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ANALYTIC APPROXIMATIONS TO THE COHERENT
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DISSERATION

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

By
Pisistha Ratanavararaksa, B.Sc., M.Sc.

...*

The Ohio State University

1977

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# Table of Contents

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acknowledgments</td>
<td>i</td>
</tr>
<tr>
<td>Vita</td>
<td>iii</td>
</tr>
<tr>
<td>List of Figures</td>
<td>vi</td>
</tr>
<tr>
<td>List of Tables</td>
<td>viii</td>
</tr>
<tr>
<td>Chapter 1: Introduction</td>
<td>1</td>
</tr>
<tr>
<td>Chapter 2: Previous Work</td>
<td>7</td>
</tr>
<tr>
<td>A. Electronic States in a Binary Substitutional Alloy</td>
<td>7</td>
</tr>
<tr>
<td>B. Methods of Approximation for $&lt;\mathcal{Q}&gt;$</td>
<td>10</td>
</tr>
<tr>
<td>B.1 Virtual Crystal Approximation (VCA)</td>
<td>10</td>
</tr>
<tr>
<td>B.2 Average $t$-Matrix Approximation (ATA)</td>
<td>11</td>
</tr>
<tr>
<td>B.3 Cumulant and Corrected Cumulant Expansion</td>
<td>13</td>
</tr>
<tr>
<td>B.4 Diagrammatic Methods</td>
<td>17</td>
</tr>
<tr>
<td>B.5 The Coherent Potential Approximation (CPA)</td>
<td>19</td>
</tr>
<tr>
<td>Chapter 3: Theory</td>
<td>22</td>
</tr>
<tr>
<td>A. The Herglotz Property of The Resolvent and The Coherent Potential</td>
<td>22</td>
</tr>
<tr>
<td>B. The Traveling Cluster Approximation (TCA)</td>
<td>26</td>
</tr>
<tr>
<td>B.1 General Idea and The Meaning of The TCA</td>
<td>26</td>
</tr>
<tr>
<td>B.2 Formalism of The TCA</td>
<td>37</td>
</tr>
<tr>
<td>B.2.1 Single-Site Approximation (TCA(1))</td>
<td>37</td>
</tr>
<tr>
<td>B.2.2 The Traveling Cluster Approximation</td>
<td>40</td>
</tr>
<tr>
<td>Chapter 4: Method of Calculation for the Nearest-Neighbor Approximation (TCA(nn))</td>
<td>56</td>
</tr>
<tr>
<td>A. Two-Dimensional System</td>
<td>57</td>
</tr>
<tr>
<td>B. Three-Dimensional System</td>
<td>68</td>
</tr>
<tr>
<td>Chapter 5: Results, Discussion and Conclusion</td>
<td>84</td>
</tr>
<tr>
<td>A. Results and Discussion</td>
<td>84</td>
</tr>
<tr>
<td>B. Conclusion</td>
<td>101</td>
</tr>
</tbody>
</table>
# LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Graphs for $\langle G \rangle$ up to third order, using cumulant average.</td>
</tr>
<tr>
<td>2.2</td>
<td>Some of the correction factors to be included in the fourth and the fifth order cumulant</td>
</tr>
<tr>
<td>2.3</td>
<td>Fourth-order corrected cumulant average</td>
</tr>
<tr>
<td>2.4</td>
<td>Graphs appearing in the ATA</td>
</tr>
<tr>
<td>3.1</td>
<td>Cumulant graphs up to fourth order, representing the terms in the expansion of $W^{(1)}$ in Eq.(3.17)</td>
</tr>
<tr>
<td>3.2</td>
<td>Modified cumulant graphs up to fourth order, representing the terms in the expansion of $W^{(1)}$ in Eq.(3.18)</td>
</tr>
<tr>
<td>3.3</td>
<td>(a) Graph 'm' in $W^{(1)}$. (b) Graph in many-site problem involving 'm' for site i</td>
</tr>
<tr>
<td>3.4</td>
<td>The result for MCA involving two different site in CA's</td>
</tr>
<tr>
<td>3.5</td>
<td>An example of overlapping MCA's</td>
</tr>
<tr>
<td>3.6</td>
<td>MCA graphs representing contributions to the coherent potential up to fourth order</td>
</tr>
<tr>
<td>3.7</td>
<td>Some modified cumulant graphs in compact form</td>
</tr>
<tr>
<td>3.8</td>
<td>A cut and reflection for a particular modified cumulant graph</td>
</tr>
<tr>
<td>3.9</td>
<td>The expansion of $W_{xy}$</td>
</tr>
<tr>
<td>Figure</td>
<td>Page</td>
</tr>
<tr>
<td>--------</td>
<td>-------</td>
</tr>
<tr>
<td>3.10</td>
<td>41</td>
</tr>
<tr>
<td>3.11</td>
<td>42</td>
</tr>
<tr>
<td>4.1</td>
<td>60</td>
</tr>
<tr>
<td>5.1</td>
<td>87</td>
</tr>
<tr>
<td>5.2</td>
<td>89</td>
</tr>
<tr>
<td>5.3</td>
<td>91</td>
</tr>
<tr>
<td>5.4</td>
<td>93</td>
</tr>
<tr>
<td>5.5</td>
<td>97</td>
</tr>
<tr>
<td>5.6</td>
<td>99</td>
</tr>
<tr>
<td>B.1</td>
<td>106</td>
</tr>
<tr>
<td>B.2</td>
<td>109</td>
</tr>
<tr>
<td>C.1</td>
<td>112</td>
</tr>
</tbody>
</table>

The expansion of \( \chi_{xy} \)

Graphs representing contributions to \( \chi_{SS} \)

Two sets of sites needed in calculating \( (g(\epsilon_0))^{-1} \)

Density of states for a two-dimensional lattice with \( V^A = 3.8, V^B = 0, c_A = .0001, c_B = .9999 \)

Density of states for a three-dimensional lattice with \( V^A = 3.8, V^B = 0, c_A = .0001, c_B = .9999 \)

Density of states for a two-dimensional alloy with \( V^A = 1.75, V^B = 0, c_A = .25, c_B = .75 \)

Density of states in the B-subband for a two-dimensional alloy with \( V^A = 20, V^B = 0 \). (a) \( c_A = .285, c_B = .715 \). (b) \( c_A = .499, c_B = .501 \). (c) \( c_A = .713, c_B = .287 \)

Density of states for a three-dimensional alloy with \( V^A = .4, V^B = -.4, c_A = .16, c_B = .84 \)

Density of states for a three-dimensional alloy with \( V^A = .75, V^B = -.75, c_A = .1, c_B = .9 \)

Linear fit for \( f \) for the two-dimensional case

Linear fit for \( f \) for the three-dimensional case

Block diagram of the procedure for calculating \( Q_d \)
LIST OF TABLES

Table | Page
-----|-----
4.1  | Solutions of $x' - x = \Sigma \mu x - x$ for the two-dimensional system, for $\Sigma = \Sigma_0$ ................................. 58
4.2  | Solutions of $x' - x = \Sigma \mu x - x$ for the three-dimensional system, for $\Sigma = \Sigma_0$ ................................. 68
CHAPTER I
INTRODUCTION

During the last decade, there has been considerable interest in the electronic properties of alloys and in the development of theories for their description. Because of the loss of lattice periodicity in alloys, the methods of group theory which one relies on because of translational symmetry, are no longer applicable, so energy eigenstates are not simply characterized by their wave vectors $\mathbf{K}$; of course it follows that "$\mathbf{K}$-selection rules" are lost. This leads to lack of knowledge about eigenstates and the lack of any obvious systematic approximation scheme, like perturbation theory. In an amorphous alloy, as in a static model of a liquid, the structural disorder is fundamental—no basis lattice exists; this make them very complicated to study. We shall restrict attention to a substitutional alloy only.

