{m \sigma}(\hat{k}).
$$

(C.3)
The coefficients \( c_{\text{om}} \) follow from symmetry arguments and can be deduced from the following array:

\[
\begin{align*}
|7, +1 \rangle &= -\sqrt{\frac{1}{6}} | -\frac{5}{2} \rangle + \sqrt{\frac{5}{6}} | \frac{3}{2} \rangle \quad (C.4) \\
|7, -1 \rangle &= -\sqrt{\frac{1}{6}} | \frac{5}{2} \rangle + \sqrt{\frac{5}{6}} | -\frac{3}{2} \rangle \quad (C.5) \\
|8, +2 \rangle &= \sqrt{\frac{5}{6}} | \frac{5}{2} \rangle + \sqrt{\frac{1}{6}} | -\frac{3}{2} \rangle \quad (C.6) \\
\langle 8, +1 \rangle &= | \frac{1}{2} \rangle \quad (C.7) \\
\langle 8, -1 \rangle &= | -\frac{1}{2} \rangle \quad (C.8) \\
\langle 8, -2 \rangle &= \sqrt{\frac{5}{6}} | -\frac{5}{2} \rangle + \sqrt{\frac{1}{6}} | \frac{3}{2} \rangle. \quad (C.9)
\end{align*}
\]

We now write the angular function in detail

\[
\beta_{m\sigma}(\hat{k}) = \sqrt{\frac{4\pi}{3}} (3(m - \frac{\sigma}{2}) \frac{1}{2}(\frac{\sigma}{2}) | \frac{5}{2} m \rangle Y_{3,-\frac{5}{2}}(\hat{k}), \quad (C.10)
\]

where the Clebsch-Gordan coefficient arises from the spin-orbit coupling on the Ce ion. In this case, for a \( 4f^1 \) configuration, Hund's rules are trivial and give an orbital angular momentum of \( L = 3 \) with a spin of \( S = 1/2 \). Further, since the \( 4f \) shell is less than half-filled, we take the total angular momentum given by \( J = |L - S| = 5/2[1] \). Equation C.1 now becomes

\[
\left(\frac{4\pi}{3}\right)^2 \sum_{\sigma' \sigma m_1 m_2 m_3 m_4} c_{\Gamma m_1} c_{\Gamma' \sigma' m_2} c_{\Gamma' \sigma' m_3} c_{\Gamma m_4} \times (3(m_1 - \frac{\sigma}{2}) \frac{1}{2}(\frac{\sigma}{2}) | \frac{5}{2} m_2 \rangle (3(m_2 - \frac{\sigma}{2}) \frac{1}{2}(\frac{\sigma}{2}) | \frac{5}{2} m_2 \rangle \\
\times 3(m_3 - \frac{\sigma'}{2}) \frac{1}{2}(\frac{\sigma'}{2}) | \frac{5}{2} m_3 \rangle (3(m_4 - \frac{\sigma'}{2}) \frac{1}{2}(\frac{\sigma'}{2}) | \frac{5}{2} m_4 \rangle \\
Y_{3,m_1 - \frac{\sigma}{2}}(\hat{k}') Y_{3,m_2 - \frac{\sigma}{2}}(\hat{k}') Y_{3,m_3 - \frac{\sigma'}{2}}(\hat{k}') Y_{3,m_4 - \frac{\sigma'}{2}}(\hat{k}). \quad (C.11)
\]

Next, we use the following property of the spherical harmonics:

\[
Y_{3,m_2 - \frac{\sigma}{2}} = (-1)^{m_2 - \frac{\sigma}{2}} Y_{3,-m_2 + \frac{\sigma}{2}}, \quad (C.12)
\]
to write the products of spherical harmonics as

\[ (-1)^{m_2 - \frac{q}{2}} (-1)^{m_4 - \frac{q'}{2}} Y_{3, -m_2 + \frac{q}{2}}(\hat{k}') Y_{3, m_1 - \frac{q}{2}}(\hat{k}) Y_{3, -m_4 + \frac{q'}{2}}(\hat{k}) Y_{3, m_3 - \frac{q'}{2}}(\hat{k}). \]

It is a well-known property of the spherical harmonics that their product can be written as a linear combination of a single harmonic[2]:

\[
Y_{3, -m_2 + \frac{q}{2}} Y_{3, m_1 - \frac{q}{2}} = \sum_L \sqrt{\frac{49}{4\pi(2L + 1)}} \langle 3(0)3(0)|L(0) \rangle \\
\times \langle 3(-m_2 + \frac{\sigma}{2})3(m_1 - \frac{\sigma}{2})|L(m_1 - m_2) \rangle Y_{L, m_1 - m_2}, \tag{C.13}
\]

where we have introduced two new Clebsch-Gordan coefficients. Putting everything together, we see that we'll have only two spherical harmonics in total. Writing one of the harmonics in terms of its complex conjugate means we pick up another phase factor. The result is

\[
\sum_{\sigma' L' \sigma_1} \sum_{m_1 m_2 m_3 m_4} \left( \frac{4\pi}{3} \right)^2 (-1)^{-(\frac{q}{2} + \frac{q'}{2})} (-1)^{m_3 - m_2} \sqrt{\frac{49}{4\pi(2L + 1)}} \sqrt{\frac{49}{4\pi(2L' + 1)}} \\
\times c_{\Gamma \alpha_1 \Gamma' \sigma' \sigma_2} c_{\Gamma' \sigma_2 \sigma_3} c_{\Gamma \alpha_3 \sigma_4} c_{\Gamma \alpha_4 \sigma_1} \langle 3(0)3(0)|L(0) \rangle \\
\times \langle 3(0)3(0)|L'(0) \rangle \langle 3(m_1 - \frac{\sigma}{2})|\frac{5}{2} m_1 \rangle \langle 3(m_2 - \frac{\sigma}{2})|\frac{5}{2} m_2 \rangle \\
\times \langle 3(m_3 - \frac{\sigma'}{2})|\frac{5}{2} m_3 \rangle \langle 3(m_4 - \frac{\sigma'}{2})|\frac{5}{2} m_4 \rangle \\
\times \langle 3(-m_2 + \frac{\sigma}{2})3(m_1 - \frac{\sigma}{2})|L(m_1 - m_2) \rangle \\
\times \langle 3(-m_4 + \frac{\sigma'}{2})3(m_3 - \frac{\sigma'}{2})|L'(m_3 - m_4) \rangle Y_{L', m_4 - m_3}(\hat{k}) Y_{L, m_1 - m_2}(\hat{k}'). \tag{C.14}
\]

Now we can combine the fourth and seventh Clebsch-Gordan coefficients in equation C.14, using the identity in Morrison's book, equation 2.7(b)[2],

\[
\langle 3(m_2 - \frac{\sigma}{2})|\frac{5}{2} m_2 \rangle \langle 3(-m_2 + \frac{\sigma}{2})3(m_1 - \frac{\sigma}{2})|L(m_1 - m_2) \rangle
\]
\[
\begin{align*}
= (-1)(-1)^{\frac{1}{2}} & - \frac{\sigma}{2} \sqrt{\frac{6}{7}} \left( \frac{1}{2} \left( \frac{\sigma}{2} \right)^{\frac{5}{2}} \right) (-m_2)|3(\frac{\sigma}{2} - m_2)) \\
\times (3(\frac{\sigma}{2} - m_2)3(m_1 - \frac{\sigma}{2} | L(m_1 - m_2)).
\end{align*}
\]

With this result we sum everything in equation C.14 dependent on the spin variable \( \sigma \). Using equation 6.5(a) in Rose's book[3] yeilds, after summing over \( \sigma \):

\[
i \sqrt{\frac{6}{7}} \frac{R_{\frac{L}{2}}^{(L)}}{2} (-m_2)^{\frac{5}{2}} (m_1 | L(m_1 - m_2)),
\]

where \( R_{\frac{L}{2}}^{(L)} \) is a so-called Racah coefficient and can be easily calculated. Using a standard table of 6j symbols[4], we find that

\[
\begin{align*}
R_{\frac{L}{2}}^{(0)} &= 1 \\
R_{\frac{L}{2}}^{(2)} &= \sqrt{\frac{5}{7}} \\
R_{\frac{L}{2}}^{(4)} &= \frac{\sqrt{11}}{21}
\end{align*}
\]

For future reference, we also give the result for the \( L \) dependent Clebsch-Gordan coefficient,

\[
\begin{align*}
(3(0)3(0)|L(0)) &= (-1)^{3+\frac{L}{2}} \sqrt{\frac{2L + 1}{7 + L}} \frac{L!}{[(\frac{L}{2})!]^2} \sqrt{\frac{(6 - L)!}{(6 + L)!} \frac{(3 + \frac{L}{2})!}{(3 - \frac{L}{2})!}},
\end{align*}
\]

which comes from equation 2.9 in reference[2]. A similar sum over \( \sigma' \) finally gives the result