Electronic properties of a substitutional alloy which are associated with the entire system, e.g., the density of states, contain within them a sampling of all configurations in the system. In calculating such properties, therefore, it is admissible to carry out averages over an ensemble of systems having all possible configurations. However, because of the lack of crystal symmetry, these properties, evaluated by statistical average over all configurations are difficult to calculate, so that various approximation have emerged. These approximations differ in the way the ensemble average is inserted into the structure of the calculations.
In 1931, Nordheim\textsuperscript{1} introduced the virtual crystal approximation. This assumes that the electrons in a binary alloy behave identically, as far as macroscopic properties are concerned, to the electrons in a hypothetical ordered material in which the crystalline potential is the average of the potentials of the pure materials. This approximation represents the lowest order term in a perturbation expansion of the coherent potential $W$ and is fairly successful in the case of the rigid band limit where the perturbed wave functions are quite extended in space so that each electron sees nearly the average perturbation. Progress in metallurgical science, as well as in the physics of dilute magnetic and nonmagnetic alloys, led to the need for a more realistic description than this approximation. Korringa\textsuperscript{2}, in 1958, and, independently, Beeby\textsuperscript{3}, in 1964, suggested the average $t$-matrix approximation, based on the assumption that the electrons in an alloy behave as if they were moving in a particular ordered system of localized potentials, the scattering matrix of which is the average of the scattering matrices of the localized potential corresponding to each constituent. This approximation was considered by Soven\textsuperscript{4}, who found that it is not a reasonable one for the case where the localized potentials have a strength approaching that found in transition metals.

In 1966, Yonezawa and Matsubara\textsuperscript{5}, by using what they called a 'cumulant expansion,' which is described in some detail below, gave a formal perturbation theory analysis leading to a systematic expansion of the coherent potential $W$. They found an approximation for $W$ by use of this method. Subsequently, Yonezawa\textsuperscript{6} found that the cumulant expansion method gives rise to spurious poles in the coherent potential and, indeed, that the coherent potential cannot be defined in an analytic
sense in that approximation. She therefore introduced the corrected or self contained cumulant expansion. In 1968, Leath\textsuperscript{7}, and Leath and Goodman\textsuperscript{8} gave the diagrammatic expansions paralleling Yonezawa's work.

The method called the coherent potential approximation (CPA) was proposed in 1967 by Soven\textsuperscript{4}, and independently by Taylor\textsuperscript{9} who called the method the self-consistent method in dealing with the phonon spectrum. This method was developed within the framework of multiple scattering theory as developed by Lax.\textsuperscript{10} It is based on replacing the atomic potential at each lattice site by an undetermined effective potential, to be known as the 'coherent potential.' The self-consistency condition is introduced by requiring that the coherent potential, when placed at each lattice site of the ordered lattice, will reproduce some of the macroscopic properties of the actual alloy. To determine the coherent potential in the original and simplest form of this approximation, one requires that a single scatterer imbedded in this effective medium should produce no further scattering on the average. Many authors\textsuperscript{11-13} agree that the CPA is the best method for a single-site approximation: the CPA is invariant with respect to the choice of the host lattice and has the correct limiting value for the perfect crystal and the split band case. It can serve as an interpolating scheme for the entire range of impurity concentration and scattering strengths. Furthermore, the CPA always yields a properly analytic mean resolvent.\textsuperscript{14,15} Nevertheless, the CPA is a single-site approximation and is thus incapable of describing effects due to multi-site scattering processes and correlations.

Many authors\textsuperscript{16-23} have attempted to generalize the CPA by including pair and cluster scattering. The first study of self-consistent pair scattering was by Aiyer et al\textsuperscript{16}, in 1969, who produced a general
diagrammatic technique for summing pair and other diagrams. There were some errors (not in the technique, but in the counting of pair diagrams) in the last section of this paper which have recently been corrected by Nickel and Krumhansl in 1971 and Leath in 1972. Nickel and Krumhansl also generalized the method to n-site approximation, which will be referred to as the 'n-site CPA,' or 'CPA(n).' In 1973, Nickel and Butler studied the CPA(n), and pointed out that in many cases the analyticity of the true mean resolvent is lost in this approximation. The presence of branch points off the real energy axis makes the approximation unacceptable, since physical quantities, such as the density of states, cannot be uniquely defined. Mills gave a more general formulation of the n-site CPA, and discussed briefly the problem of analyticity of the mean resolvent raised by Nickel and Butler.

In 1973, Leath found the condition for the equivalence of localized state and Bloch state expansions in generalized coherent potential approximations. This condition is that the coherent potential be cluster-diagonal. In the CPA this is satisfied since the coherent potential is site-diagonal. This condition is met also in the molecular CPA (MCPA) model of Tsukada. In this model, the crystal is divided into cells and considered as if it were a 'molecular crystal' composed of the cells and, then, the single-site CPA is applied to this 'mixed molecular crystal.' It has been proved that the MCPA is analytic. However the translational invariance of the coherent potential is not satisfied in the MCPA. The MCPA leads to rather heavy computations, and simplified forms of this approximation have therefore been used recently. Basically, the idea is to neglect the off-diagonal matrix elements of the coherent potential within a cluster and to keep a single
scalar self-consistent equation. Then the theory depends only on a single parameter $\mathcal{C}$, the site-diagonal coherent potential.

In Chapter 3, we shall discuss the approximation proposed by Mills in 1974, to deal with the problem of analyticity. In this approximation, the graphs of the corrected cumulant expansion are partially summed in such a way that the Herglotz property of the mean resolvent can be analyzed easily at each stage, and the proper modified graphs combined in such a way as to preserve this property in any desired level of approximation. In an n-site approximation ($n \geq 2$), it is found that any number of sites may be involved in a given graph, but in such a way that no more than $n$ cumulant averages overlap in any place along the graph. Each particular approximation in this scheme, like those in the n-site CPA, is characterized by some family $T$ of sets of sites $S$, but whereas the CPA(n) consists in allowing each entire graph to involve only sets $S$ belonging to $T$, the corresponding approximation in this scheme includes all graphs for which the overlapping cumulant averages involve only sets $S$ belonging to $T$. Because of the fact that a single graph may involve a sequence of clusters traveling arbitrarily large distances through the sample, such a specific approximation will be referred to hereafter as the 'Traveling Cluster Approximation (TCA).'

The single-site TCA, for which $T$ consists of all single-site sets, will be shown to be exactly equivalent to the single-site CPA.

In Chapter 4 the method is applied to a single band calculation, with nn interaction, and site diagonal disorder only, for the nearest-neighbor approximation (TCA(nn)) for both a two-dimensional and a three-dimensional binary alloy. By the nearest-neighbor approximation, we mean that $T$ is a family consisting of two classes of sets, namely sets
consisting of a single site and sets consisting of a nearest-neighbor pair, \( T=\{i\}, \{i,j\}, i \) adjacent to \( i \). Finally, Chapter 5 is devoted to results, discussion and conclusions. The nearest neighbor TCA gives a noticeably better fit to exact results than does the single-site CPA, showing somewhat more detail in the substructure of the density of states, and a better fit for the location of the band edges.
CHAPTER II
PREVIOUS WORK

A. Electronic States in a Binary Substitutional Alloy

Consider a binary substitutional A-B alloy. The resolvent $G$ is defined by

$$G(Z) = \frac{1}{Z - H}$$

or

$$G(z) = \sum_n \frac{|n\rangle \langle n|}{Z - E_n}$$

where $Z$ is a complex energy variable, $H$ a Hamiltonian for the alloy with a random potential $V$, and $n$ an energy eigenstate of the whole system, i.e., an eigenvector of $H$,

$$H = H_0 + V,$$

where $H_0$ is a Hamiltonian for a system with crystalline symmetry. The line under any quantity will be used to denote an operator or a matrix, and $I$ is the identity operator or matrix depending on the problem being considered.

We suppose that $H_0$ can be chosen in such a way that $V$ is a sum of single-site terms;

$$V = \sum_i V_i,$$

where $\sum_i$ is a sum over site $i$. We restrict ourselves to the case that there is no correlation among $V_i$'s at different site $i$. $V_i$ can be $V_i^A$ or $V_i^B$ with probability $c_A$ or $c_B (=1-c_A)$ respectively; $V_i^A$ is the potential
due to the presence of species A at site i and \( c_A \) is the concentration of species A.

The density of states \( \rho(E) \) can be expressed in terms of the resolvent defined above, as follows:

Consider

\[
\mathcal{G}(E) = \sum_n \frac{|n\rangle \langle n|}{E - E_n + i\epsilon},
\]

where \( \epsilon \) is a positive infinitesimal. By using the familiar relationship

\[
\frac{1}{E - E_n + i\epsilon} = \frac{P}{E - E_n} - i\pi \delta(E - E_n),
\]

where \( \frac{P}{E - E_n} \) indicates the principle value of \( \frac{1}{E - E_n} \), one gets

\[
\text{Im} \mathcal{G}(E) = -\pi \sum_n |n\rangle \delta(E - E_n) \langle n|,
\]

\[
-\frac{1}{\pi} \text{Tr}(\text{Im} \mathcal{G}(E)) = \text{Tr} \sum_n |n\rangle \delta(E - E_n) \langle n|,
\]

\[
= \sum_n \delta(E - E_n)
\]

\[
= \rho(E);
\]

the notation \( \text{Im} A \) is used for the antihermitian part of \( A \).

It is impractical to deal with the actual density of states, but experimental quantities of a disordered system have an essential common feature—they all involve sums involving all sites in a macroscopic sample. If the sample is sufficiently large, the sum samples all possible local environments, so that in the limit of infinite sample size it is the same as that which would be calculated by fixing sites but taking a configuration average over all possible configurations of arbitrary but finite size.
The average density of states is simply

\[ \langle \mathcal{P}(E) \rangle = -\frac{1}{\mathcal{V}} \text{Tr} \left( \text{Im} \langle \mathcal{G}(E) \rangle \right) , \]

where the average \( \langle \ldots \rangle \) is over all configurations of \( \mathcal{V} \).

Let

\[ \mathcal{G}_0 = \frac{1}{\mathcal{Z} - \mathcal{H}_0} ; \]

hence Eq.(2.1) yields,

\[ \mathcal{G} = \frac{1}{\mathcal{G}_0 - \mathcal{V}} \]

\[ = \mathcal{G}_0 (1-\mathcal{V}\mathcal{G}_0)^{-1} \] (2.3)

\[ \langle \mathcal{G} \rangle = \langle \mathcal{G}_0 (1-\mathcal{V}\mathcal{G}_0)^{-1} \rangle \]

\[ = \langle \mathcal{G}_0 \rangle + \langle \mathcal{G}_0 \mathcal{V}\mathcal{G}_0 \rangle + \langle \mathcal{G}_0 \mathcal{V}\mathcal{G}_0 \mathcal{V}\mathcal{G}_0 \rangle + \ldots . \] (2.4)

Various methods of approximate calculation of \( \langle \mathcal{G} \rangle \) differ in the way the configuration average is inserted into the structure of the calculation, and correspond to summations over certain sets of terms in this perturbation expansion. \( \mathcal{G}_0 \) is not involved in the average in Eq.(2.4) since it is nonrandom, so that

\[ \langle \mathcal{G} \rangle = \mathcal{G}_0 + \mathcal{G}_0 \langle \mathcal{V} \rangle \mathcal{G}_0 + \mathcal{G}_0 \langle \mathcal{V}\mathcal{G}_0 \mathcal{V} \rangle \mathcal{G}_0 \]

\[ + \mathcal{G}_0 \langle \mathcal{V}\mathcal{G}_0 \mathcal{V}\mathcal{G}_0 \mathcal{V} \rangle \mathcal{G}_0 + \ldots ; \] (2.5)

in general, of course, \( \mathcal{G}_0 \) and \( \mathcal{V} \) do not commute.

In order to find the average density of states, it suffices to know \( \langle \mathcal{G} \rangle \). In the next section we are going to discuss methods of
approximation for $\langle G \rangle$.

B. **Methods of Approximation for $\langle G \rangle$**

We define an equivalent effective potential $\bar{W}$, known as the coherent potential, by

$$\langle G \rangle = \frac{1}{G_0^{-1} - \bar{W}} ;$$ (2.6)

hence our problem is equivalent to finding an approximation for $\bar{W}$.

B.1 **Virtual Crystal Approximation (VCA)**

In 1931, Nordheim\(^1\) introduced the virtual crystal approximation. This assumes that the electrons in a binary alloy behave identically, as far as macroscopic properties are concerned, to the electrons in a hypothetical ordered material in which the crystalline potential is the average of the potentials of the pure materials.

This approximation, then, simply uses

$$\bar{W} = \sum_i V_i ,$$ (2.7)

where

$$V_i = c_A V_i^A + c_B V_i^B ,$$ (2.8)

and hence,

$$\langle G \rangle = \left( G_0^{-1} - \sum_i V_i \right)^{-1} .$$ (2.9)

This approximation represents the lowest order term in a perturbation series of $\bar{W}$, as will be seen later, and is fairly successful in the rigid band limit where the perturbed wave functions are quite extended in space so that each particle sees nearly the average perturbation. The usefulness of low-order perturbation theory is
very limited. 31

B.2 Average t- Matrix Approximation (ATA)

If a single-site t-matrix is defined by

$$t_i = V_i + V_i G_0 t_i$$  \hspace{1cm} (2.10)

$$= V_i (1 - G_0 V_i)^{-1}.$$  \hspace{1cm} (2.11)

Then the resolvent may be expressed (see Eq.(2.3)) by

$$G = G_0 + \sum_i G_0 t_i G_0 + \sum_{i \neq j} G_0 t_i G_0 t_j G_0 + \ldots.$$  \hspace{1cm} (2.12)

The mean resolvent, then, is

$$\langle G \rangle = G_0 + \sum_i G_0 \langle t_i \rangle G_0 + \sum_{i \neq j} G_0 \langle t_i t_j \rangle G_0 + \ldots.$$  

The restriction on the summation for the successive scatterings is because \( t \) contains all the scattering from a single site and further scattering must therefore be from another site.

The ATA was suggested independently by Korringa 2 and by Beeby 3; they calculated the \( t_i \)-matrices \( t_i^A \) and \( t_i^B \) for scattering off the potential \( V_i^A \) and \( V_i^B \) respectively, and then associating with each lattice site of the crystal the average t-matrix

$$\langle t_i \rangle = c_{A-1}^A t_i^A + c_{B-1}^B t_i^B.$$  

Thus the approximation for \( \langle G \rangle \) is made by using the replacement of the average of products of t-matrices by the products of the average t-matrix. One writes
\[ \langle G \rangle = G_0 + \sum_i G_0 \langle t_i \rangle G_0 + \sum_{j>i} \sum_k G_0 \langle t_j \rangle G_0 \langle t_k \rangle G_0 + \ldots \]  \hspace{1cm} (2.13)

From Eqs. (2.6) and (2.13), one gets

\[ \langle t_i \rangle = W_i (1 - G_0 W_i)^{-1}, \]  \hspace{1cm} (2.14)

this is the t-matrix for scattering from \( W \) at \( i \)th site,

or

\[ W_i = \langle t_i \rangle (1 + G_0 \langle t_i \rangle)^{-1}. \]  \hspace{1cm} (2.15)

We observe that the potential \( \sum_i W_i \) yields a resolvent equal to the mean resolvent \( \langle G \rangle \) in this approximation. This shows that it is a single-site approximation, in the sense that \( W \) is a sum of single-site terms involving only single-site scattering:

\[ W = \sum_i W_i \]

\[ = \sum_i \langle t_i \rangle (1 + G_0 \langle t_i \rangle)^{-1}. \]  \hspace{1cm} (2.16)

For a single band calculation, one gets

\[ \langle t_i \rangle = c_A t_i^A + c_B t_i^B \]

by Eq. (2.11),

\[ = c_A v_i^A (1 - (G_0)_{00} v_i^A)^{-1} + c_B v_i^B (1 - (G_0)_{00} v_i^B)^{-1} \]  \hspace{1cm} (2.17)

and

\[ W_i = \langle t_i \rangle (1 + (G_0)_{00} \langle t_i \rangle)^{-1}. \]  \hspace{1cm} (2.18)

Detailed numerical results on Eq. (2.17) are discussed by Elliot et al.\(^ {32} \) Soven\(^ {4} \) found that the ATA is not a reasonable approximation for the case where the localized potentials have a strength approaching that found in transition metals.
B.3 Cumulant and Corrected Cumulant Expansion

We now review the meaning of cumulant and corrected cumulant averages, which will be used here and later.