\[
\begin{align*}
&-\frac{6}{7} \left( \frac{4\pi}{3} \right)^2 \sum_{L} \sum_{m_1 m_2 m_3 m_4} (-1)^{m_2} (-1)^{m_3} c_{\Gamma_1 \alpha_1} c_{\Gamma_2 \alpha_2} c_{\Gamma_3 \alpha_3} c_{\Gamma_4 \alpha_4} \\
\times \sqrt{\frac{49}{4\pi(2L + 1)}} \sqrt{\frac{49}{4\pi(2L' + 1)}} R_{\frac{L^3}{2}} \! \! R^L_{\frac{L^3}} (3(0)3(0)|L(0))(3(0)3(0)|L'(0)) \\
\times (\frac{5}{2} (-m_2)^{\frac{5}{2}} (m_1 | L(m_1 - m_2))(\frac{5}{2} (-m_3)^{\frac{5}{2}} (m_4 | L'(m_4 - m_3))
\end{align*}
\]
Note that the coefficient \( \langle 3(0)3(0)|L(0) \rangle \) vanishes unless \( L \) is even. Further, from the triangle inequality we know that \( 0 \leq L \leq 6 \). In spherical symmetry, we would have free sums over the \( m_i (i = 1, 2, 3, 4) \), and the sum rule of spherical harmonics would eventually leave us with Legendre polynomials of the form \( P_l (\hat{k} \cdot \hat{k}') \), where \( l = 0, 2, 4 \) and the polynomial is a function of the angle between the two vectors \( \hat{k} \) and \( \hat{k}' \). This is in agreement with the results of Zhang and Lee[5], who calculated the quasiparticles interactions in the infinite-U Anderson lattice in the presence of spherical symmetry.

In the presence of crystal fields of cubic symmetry, we first specify the crystal field quantum numbers, \( \Gamma, \alpha, \Gamma', \alpha' \), and then we sum over the remaining variables in equation C.14. The coefficients \( \alpha_{\Gamma m} \) will automatically pick out the correct values of \( m_i \) for a given set of crystal field quantum numbers. We'll show explicitly how this works for the case of \( \Gamma, \alpha = \Gamma', \alpha' = \Gamma_7, +1 \). A close look at equation C.14 reveals that the expression is separable in \( \hat{k} \) and \( \hat{k}' \). Thus we need look only at one of the two variables. We shall on all variables connected with the \( \hat{k} \) dependence of equation C.14. Sum, first, over \( m_3 \) and \( m_4 \); we present the result, but for convenience do not show the constant prefactors:

\[
-i \sum_{L} \sqrt{\frac{49}{4\pi(2L+1)}} R_{23}^{L} \left[ \frac{1}{6} \left( \frac{5}{2} \frac{5}{2} \frac{5}{2} \right) |L'(0)\rangle Y_{L'=0}^{*} + \frac{5}{6} \left( \frac{3}{2} \frac{3}{2} \frac{3}{2} \right) |L'(0)\rangle Y_{L'=0}^{*} \right. \\
- \left. \frac{\sqrt{5}}{6} \left( \frac{5}{2} \frac{3}{2} \frac{5}{2} \right) |L'(-4)\rangle Y_{L'=-4}^{*} - \frac{\sqrt{5}}{6} \left( \frac{5}{2} \frac{3}{2} \frac{3}{2} \right) |L'(-4)\rangle Y_{L'=-4}^{*} \right].
\]  

\( (C.21) \)

Next, we sum over \( L' \). It turns out that only non-zero contributions to the sum come from \( L = 0 \) and \( L = 4 \). Using equation C.19 and the values for the Racah coefficients presented above, we find the following final result for
equation C.1 evaluated for the $\Gamma_7, +1$ crystal field state:

$$-\frac{4\pi}{9} V_{\sigma}^4(k) \left[ Y_0^*(\hat{k}) - \frac{1}{3} Y_{40}^*(\hat{k}) - \frac{1}{3} \sqrt{\frac{5}{14}} \left( Y_{44}^*(\hat{k}) + Y_{-4}^*(\hat{k}) \right) \right]$$

$$\times \left[ Y_0(\hat{k}') - \frac{1}{3} Y_{40}(\hat{k}') - \frac{1}{3} \sqrt{514} \left( Y_{44}(\hat{k}') + Y_{-4}(\hat{k}') \right) \right]. \quad (C.22)$$

In chapter 5, we defined a function

$$\mu_{\Gamma_7, \sigma'}(\hat{k}) = \sum_{\sigma} V_{\sigma}^*(\hat{k}) V_{\sigma', \alpha'}(\hat{k}). \quad (C.23)$$

Using this notation, equation C.1 becomes

$$\mu_{\Gamma_7, \sigma'}(\hat{k}) \mu_{\Gamma_7, \sigma}(\hat{k}), \quad (C.24)$$

and with the result from equation C.22, we can write

$$\mu_{71, 71}(\hat{k}) = -\frac{2\sqrt{\pi}}{3} V_{\sigma}(k) \left[ Y_0(\hat{k}) - \frac{1}{3} Y_{40}(\hat{k}) - \frac{1}{3} \sqrt{514} \left( Y_{44}(\hat{k}) + Y_{-4}(\hat{k}) \right) \right]. \quad (C.25)$$

It is tedious but straightforward to calculate the matrix elements for all possible combinations of the crystal field quantum numbers. The results have already been presented, in Table 5.2.