Suppose we want to find \( \langle \prod A_i \rangle \), where \( A_i \)'s are random variables, when there are correlations among the \( A_i \)'s, including the fact that several factors \( A_i \) may be associated with the same site \( i \). This can be written

\[
\langle \prod A_i \rangle = \prod \langle A_i \rangle + \text{correlations due to the correlation among the } A_i \text{'s}.
\]

These correlations give rise to terms that we call cumulant averages. The cumulant average is not the real average of anything, but a difference between the actual average and a sort of uncorrelated average. It is zero unless all of the factors are correlated in some way. Any average of a product of factors can be broken down into a sum of products of cumulant averages. Thus

\[
\langle A \rangle = \langle A \rangle^c \\
\langle AB \rangle = \langle A \rangle^c \langle B \rangle^c + \langle AB \rangle^c
\]

or \( \langle AB \rangle^c = \langle AB \rangle - \langle A \rangle^c \langle B \rangle^c \)

\[
\langle ABC \rangle = \langle A \rangle^c \langle B \rangle^c \langle C \rangle^c + \langle AB \rangle^c \langle C \rangle^c + \langle A \langle B \rangle^c \langle C \rangle^c \\
+ \langle A \rangle^c \langle BC \rangle^c + \langle ABC \rangle^c
\]

or \( \langle ABC \rangle^c = \langle ABC \rangle - \langle A \rangle^c \langle B \rangle^c \langle C \rangle^c - \langle AB \rangle^c \langle C \rangle^c \\
- \langle A \langle B \rangle^c \langle C \rangle^c - \langle A \rangle^c \langle BC \rangle^c, \)

and so forth. The suffix \( c \) indicates the 'cumulant average.' If two factors in a single cumulant average are statistically independent, then the cumulant average is zero.
By use of this kind of average, one gets, from Eq. (2.5),

\[
\langle \mathcal{G} \rangle = G_0 + G_0 \langle V \rangle \mathcal{G}_0 + G_0 \langle V \rangle \mathcal{G}_0 \langle V \rangle \mathcal{G}_0 + G_0 \langle VG_0 V \rangle \mathcal{G}_0 \\
+ G_0 \langle V \rangle \mathcal{G}_0 \langle V \rangle \mathcal{G}_0 \langle V \rangle \mathcal{G}_0 + G_0 \langle VG_0 V \rangle \mathcal{G}_0 \langle V \rangle \mathcal{G}_0 \\
+ G_0 \langle V \rangle \mathcal{G}_0 \langle VG_0 V \rangle \mathcal{G}_0 + G_0 \langle VG_0 \rangle \mathcal{G}_0 \langle V \rangle \mathcal{G}_0 \\
+ G_0 \langle VG_0 V \rangle \mathcal{G}_0 \langle V \rangle \mathcal{G}_0 + \cdots \quad \text{(2.19)}
\]

It is convenient to use graphs to represent the terms in the expansion of \( \langle \mathcal{G} \rangle \) in Eq. (2.19) as shown in Fig. (2.1).

![Graphs](image)

**Fig. 2.1** Graphs for \( \langle \mathcal{G} \rangle \) up to third order, using cumulant average.

In Fig. (2.1), each horizontal line segment represents a factor \( G_0 \), each vertex of the horizontal line represents a factor \( V \) and each point above the horizontal line represents a cumulant average involving the vertices that it connects. The graphs a-i represent the terms given explicitly in Eq. (2.19). In each graph, we refer to a portion joined to the rest of the graph by just one or two \( G_0 \) lines as 'a self-energy subgraph', and a self-energy subgraph which cannot be divided into smaller self-energy subgraphs joined only by \( G_0 \) lines, is called a 'proper self-energy graph.' A graph which involves no internal self-energy
subgraphs, such as Fig. (2.1(i)), is called an 'irreducible graph.'

We shall now obtain the expansion of $\mathcal{W}$ in terms of cumulant averages.

From Eq. (2.6), one gets

$$\langle G \rangle = G_0 + G_0 W G_0 + G_0 W G_0 W G_0 + \ldots .$$  \hspace{1cm} (2.20)

Comparing the graphical expansion of $\langle G \rangle$ in Fig. (2.1) with the expansion of $\langle G \rangle$ in terms of $W$'s in Eq. (2.20), one sees that $W$ is equal to the summation of the terms represented by all proper self-energy graphs only,

$$W = \sum_{n=1}^{\infty} \langle V (G_0 V)^{n-1} \rangle^P,$$

where $P$ indicates the sum of all proper self-energy graphs of the given order or, in a compact notation,

$$W = \langle V (1 - G_0 V)^{-1} \rangle^P .$$  \hspace{1cm} (2.21)

The cumulant average of arbitrary order cannot be expressed in closed form, and for an uncorrelated alloy, each cumulant average involves only a single site. A generating function for cumulant averages for a single band model was found by Yonezawa and Matsubara. They used the cumulant expansion and found $W$ in the level of what they called the first-order approximation, so called because only terms involving a single cumulant average are included in $W$, even though terms of all orders in $V$ are in fact included. This approximation includes all the effects of electron scattering caused by a single impurity, but does not take account of effects such that an electron scattered by an impurity is appreciably influenced by other impurities before the first scattering is completed.

Yonezawa found that there were some deficiencies in this 'first-order approximation', in that there appear spurious poles, and also that...
\( W \) is found not to be an analytic function of \( Z \). The difficulties result from the fact that the relation between the degree of approximation and the correction factors to the cumulant is not properly appreciated. This can be understood easily by considering the examples shown in Figs.(2.2(a)) and (2.2(b)).

![Diagram](attachment:image.jpg)

**Fig. 2.2** Some of the correction factors to be included in the fourth and the fifth order cumulant.

The graph in Fig.(2.2(a)) is not included in the first-order approximation, although the corrections to it are taken into account when the fourth order cumulant \( \langle V_G V_G V_G V_G \rangle^C \) is evaluated; similarly, the corrections to the five graphs in Fig.(2.2(b)) are included when the fifth order cumulant \( \langle V_G V_G V_G V_G V_G \rangle^C \) is evaluated, though the graphs themselves are not included.

This difficulty can be avoided by including such graphs as shown in Fig.(2.2) in the approximation. Yonezawa called this new approximation the 'self-contained first-order approximation', and it is generally known as a single-site approximation. Because of the necessity of including such graphs as shown in Fig.(2.2), Yonezawa introduced a 'corrected
cumulant average.' This average includes the cumulant average and the corresponding corrections of the same order, as shown, for example, in Fig. (2.3).

\[ \begin{align*}
&\text{i} \\
\equiv &\text{ } \\
&\text{i} \\
+ &\text{i} \\
\end{align*} \]

Fig. 2.3 Fourth-order corrected cumulant average.
A cross above the horizontal line refers to the corrected cumulant average.