In the presence of spherical symmetry, equation C.20 becomes

$$\frac{6}{7} \left( \frac{4\pi}{3} \right)^2 \sum_{L_{mm'}} \frac{49}{4\pi(2L + 1)} \left( R_{\frac{L}{23}} \right)^2 \langle 3(0)3(0)|L(0) \rangle^2$$

$$\times \left( \frac{5}{2} \right)^2 \langle -m | 5/2(m + m')|L(m') \rangle^2 Y_{L_{mm'}}^*(\hat{k}') Y_{L_{mm'}}(\hat{k}). \quad (C.26)$$

Consider the case of $L = 0$. We then have

$$\frac{16\pi^2}{9} \frac{49}{4\pi} \left( R_{\frac{L}{23}}^0 \right)^2 \langle 3(0)3(0)|0(0) \rangle^2$$

$$\times \sum_{m'm'} \left( \frac{5}{2} \right)^2 \langle -m | 5/2(m' + m)|0(m') \rangle^2 Y_{m'm'}^*(\hat{k}') Y_{m'm'}(\hat{k}).$$
Now
\[ \sum_m \frac{5}{2} (-m) \frac{5}{2} (m' - m) |0(m')|^2 = 1, \]
and
\[ \sum_{m'} Y_{0m'}^* (\hat{k}') Y_{0m'} (\hat{k}) = \frac{1}{4\pi} P_0 (\hat{k}' \cdot \hat{k}). \]
So the final result for \( L = 0 \) is
\[ \frac{2}{3} P_0 (\hat{k}' \cdot \hat{k}). \] (C.27)
A similar procedure for \( L = 2 \) yields
\[ \frac{16}{21} P_2 (\hat{k}' \cdot \hat{k}), \] (C.28)
while for \( L = 4 \) we have
\[ \frac{4}{7} P_4 (\hat{k}' \cdot \hat{k}). \] (C.29)
These numbers agree with those of Zhang and Lee[5], so we have a way of checking this procedure. In terms of the function \( B (\hat{k} \cdot \hat{k}') \), defined in equation 5.46, equations C.27- C.29 give
\[ B (\hat{k} \cdot \hat{k}') = \frac{2}{3} P_0 (\hat{k} \cdot \hat{k}') + \frac{16}{21} P_2 (\hat{k} \cdot \hat{k}') + \frac{4}{7} P_4 (\hat{k} \cdot \hat{k}'). \] (C.30)

APPENDIX C  REFERENCES


APPENDIX D: A Simple Identity for the Quasiparticle Bands in Spherical Symmetry

In this appendix we wish to prove the following identity, first seen in equation 4.78:

\[(E_{2\mathbf{k'}} - E_{1\mathbf{k}})(E_{1\mathbf{k'}} - E_{1\mathbf{k}}) = (\xi_{\mathbf{k'}} - \xi_{\mathbf{k}})(T_o - E_{1\mathbf{k}}),\]  

(D.1)

where \(E_{nk}\) is the quasiparticle energy for band \(n\), where \(\xi_{\mathbf{k}}\) is the free conduction electron energy, and where \(T_o\) is the Kondo temperature. In spherical symmetry, the quasiparticles bands come from the diagonalization of a \(2 \times 2\) matrix, and so are the solutions of a quadratic equation. The energies are given by

\[E_{nk} = \frac{\xi_{\mathbf{k}} + T_o \pm \sqrt{(\xi_{\mathbf{k}} - T_o)^2 + 4s_o^2V_o^2}}{2}.\]  

(D.2)

To prove the identity, we start with the left hand side of equation D.1 and substitute for the band energies from equation D.2:

\[(E_{2\mathbf{k'}} - E_{1\mathbf{k}})(E_{1\mathbf{k'}} - E_{1\mathbf{k}}) = \]

\[
\frac{1}{4}(\alpha + \beta)(\alpha - \beta),
\]  

(D.3)

where

\[\alpha \equiv \xi_{\mathbf{k'}} - \xi_{\mathbf{k}} + \sqrt{(\xi_{\mathbf{k}} - T_o)^2 + 4s_o^2V_o^2},\]
Next, we note that the combination of \( \alpha \) and \( \beta \) is equivalent to \( \alpha^2 - \beta^2 \) to write equation D.3 as

\[
\frac{1}{4} \left[ (\xi_{k'} - \xi_k) \left( (\xi_{k'} - \xi_k) + 2\sqrt{(\xi_k - T_o)^2 + 4s_o^2V_o^2} \right) \right.
\]

\[
\left. + (\xi_k - \xi_{k'}) (x_{k'} + \xi_k) + 2T_o (\xi_{k'} - \xi_k) \right]
\]

\[
= \frac{1}{2} (\xi_{k'} - \xi_k) [\xi_k - \sqrt{(\xi_k - T_o)^2 + 4s_o^2V_o^2}].
\]

(D.4)

(D.5)

Finally, from equation D.2 we can write

\[
\xi_{k'} - \sqrt{(\xi_k - T_o)^2 + 4s_o^2V_o^2} = 2E_{1k} - T_o,
\]

which, when substituted into equation D.5 gives

\[
(\xi_{k'} - \xi_k) (T_o - E_{1k}).
\]

This is the result we wished to prove.
APPENDIX E: Details of the Numerical Fermi Surface Averages

In this appendix, we discuss details of the numerical integrations used in the calculation of the Fermi-surface averaged quasiparticle scattering amplitude, (see equation 5.69), (\Gamma)\eta, where \eta = A_{1g}, E_g, T_{1g}, T_{2g} are the representations of Oh symmetry. In Chapter 5, we said that there are two important integrals to perform in this calculation: the (double) Fermi surface average of the scattering amplitude,

$$\int_{FS} \frac{d\vec{k}}{4\pi} \int_{FS} \frac{d\vec{k}'}{4\pi} \Phi^*_{\eta}(\vec{k}') \Gamma_{QP}(\vec{k}, \vec{k}') \Phi_{\eta}(\vec{k});$$  \hspace{1cm} (E.1)

and the Brillouin zone integration that calculates the dressed (to order 1/N) Bosonic Green function, which is, in turn, fed into \Gamma_{QP}(\vec{k}, \vec{k}')$. The Brillouin zone integration was discussed extensively in Chapter 4. Here we focus on equation E.1.

The expression for the scattering amplitude was given in equation 5.35. At first, we focus on the strongly anisotropic normalization function,

$$A^2_{1}(\vec{k}) = \left[1 + \frac{1}{2} \sum_{\gamma \alpha \sigma} \frac{\delta^{2}_{\gamma\sigma} |\hat{V}_{\gamma\alpha\sigma}(\vec{k})|^2}{(\epsilon_{\gamma} - E_{1\vec{k}})^2}\right]^{-1}. \hspace{1cm} (E.2)$$

As can be seen in figure 5.3, near the coordinate axes of the Brillouin zone, the function $A^2_{1}$ is very sharply peaked. This is due to the vanishing of the $\Gamma_{\gamma}$
matrix elements, $V_{\gamma\alpha\sigma}$, at the axes. In fact, $A_1^2$ is varying so rapidly over such small regions of $k$-space, that we proceed as follows. When equation 5.35 is averaged over the (assumed) spherical Fermi surface, everything but the normalization functions $A_1^2(\vec{k})A_1^2(\vec{k}')$ is treated as constant over small regions of the surface near where the axes intersect the sphere. The normalization functions are integrated essentially exactly over these small regions, which are taken to have angular sizes of $\Delta\phi = \pi/10$ and $\Delta\theta = \pi/10$. $\theta$ and $\phi$ are the usual angular variables of spherical coordinates. Outside of these small patches of the Fermi surface, all elements of the integrand are treated equally in the numerical integration.

As discussed briefly in Chapter 5, the normalization function can be written as

$$A^2 = \frac{\left(\frac{T_{\gamma\ell}/s_0V_0}{s_0V_0}\right)^2}{\frac{1}{3} + \frac{2}{3}\left(\frac{T_{\alpha\sigma}}{T_{\alpha\sigma}}\right)^2 - \frac{2\sqrt{\pi}}{9}\left[1 - \left(\frac{T_{\alpha\sigma}}{T_{\alpha\sigma}}\right)^2\right]\left[Y_{40} + \sqrt{\frac{5}{14}}(Y_{44} + Y_{4-4})\right]}, \quad (E.3)$$

where the sums over $\Gamma$, $\alpha$, and $\sigma$ were performed exactly. Since $A_1^2$ will be evaluated on the surface of a sphere far from the zone center, we shall not worry about the dependence of equation E.3 on the magnitude of $\vec{k}$. Note that at any point on one of the axes, the combination of spherical harmonics reduces to $3/2\sqrt{\pi}$ and $A_1^2$ becomes

$$A_1^2 \approx \left(\frac{T_{\alpha\ell}}{s_0V_0}\right)^2. \quad (E.4)$$

If, at a general $k$-point, $A_1^2 \approx (T_{\alpha\ell}/s_0V_0)^2$, we see that the normalization can increase by a couple of orders of magnitude for points on the axes.