B.4 Diagrammatic Methods

In 1958, Edwards introduced diagrammatic notation for classifying and collecting the terms in the perturbation expansion of the electronic properties of liquid metals and alloys. After that many authors have used such diagrams to help study the properties of disordered systems.

We have already used diagrammatic notation in the last section to keep track of interconnected cumulant averages. In this section it will be shown that the coherent potential in a single-site approximation can be found without using explicit forms for the cumulant averages, by using a diagrammatic analysis.

Eq. (2.21) can be changed into a self-consistent form involving \( \langle G \rangle \) itself by summing over internal self-energy subgraphs of \( W \), such as that appearing in Fig. (2.1(h)). We shall get the expansion of \( W \) in the terms corresponding to all irreducible graphs only, with \( G_0 \) replaced by \( \langle G \rangle \) everywhere in the graphs.
Hence Eq.(2.21) can be written as

\[ W = \langle V(1 - \langle G \rangle V)^{-1}\rangle^I, \]  

(2.22)

where I refers to all irreducible graphs.

Expanding Eq.(2.22), we get

\[ W = \langle V \rangle + \langle V \langle G \rangle V \rangle^I + \langle V \langle G \rangle V \langle G \rangle V \rangle^I + \ldots, \]  

(2.23)

or in the case of a single-site approximation,

\[
\begin{align*}
W & = \frac{1}{\xi} \sum W_i \\
W_i & = \langle V_i \rangle + \langle V_i \langle G \rangle V_i \rangle^I + \langle V_i \langle G \rangle V_i \langle G \rangle V_i \rangle^I + \ldots \\
& \quad + \ldots
\end{align*}
\]  

(2.24)

By using diagrammatic techniques, it can be shown that, by replacing \( \langle G \rangle \) by \( G_0 \), this leads to the ATA in section B.2 as shown in the following.

\[ <G> \]

![Diagram](image)

Fig. 2.4 Graphs appearing in the ATA. Circles above horizontal lines refer to true averages.
Each term of the right-hand side of Eq. (2.24) is associated with the corresponding row in Fig. (2.4), with the rule that $\langle G \rangle$'s are substituted for $G_0$'s.

In Fig. (2.4), each row contains graphs of a given order in $V$; the first column contains graphs which, by using Eq. (2.11), sum to $t_1$, the $n$th column $(n > 2)$ contains graphs with $n$ irreducible parts whose sum is given at the bottom of the column.

From Fig. (2.4), one gets

$$W_1 = \langle t_1 \rangle - W_1 G_0 W_1 - W_1 G_0 W_0 W_1 - W_1 G_0 W_1 C_0 W_1 - \ldots,$$

$$\langle t_1 \rangle = W_1 (1 + C_0 W_1 + C_0 W_1 C_0 W_1 + C_0 W_1 C_0 W_1 + \ldots),$$

$$\langle t_1 \rangle = W_1 (1 - G_0 W_1)^{-1}. \quad (2.25)$$

This is exactly the defining equation Eq. (2.14) for the ATA.

It can be shown that if $\langle G \rangle$ is inserted self-consistently into the internal lines, the result is exactly equivalent to the coherent potential approximation which will be discussed in the next section.

B.5 The Coherent Potential Approximation (CPA)

In 1967, Taylor and Soven developed a new method, within the framework of multiple scattering theory introduced by Lax, for the calculation of the mean resolvent. They introduced the concept of an effective or coherent potential which, when placed at each lattice site of the alloy lattice, will stimulate the electronic density of states in the case of Soven's work, or the phonon spectrum in the case of Taylor's, of the actual alloy. Soven called his method the coherent potential model while Taylor called his the self-consistent one.
Their method is equivalent to viewing the actual scattering potential as an impurity imbedded in an effective medium, whose propagator has a self-energy adjusted so that the t-matrix for scattering by a single site impurity in this medium is zero on the average; the scattering we are neglecting is that by pairs and higher clusters. One of the most interesting and useful points about the CPA is its invariance with respect to the choice of the host lattice and its correct limiting value in the perfect crystal and split band limits. Furthermore the CPA always yields a properly analytic mean resolvent.

In this approximation, we assume that there is an effective medium characterized by a resolvent \( G^0 \) which is related to a coherent potential \( \mathcal{W} \) through the Dyson equation

\[
G^0 = G_0 + G^0 \mathcal{W} G^0. \tag{2.26}
\]

In the ordinary, or single-site CPA, the coherent potential is assumed to be site-diagonal, but in general there will be off-diagonal elements. Now we write Eq.(2.3) for \( G \) in terms of \( G^0 \), eliminating \( G_0 \) via Eq.(2.26) with the result

\[
G = G^0 + G^0 (V - \mathcal{W}) G. \tag{2.27}
\]

By iterating and averaging Eq.(2.27), one gets

\[
\langle G \rangle = G^0 + G^0 \langle V - \mathcal{W} \rangle G^0 + G^0 \langle V - \mathcal{W} \rangle G^0 \langle V - \mathcal{W} \rangle G^0 + \ldots \ldots . \tag{2.28}
\]

There is an extra degree of freedom in that the coherent potential is arbitrary. Therefore, we choose \( \mathcal{W} \) in such a way as to best improve the convergence of Eq.(2.28). If \( \mathcal{W} \) is chosen to be the exact self-energy of \( \langle G \rangle \) in Eq.(2.26) then we would have \( \langle G \rangle = G^0 \) and the scattering terms in
Eq. (2.28) must cancel, that is the average $T$-matrix for the system must be zero. The CPA method is to calculate $\langle T \rangle$ in some approximation and set this to zero as a determining equation for $\hat{W}$.

In the single-site CPA, one decouples $\langle T \rangle$ into products of single-site $t$-matrices which are set to zero on average,

$$\langle t_t \rangle = \langle (v_i - \hat{W})(1 - G^0(v_i - \hat{W}))^{-1} \rangle = 0.$$  \hfill (2.29)

This equation is then solved simultaneously with Eq. (2.26) to find $G^0$ as the approximation for $\langle G \rangle$.

The CPA is a single-site approximation and is thus incapable of describing effects due to multi-site scattering processes and correlations. Many authors have attempted to generalize the CPA by including pair and cluster scattering. Nickel and Krumhansl generalized the method to an n-site approximation. Mills gave a more general formulation of the n-site CPA, and discussed briefly the problem of analyticity of the mean resolvent raised by Nickel and Butler.

Nickel and Butler discovered through numerical computations that these approximations give rise to a mean resolvent that lacks the required analyticity off the real axis for strong disorder; which means in particular that it is impossible to define a single solution of the self-consistent equations. It should be pointed out that this problem had previously been reported in a somewhat similar calculation by Šapek.

In the next chapter, we shall review the analyticity properties of the resolvent and the coherent potential, and discuss in detail an approximation which keeps these analyticity properties.
A. The Herglotz Property of The Resolvent and The Coherent Potential

An operator or matrix-valued function \( f(Z) \) will be referred to as Herglotz if for all \( Z \) in the cut plane, \( \text{Im} \, Z \neq 0 \), it has the following properties:

1. \( f(Z) \) is analytic,
2. \( \text{Im} \, f(Z)/\text{Im} \, (Z) < 0 \),
3. \( f(Z) \) satisfies the reality condition

\[
\dagger f(Z) = f(Z^*)
\]

Following Ducastelle, we show that \( G \) and \( W \) have these properties.

The resolvent \( G \) is given [Eq.(2.1)] by

\[
G(Z) = \frac{1}{ZI - H} = \sum_n \frac{|n\rangle \langle n|}{Z - E_n} = \int \frac{1}{Z - \omega} P(\omega) \, d\omega,
\]

where

\[
P(\omega) = \sum_n |n\rangle \delta(\omega - E_n) \langle n|.
\]

It is immediately evident that \( G(Z) \) obeys conditions (1) and (3) above. We now study condition (2). We have

\[
\text{Tr} P(\omega) = \text{Tr} \sum_n |n\rangle \delta(\omega - E_n) \langle n|
\]
where $\rho(\omega)$ is the density of states.

For any state $\psi$, we have, by Eq.(3.3),

$$
\langle \psi | \mathcal{F} | \psi \rangle = \sum_n \langle n | \psi \rangle^2 \delta(\omega - E_n) > 0; \quad (3.4)
$$

so that $\mathcal{F}$ is a positive semi—definite operator. From Eq.(3.2), we get

$$
G(Z) = \int_{-\infty}^{\infty} \frac{(E - iY - \omega) \rho(\omega) d\omega}{|Z - \omega|^2},
$$

where $Z = E + iY$,

$$
\text{Im } G(Z) = \int_{-\infty}^{\infty} \frac{-Y \rho(\omega) d\omega}{|Z - \omega|^2}. \quad (3.5)
$$

Suppose for some $|\psi\rangle$, we have

$$
\int_{-\infty}^{\infty} \frac{\langle \psi | \mathcal{F} | \psi \rangle d\omega}{|Z - \omega|^2} = 0,
$$

this implies $\langle \psi | \mathcal{F} | \psi \rangle = 0$ for all $\omega$; substituting $\rho(\omega)$ from Eq. (3.3), we get

$$
\sum_n \delta(\omega - E_n) |\langle n | \psi \rangle|^2 = 0
$$

$$
\langle n | \psi \rangle = 0 \quad \text{for all } n
$$

or

$$
\psi = 0,
$$

which is not a state as supposed. Hence we have, from Eq.(3.5),

$$
\text{Im } G(Z) \leq 0 \quad \text{for } \text{Im } Z \geq 0. \quad (3.6)
$$
From Eq. (3.1), for any given point \( Z \) off the real axis \( G^{-1}(Z) \) is analytic, with \( \| G^{-1}\psi \| \geq Y \) for all vectors \( \psi \), from which it follows that \( \| G(Z) \| \) cannot become infinite, and that \( G(Z) \) is analytic. It does not matter which sign of \( Y \) we consider but \( \text{Im} \ G(Z)/Y \) must keep its negative definiteness for all \( Y \neq 0 \). (\( A \) is a positive definite if \( \langle A\psi|\psi \rangle > 0 \) for all states \( |\psi \rangle \) of the Hilbert space; here the notation \( A > 0 \) will always mean that \( A \) is positive definite.)

Let us consider \( Z \) in the upper-half plane. In Chapter 2, the coherent potential \( W \) is defined by

\[
\langle G(Z) \rangle = \langle (G_0^{-1} - Y)^{-1} \rangle
\]

\[
= (G_0^{-1} - Y)^{-1}
\]

where

\[
G_0^{-1} = ZI - H_0.
\]

\( \langle G \rangle \) can have no zero eigenvalue, for \( \text{Im} \ Z \neq 0 \), and therefore, basically because \( \langle G \rangle^{-1} \) is nonsingular, \( W \) is found also to be analytic.

Now we are going to find the sign of \( \text{Im} \ W(Z) \).

Consider

\[
\text{Im} \langle G \rangle = \langle G^\dagger \text{Im} (\langle G \rangle^\dagger)^{-1} \langle G \rangle \rangle
\]

\[
= \langle G^\dagger \text{Im} (G_0^{-1} - W^\dagger) \langle G \rangle \rangle
\]

\[
= - \langle G^\dagger (YI - W_2) \langle G \rangle \rangle,
\]

where

\[
W_2 = \text{Im} W.
\]

For \( Z = E + i0 \), we get

\[
\text{Im} \langle G \rangle = \langle G \rangle^\dagger W_2 \langle G \rangle,
\]

by Eq. (3.6), \( \leq 0 \)

or \( W_2(E + i0) \leq 0 \). (3.7)
Since $\mathbb{W}$ is analytic and, by Eq. (2.21), $\mathbb{W} \to \mathbb{V}$ when $|Z|$ becomes infinite, it follows that for $Y > 0$, $\mathbb{W}(Z)$ can be expressed by a dispersion relation:

$$\mathbb{W}(Z) = \langle \mathbb{V} \rangle - \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\mathbb{W}_2(E + i0) \, dE'}{Z - E'}$$

$$\mathbb{W}_2(Z) = -\frac{1}{\pi} \text{Im} \int_{-\infty}^{\infty} \frac{(E - E' - iY) \, \mathbb{W}_2(E' + i0) \, dE'}{|E - E' + iY|^2}$$

$$= \frac{Y}{\pi} \int_{-\infty}^{\infty} \frac{\mathbb{W}_2(E + i0) \, dE'}{|Z - E'|^2}$$

by Eq. (3.7), $\langle 0 \rangle$, (3.8)

unless $\mathbb{W}_2(E + i0) = 0$ for all $E$, which is the case only for a perfect crystal.

Eq. (3.1) shows that $\mathbb{G}^{\dagger}(Z)$ is equal to $\mathbb{G}(Z^*)$ or $\langle G(Z) \rangle^* = \langle G(Z^*) \rangle$.

It follows readily that $\mathbb{W}$ has the same property:

$$\mathbb{W}(Z) = Z I - H_0 - \langle G(Z) \rangle^{-1}$$

$$\mathbb{W}(Z^*) = Z^* I - H_0 - \langle G(Z^*) \rangle^{-1}$$

$$= (Z I - H_0 - \langle G(Z) \rangle^{-1})^\dagger$$

$$= \mathbb{W}^{\dagger}(Z).$$

In the same way, these properties can be shown for $Z$ in the lower-half plane. This completes our proof for the Herglotz property of the resolvent and the coherent potential.
B. The Traveling Cluster Approximation (TCA)

B.1 General Idea and The Meaning of The TCA

In section A, it was shown that off the real axis \( G \) and \( W \) are analytic. Now we come to the problem how to keep \( W \) analytic formally in an approximation for \( G \).

From the expression (2.21) for \( W \), we see that the perturbation expansion of \( W \) has the general form

\[
W = \sum f_{ij...kl} V_i G_0 V_j G_0 ... G_k G_0 V_1,
\]

where the coefficients \( f_{ij...kl} \) are real factors arising from the various cumulant averages appearing in \( \langle \mathcal{V}(1 - G_0 V) \rangle^{-1} \). Hence we have

\[
\text{Im } W = \frac{1}{2i} \left[ \sum f_{ij...kl} V_i G_0 V_j G_0 ... G_k G_0 V_1 \right. \\
- \left. \sum f_{1k...ji} V_{i0} G_0 V_{j0} ... G_{k0} G_0 V_{1} \right]
\]

Because of the left-right symmetry of the graphical expansion, we get

\[
f_{1k...ji} = f_{ij...kl}.
\]

Hence, since \( \frac{1}{2i} (G_0 - G_0^+) = -G_0^+(\text{Im } G_0^{-1})G_0 \), we have

\[
\text{Im } W = \frac{1}{2i} \sum f_{ij...kl} \left[ V_i (G_0 - G_0^+) V_j G_0 ... G_k G_0 V_1 \right.
- \left. V_{i0} G_0 V_{j0} ... G_{k0} G_0 V_{1} \right]
\]
where $Y = G_{0}^{+}(\Im G_{0}^{-1})G_{0} > 0$, for $\Im Z > 0$.

Each term within the brackets in Eq.(3.9) can be separated into two parts, separated by a factor $Y$, which we shall call $R_{\beta}$ and $R_{\alpha}$. Hence, from Eq.(3.9), we can write
\begin{equation}
\Im \tilde{W} = - \sum_{ij...kl} c^{\alpha}_{\beta} R^{\alpha}_{\beta} Y R_{\alpha},
\end{equation}
where $c^{\alpha}_{\beta}$ is a real symmetric coefficient. From (3.8) $\Im \tilde{W}$ must be negative-definite in order to preserve the Herglotz property of $G(Z)$.