To integrate $A_1^2(\vec{k})$, we expand equation E.3 for an azimuthal angle near the equator, i.e. near $\theta = \pi/2$. Let $\delta\theta \equiv \theta - \pi/2$. Expanding the spherical
harmonics to order $\delta \theta^2$ gives

$$A_1^2 \approx \frac{(T_0/T_0')^2}{\frac{1}{3} + \frac{2}{3}(1 - \delta T)^{2}} - \frac{\delta T}{24} \left[ 3 - 30 \delta \theta^2 + (5 - 10 \delta \theta^2) \cos(4\phi) \right],$$  \hspace{1cm} (E.5)

where $\delta T \equiv 1 - (T_0/T_0')^2 \approx 0.9993725$. We now perform the integral over the solid angle subtended by a small region of surface area,

$$\int d\Omega A_1^2(\Omega) = 3\left(\frac{T_0'}{s_0 V_o}\right)^2 \int_{(\pi + \Delta \theta)/2}^{(\pi - \Delta \theta)/2} d\theta \sin \theta \int_{0}^{\Delta \phi/2} 2d\phi \frac{1}{a + b \cos(4\phi)},$$  \hspace{1cm} (E.6)

where

$$a = 3 - \frac{\delta T}{8} (19 - 30 \delta \theta^2),$$

$$b = -\frac{5}{8} \delta T (1 - 2 \delta \theta^2).$$

We can perform the $\phi$ integral analytically. The result is

$$\frac{1}{\sqrt{\alpha \delta \theta^2 + \beta}} \tan^{-1} \left[ \frac{\sqrt{\alpha \delta \theta^2 + \beta} \tan(\Delta \phi)}{\gamma \delta \theta^2 + \Delta} \right],$$  \hspace{1cm} (E.7)

where

$$\alpha = \frac{5}{2} \delta T (9 - \frac{13}{2} \delta T),$$

$$\beta = \frac{3}{4} \delta T (7 \delta T - 19),$$

$$\gamma = 5 \delta T,$$

$$\Delta = 3(1 - \delta T).$$

We are left with the theta integral, which can be written as

$$6\left(\frac{T_0'}{s_0 V_o}\right)^2 \int_{0}^{\Delta \phi/2} du \frac{\cos u}{\sqrt{\alpha u^2 + \beta}} \tan^{-1} \left[ \frac{\tan(\Delta \phi) \sqrt{\alpha u^2 + \beta}}{\gamma u^2 + \Delta} \right],$$  \hspace{1cm} (E.8)

and which is straightforward to evaluate numerically. This gives us the result for the four special regions along the equator of the Fermi surface.
Next, we expand the normalization function for $\theta$ near 0 (or $\pi$). In this case, $\delta\theta = \theta$, and to order $\theta^2$ we find

$$A_1^2 \approx \frac{3(T_o^2 s_o V_o)^2}{3 - 2\delta T - \delta T(1 - 5\theta^2)},$$

where the $\phi$ dependence has completely disappeared. Integrating about a small solid angle at the polar caps, gives

$$2 \times 2\pi \int_0^{\Delta \theta/2} d\theta \sin \theta \frac{3\left(\frac{F_{k^*}}{s_0 V_o}\right)^2}{a + b\theta^2},$$

where $a = 3(1 - \delta T)$ and $b = 5\delta T$. The prefactor of 2 in equation E.10 accounts for both poles, and the factor of $2\pi$ results from the $\phi$ integration. The remaining $\theta$ integral can be evaluated analytically and gives

$$\int d\Omega A_1^2 \approx 12\pi \left(\frac{T_o^2}{s_o V_o}\right)^2 \frac{1}{5\delta T} \ln \left| 1 + \frac{5\delta T}{3(1 - \delta T)} \left(\frac{\Delta \theta}{2}\right)^2 \right|.\quad (E.11)$$

This grafting-like procedure for the normalization function can be tested as follows. In the local limit, in which the functions $F(k' - k)$ and $F(k' + k)$ of equation 5.36 are set to zero, the scattering amplitude is separable in the variables $k$ and $k'$. In this case, it is easy to calculate the Fermi surface averages numerically by merely taking a very fine mesh. In this way, no approximations about the normalization function need to be made. Of course, the inclusion of the Boson self-energies through the function $F(k \pm k')$ ruins the separability of the scattering amplitude, and we truly have, in that case, a double surface average to perform, which in turn means we can not afford a very fine mesh. Thus we must utilize this grafting procedure for the normalization function in order to prevent the averaging mesh from becoming too large. In Table E.1, we
Table E.1:
A check of the grafting procedure for the Fermi surface averaged local quasiparticle scattering amplitude. Column 1 gives the "exact" results, with no approximations; notice the fine mesh required. Column 2 treats the normalization function carefully near the special points of $\Gamma_7$ symmetry. The averaging mesh for column 2 has only 102 points. These numbers come from the following mean field parameters: $\epsilon_7 = -0.704086$ eV; $T_{07} = 12.4$ K; $s_0 = 0.246393$; $V_0 = 0.375$ eV.