In any approximation to $\tilde{W}$, if we can select the factor $f_{ij...kl}$ in Eq.(3.9) in such a way that $\Im \tilde{W}$ has the form
\begin{equation}
\Im \tilde{W} = - \sum_{\alpha\beta} R^{\alpha}_{\beta} Y R_{\alpha},
\end{equation}
this will make $\Im \tilde{W} < 0$, and thus satisfy a crucial necessary (though not sufficient) condition for Herglotzicity. If we can do this, then we shall at least have some hope of keeping $G(Z)$ analytic, which we need in order to have $\langle G(Z) \rangle$ yield meaningful physical quantities, in an approximation of $\tilde{W}$.

In order to look for a suitable rearrangement of terms of the form we want, we shall study first the one-site problem, the system
which consists of only one site with the potential $V^A$ or $V^B$ with the probability $c_A$ or $c_B$ respectively, $c_A + c_B = 1$.

Letting $\mathcal{G}^{(1)}$ and $\mathcal{W}^{(1)}$ be the resolvent and the coherent potential respectively for a one-site problem, we have

$$\mathcal{G}^{(1)} = (\mathcal{G}_0^{-1} - \mathcal{W}^{(1)})^{-1}$$

$$= \langle (\mathcal{G}_0^{-1} - \gamma)^{-1} \rangle$$

$$= c_A (\mathcal{G}_0^{-1} - \gamma^A)^{-1} + c_B (\mathcal{G}_0^{-1} - \gamma^B)^{-1},$$

where $\gamma^A = V^A_{\text{I}}$ and $\gamma^B = V^B_{\text{I}}$. Rearranging terms, we get

$$(\mathcal{G}_0^{-1} - \gamma^{(1)})^{-1} = (\mathcal{G}_0^{-1} - \gamma^A)^{-1} \left[ c_A (\mathcal{G}_0^{-1} - \gamma^B) + c_B (\mathcal{G}_0^{-1} - \gamma^A)^{-1} \right]$$

$$= (\mathcal{G}_0^{-1} - \gamma^A)^{-1} \left[ (\mathcal{G}_0^{-1} - (c_A \gamma^B + c_B \gamma^A)) (\mathcal{G}_0^{-1} - \gamma^B)^{-1} \right]$$

where $\gamma = c_A \gamma^B + c_B \gamma^A$.

Inverting, we get

$$(\mathcal{G}_0^{-1} - \mathcal{W}^{(1)}) = (\mathcal{G}_0^{-1} - \gamma^B)(\mathcal{G}_0^{-1} - \gamma^A)^{-1}(\mathcal{G}_0^{-1} - \gamma^A)$$

$$= \left[ 1 - (\gamma^B - \gamma^A)(\mathcal{G}_0^{-1} - \gamma^A)^{-1} \right](\mathcal{G}_0^{-1} - \gamma^A)$$

$$= \mathcal{G}_0^{-1} - \gamma^A - (\gamma^B - \gamma^A) \left[ 1 - (\mathcal{G}_0^{-1} - \gamma^A)^{-1}(\gamma^A - \gamma^A)^{-1} \right]$$

$$= \mathcal{G}_0^{-1} - \gamma^A - \gamma^B + \gamma^A + (\gamma^B - \gamma^A)(\mathcal{G}_0^{-1} - \gamma^A)^{-1}(\gamma^A - \gamma^A).$$

(3.12)

But

$$\gamma^A + \gamma^B - \gamma = c_A \gamma^A + c_B \gamma^B = \gamma$$

(3.13)

and

$$\gamma^B - \gamma = -c_B (\gamma^A - \gamma^B),$$

$$\gamma^A - \gamma = c_A (\gamma^A - \gamma^B).$$

(3.14)
So that, from Eqs. (3.12)-(3.15), we get
\[ W^{(1)} = \bar{\nu} + c_{A} c_{B} (\nu^{A} - \nu^{B})(\bar{\nu}_{0}^{-1} - \bar{\nu})^{-1}(\nu^{A} - \nu^{B}). \]

We let \( \Delta \nu = \sqrt{c_{A} c_{B}} (\nu^{A} - \nu^{B}) \), and get, finally,
\[ W^{(1)} = \bar{\nu} + \Delta \nu (\bar{\nu}_{0}^{-1} - \bar{\nu})^{-1} \Delta \nu \]
\[ = \bar{\nu} + \sum_{\eta=0}^{\infty} \Delta \nu \bar{\nu}_{0}^{-\eta} \Delta \nu. \] (3.16)

Now we do the same problem using the cumulant expansion method in order to see the relationship between the forms of \( W^{(1)} \) in those ways. For the one-site problem in the cumulant expansion, by use of Eq. (2.21), we get
\[ W^{(1)} = \langle v(1 - G_{0} v) \rangle^{p} \]
\[ = \langle v \rangle^{p} + \langle vG_{0} v \rangle^{p} + \langle vG_{0} vG_{0} v \rangle^{p} \]
\[ + \langle vG_{0} vG_{0} vG_{0} v \rangle^{p} + \ldots. \] (3.17)

As shown in the last chapter, this expansion can be represented by graphs as shown in Fig. (3.1).

\[ W^{(1)} = \sum_{\eta=0}^{\infty} \Delta G_{0}^{(\eta)} \]

Fig. 3.1 Cumulant graphs up to fourth order, representing the terms in the expansion of \( W^{(1)} \) in Eq. (3.17).
We have
\[ \langle V \rangle = w_1^{(1)} \]
\[ \langle VG_0V \rangle^P = w_2^{(1)} \]
\[ \langle VG_0VG_0V \rangle^P = w_3^{(1)} + w_4^{(1)} \]
\[ \langle VG_0VG_0VG_0V \rangle^P = w_5^{(1)} + w_6^{(1)} + w_7^{(1)} + w_8^{(1)} + w_9^{(1)} + w_{10}^{(1)} \]

For the new arrangement of \( \bar{W}^{(1)} \) in Eq.(3.16), it has the form
\[ \bar{W}^{(1)} = \bar{V} + \Delta VG_0AV + \Delta VG_0\tilde{V}G_0AV + \Delta VG_0\tilde{V}G_0\tilde{V}G_0AV \]
\[ + \ldots \ldots \ldots \ldots \] (3.18)

From Eqs.(3.17) and (3.18), we have
\[ \bar{V} = \langle V \rangle \]
\[ \Delta VG_0AV = \langle VG_0V \rangle^P \] (3.19)
\[ \Delta VG_0\tilde{V}G_0AV = \langle VG_0VG_0V \rangle^P \] (3.20)
\[ \Delta VG_0\tilde{V}G_0\tilde{V}G_0AV = \langle VG_0VG_0VG_0V \rangle^P \] (3.21)

This same form can be used in the analysis of the many-site problem, and permits each term in \( \bar{W} \) to be written as a sequence of simple factors whose form is independent of the order of the term. This in turn means that the components \( R_{\Lambda} \) and \( c_{\Lambda,\Phi} \) of Eq.(3.10) can be identified, and expressions of the form (3.11) obtained by a judicious choice of terms to be included in a given approximation scheme.

It is convenient for this purpose to invent a new type of graphs which includes, in a single graph, all the overlapping cumulant average graphs involving a single site. We shall call these new graphs
'modified cumulant graphs' and the average obtained in this manner 'the modified cumulant average (MCA). No MCA's involving the same site may overlap; as we shall see this facilitates an analysis of the Herglotz properties of \( \overline{y} \).

In Fig. (3.2), each horizontal line segment represents a factor \( G_0 \), and the vertex of the vertical line in the first-order MCA represents \( \overline{y} \). In a higher-order MCA the initial and final vertices represent factors \( \Delta y \), while the intervening vertices, if any, represent factors \( \overline{y} \). Each heavy dot above the horizontal line represents a modified cumulant average involving the vertices connected by it.