<table>
<thead>
<tr>
<th>$\eta$</th>
<th>Exact Average(eV)</th>
<th>Special Mesh(eV) (102 points)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_{1g}$</td>
<td>$4.9 \times 10^{-3}$ (16,625 mesh points)</td>
<td>$3.10 \times 10^{-3}$</td>
</tr>
<tr>
<td>$E_g$</td>
<td>$-6.95 \times 10^{-4}$ (34,125 points)</td>
<td>$-6.83 \times 10^{-4}$</td>
</tr>
<tr>
<td></td>
<td>$-7.20 \times 10^{-4}$ (36,425 points)</td>
<td>$-6.81 \times 10^{-4}$</td>
</tr>
</tbody>
</table>

give a comparison of the local interactions for two cases: (1) in the first column, we have the results of an exact treatment of $A_1^2(\vec{k})$ for a fine mesh; (2) in the second column, we have the results of our grafting procedure, where $A_1^2(\vec{k})$ is integrated over small surface areas of the Fermi surface. An averaging mesh of 102 mesh points was used for the results in column 2, while about 15,000 mesh points was required to get the results in the first column. The author believes, that given the approximation of treating everything but the normalization as constant inside these special regions, and given the modest number of mesh points needed, the results in column 2 are in acceptable agreement with those of column 1. Note that the state of $T_{1g}$ and $T_{2g}$ symmetry are not represented in the table, since they are relatively small in magnitude near the special regions of the Fermi surface. Note, also, that equations E.8 and E.10 are valid for any set of reasonable mean field parameters, $s_0$, $V_0$, and $T_0$. 
APPENDIX F: The Lattice Kondo Temperature in the
SU(2) Model

In this appendix, we discuss a technical matter in the SU(2) model, pertaining to the definition of the lattice Kondo temperature, $T_o$, for the case of a half-filled conduction band. Namely, if we take a half-filled conduction band (with a flat density of states), then we find that the usual definition of the Kondo temperature (see equation F.1 below) is valid only if the lowest quasiparticle band is completely filled, i.e. only if we have an insulator. We show, however, that this anomaly occurs only for the SU(2) model when the conduction band is exactly half filled. The usual definition of $T_o$ is[1]

$$T_o = \epsilon - \mu = De^{-|E|/NN(0)V^2},$$  \hspace{1cm} (F.1)

where

- $\epsilon$ is the hybridization shifted 4f multiplet energy,
- $|E|$ is the unshifted 4f multiplet energy, $E \approx 2.0$ eV,
- $\mu$ is the quasiparticle chemical potential, which we shall take to be at zero energy,
- $D$ is the conduction electron half-bandwidth,
Figure F.1:

Conduction electron density of states for a half filled band. The half-bandwidth is denoted by $D$. The lowest quasiparticle band energy is also plotted as a function of $k$ for k-points near a zone boundary. We call the largest k-point $k_{\text{max}}$ and the corresponding quasiparticle energy $E_{\text{max}}$. The unhybridized conduction electrons would have energy $D$ at $k = k_{\text{max}}$. Note that the quasiparticle chemical potential is taken to be zero. The usual definition of the Kondo temperature, $T_o = \epsilon$, is shown explicitly in the figure. Note that $\epsilon$ is the hybridization shifted 4f multiplet energy.

- $N(0)$ is the conduction electron density of states, which we shall take to be flat ($N(0) = 1/2D$),
- $V_o$ is the bare hybridization strength,
- $N$ is the degeneracy of each 4f multiplet.

We take a 2-fold degeneracy ($N = 2$) and assume a half-filled conduction band. (See figure F.1.) The quasiparticle states (for the lowest band) are also shown in figure F.1 for k-points near the zone boundary, $k_{\text{max}}$. Note that the maximum quasiparticle energy in the band is labeled as $E_{\text{max}}$. 