We have, then,

\[
\begin{align*}
\overline{y} &= \overline{w}_a^{(1)} \\
\Delta y G_0 \Delta y &= \overline{w}_b^{(1)} \\
\Delta y G_0 \overline{y} G_0 \Delta y &= \overline{w}_c^{(1)} \\
\Delta y G_0 \overline{y} G_0 \Delta y &= \overline{w}_d^{(1)}
\end{align*}
\]

Fig. 3.2 Modified cumulant graphs up to fourth order, representing the terms in the expansion of \( \overline{w}^{(1)} \) in Eq.(3.18).
The relationship between the new and the old expansion is the following:

\[ W_a^{(1)} = W_1^{(1)} \]
\[ W_b^{(1)} = W_2^{(1)} \]
\[ W_c^{(1)} = W_3^{(1)} + W_4^{(1)} \]
\[ W_d^{(1)} = W_5^{(1)} + W_6^{(1)} + W_7^{(1)} + W_8^{(1)} + W_9^{(1)} + W_{10}^{(1)} \]

We call the number of interactions in any term in the expansion of \( W \) 'the order of that term', which is also the order of the corresponding graphs; hence an MCA of order \( n \) is equal to the summation of all overlapping single-site CA's of order \( n \).

Next we shall show that we can use the one-site result to construct the generalization for the many-site problem.

Consider a graph 'm' of order \( n \) in the one-site problem, consisting of some set of overlapping CA's and corresponding to a term \( f^m_{\eta p} \cdots \nu G_0 \nu G_0 \cdots G_0 \nu \) in \( W^{(1)} \) (see Fig.(3.3(a)). If the same graph appears in the many-site problem associated with the site \( i \), say, though with vertices involving other sites interspersed (see Fig.(3.3(b))), we can sum terms
of order n involving only the same site, then the result is the same as for the one-site problem.

\[
\sum_{i-\text{CA's}} \sum_{j-\text{CA's}} = \sum_{i-\text{CA's}} \sum_{i-\text{CA's}}
\]

Fig. 3.4 The result for MCA involving two different sites in CA's, \( \bigcup \) representing all proper \( n \) graphs of order n.

It is seen that it does not matter if there are other interspersed vertices or not, and that we can still use the same notation and terminology for an MCA in this case as for the one-site problem. It is still all right even though there are any number of overlapping MCA's as illustrated in Fig. (3.5).

Fig. 3.5 An example of overlapping MCA's, 

\[ i \neq j, j \neq k, (i \text{ may equal } k). \]
Now we define that an MCA of order \( n \) is equal to the summation of all overlapping single-site CA's of order \( n \), and that no MCA's involving the same site may overlap. Hence from Eq.(2.21)

\[
W = \langle \mathbf{V}(1 - G_0\mathbf{V})^{-1} \mathbf{P} \rangle \\
= \langle \mathbf{V} \rangle + \langle G_0\mathbf{V} \rangle^P + \langle G_0\mathbf{V}G_0\mathbf{V} \rangle^P + \langle G_0\mathbf{V}G_0\mathbf{V}G_0\mathbf{V} \rangle^P + \ldots,
\]

where \( \mathbf{V} = \sum \mathbf{V}_i \), we get in terms of MCA's,

\[
W = \sum \mathbf{V}_i + \sum \Delta \mathbf{V}_i G_0 \mathbf{V}_1 + \sum \Delta \mathbf{V}_i G_0 \mathbf{V}_1 G_0 \mathbf{V}_1 + \sum \Delta \mathbf{V}_i G_0 \mathbf{V}_1 G_0 \mathbf{V}_1 G_0 \mathbf{V}_1 \\
+ \sum \Delta \mathbf{V}_i G_0 \mathbf{V}_1 G_0 \mathbf{V}_1 G_0 \mathbf{V}_1 G_0 \mathbf{V}_1 G_0 \mathbf{V}_1 + \sum \Delta \mathbf{V}_i G_0 \mathbf{V}_1 G_0 \mathbf{V}_1 G_0 \mathbf{V}_1 G_0 \mathbf{V}_1 G_0 \mathbf{V}_1 G_0 \mathbf{V}_1 + \ldots,
\]

where the terms listed explicitly, namely all the terms up to fourth order, correspond to the graphs shown in Fig.(3.6).

![MCA graphs representing contributions to the coherent potential up to fourth order.](image)

Fig. 3.6 MCA graphs representing contributions to the coherent potential up to fourth order.

We see that each MCA is a linear sequence of factors independent of the order of the term; this helps us approximate \( W \) by keeping certain classes of terms in Eq.(3.16) in such a way that \( \text{Im} \ W \) has the form
(3.11). Each term in the expansion of $\text{Im } W$ in Eq. (3.9) can be separated into two parts with $Y$ in between; in each term, we shall call the part to the right of $Y$ a 'right hand part', and the part to the left of $Y$ a 'left hand part'.

Let $S$ be a certain set of terms in the expansion of $W$, which we want to include in an approximation for $W$. It will guarantee that we have the form (3.11) if the sum of those terms satisfies the following 'consistency condition': if the terms in $\text{Im } W$ generated from $S$ that have $r_i$ as a left hand part have right hand parts adding up to $R_i$, then $R_i$ must include $r_i$, and $S$ is also such that all of the terms in $-R_i Y R_i$ are generated. The parts of a graph corresponding to $r_i$ and $r_i$ will be referred to as 'mirror images' of each other.

For greater clarity in considering complicated graphs, we now introduce a more compact graphical notation for modified cumulant graphs. We omit the electron line altogether, and replace each MCA by a single horizontal line labeled with the site involved, with dots to represent the successive vertices. This new notation is illustrated in Fig. (3.7).

Fig. 3.7 Some modified cumulant graphs in compact form.
In taking the antihermitian part of $\tilde{W}$, as we have seen in Eq. (3.9), we see that each factor $\mathcal{G}_0$ in turn gives rise to a factor $\mathcal{Y}$, which may be represented by a vertical cut in the corresponding graph for $\tilde{W}$. The parts of the graph with a cut in between will, if a cut works as a mirror for both sides, reflect and give their own image. This can be seen, for example, in Fig. (3.8), where, if graph (a) is to be included then graphs (b) and (c) must also, in order to satisfy the consistency condition.

![Graphs (a), (b), and (c)](image)

**Fig. 3.8** A cut and reflection for a particular modified cumulant graph.

(a) A cut.

(b) A reflection of the left hand part.

(c) A reflection of the right hand part.

We see that from a single graph, the consistency condition can be used to generate additional graphs by cutting and reflecting repeatedly; if we define the 'rank' of any graph in a graphical expansion of $\tilde{W}$ as the maximum number of sites overlapped, i.e., the maximum number of MCA lines that can be intersected by a vertical cut, then the consistency condition never generates graphs of greater rank than we started with, as illustrated in Fig. (3.8). In fact, if we say that the sets $S$ 'involved' in a graph are those sets of sites intersected
by different vertical cuts, then a graph involving sets \( S_1, S_2, \ldots S_r \) can only generate graphs involving the same sets \( S_1, S_2, \ldots S_r \). Such families of sets will be called \( T \).

Each particular approximation in this scheme, like those in the n-site CPA, is characterized by some family \( T \) of sets of sites \( S \), but whereas the CPA(n) consists in allowing each entire graph to involve only a single set \( S \) belonging to \( T \), the corresponding approximation in this scheme includes all graphs for which the overlapping cumulant averages involve only sets \( S \) belonging to \( T \). Because of the fact that a single graph, through cutting and reflecting repeatedly in order to preserve the consistency condition, may involve a sequence of clusters traveling arbitrarily large distances through the sample, such a specific approximation will be referred to hereafter as a 'Traveling Cluster Approximation (TCA)'.

The formalism of this approximation will be given in the next section.

B.2 Formalism of The TCA

B.2.1 Single-