In general, the quasiparticle band energy as a function of \( k \) is

\[
E_k = \frac{\xi_k + \epsilon - \sqrt{(\xi_k - \epsilon)^2 + 4s_0^2V_o^2}}{2},
\]

where

- \( \xi_k \) is the conduction electron energy, and
- \( s_0V_o \) is the renormalized hybridization strength.

For a half-filled conduction band, when \( k = k_{\text{max}} \) (at a zone boundary), \( \xi_k = D \), where \( D \gg |\epsilon| \) and \( D \gg s_0V_o \). Thus for \( k = k_{\text{max}} \), we can approximate the quasiparticle energy (equation F.2) by

\[
E_{\text{max}} \approx \epsilon - \frac{s_0^2V_o^2}{D}.
\]

If we assume the Kondo temperature is given by equation F.1, then \( \epsilon = T_o \). In this case, the solution of the mean-field self-consistency equations gives

\[
T_o = NN(0)s_0^2V_o^2,
\]

where the last equality holds for \( N = 2 \). Substituting the last line into equation F.3 requires that

\[
E_{\text{max}} = 0.
\]

In other words, if we define the Kondo temperature by equation F.1, self-consistency requires that the lowest quasiparticle band be completely filled. We have an insulator! This is bad news, if one is looking for a superconducting instability.

What happens if the conduction band is initially less than half-filled? In figure F.2, we show a conduction band with a density of states \( N(0) = 1/2D \),
Figure F.2:

Conduction electron density of states for a less than half-filled conduction band. The lower band edge is $D_L$, and the upper band edge is $D_U$. The filling is chosen such that $D_L < D < D_U$. The quasiparticle band is also shown for $k$ near $k_{max}$.

but with a lower band edge $D_L$ and an upper band edge $D_U$. The filling of the band has been chosen such that

$$D_L < D < D_U.$$  \hfill (F.6)

For $k$ near $k_{max}$, the quasiparticle band is also shown. In this case, at $k = k_{max}$, the conduction electron energy would be $\xi = D_U$, and the quasiparticle energy is

$$E_{max} \approx \epsilon - \frac{s_o^2 V_o^2}{D_U},$$  \hfill (F.7)

for $N = 2$. If we assume, once more, that $\epsilon = T_o$, then equation F.4 is still valid, where the density of states is unchanged from the value at half-filling ($N(0) = 1/2D$). Substituting for $s_o V_o$ from equation F.4 into equation F.7
gives

\[ E_{\text{max}} = \left[ 1 - \frac{D}{D_U} \right] T_o. \]  

(F.8)

We see from equation F.8 that

- \( E_{\text{max}} = 0 \) at \( D = D_U \) (half-filling),
- \( E_{\text{max}} < T_o \) for \( D > D_U \) (less than half-filling).

From figure F.2 and equation F.8, we see that \( E_{\text{max}} < T_o \) can be consistent with: (a) a partially filled quasiparticle band, and (b) the usual definition of the lattice Kondo temperature, \( \epsilon = T_o \) (equation F.1).

For concreteness, let's check the result with some numbers. Consider a quarter filled conduction band, which corresponds to \( D/D_U = 2/3 \). Taking a Kondo temperature of \( T_o = 10K \approx 1 \text{meV} \), gives \( E_{\text{max}} = 3.33 K \approx 0.333 \text{meV} \). For mean-field parameter set (a) (see page 263), we can calculate \( E_{\text{max}} \), finding \( E_{\text{max}} = 0.49 \text{meV} \). This is in reasonable agreement with the \( SU(2) \) result. It is worthwhile to remind the reader that our Hamiltonian in the presence of crystal fields (equation 3.55) is not the same as the \( SU(2) \) model, and so we should not expect exact agreement. The comparison of the \( SU(2) \) and crystal field values of \( E_{\text{max}} \) serves just to tell us that our value of \( E_{\text{max}} \) in the presence of the crystal fields is reasonable.

Thus we see that it is indeed possible to have self-consistent mean field solutions for \( N = 2 \), as long as the conduction electron band is not half-filled. One can also repeat this analysis for a half-filled conduction band and for arbitrary degeneracy \( N > 1 \). We find the result

\[ E_{\text{max}} = \left[ 1 - \frac{2}{N} \right] T_o, \]  

(F.9)

which gives \( E_{\text{max}} = 0 \) for \( N = 2 \) (as expected), and which gives \( E_{\text{max}} \to T_o \) for \( N \to \infty \). It is interesting to note that the structure of equation F.9 is the same
as that for $N = 2$ and less than half-filling, equation F.8.

APPENDIX F REFERENCES

LIST OF REFERENCES

1 A. A. Abrikosov, Physics 2, 5 (1965).


38 see, e.g., D. L. Cox, Ph. D. Thesis (Cornell University, 1985) unpublished.


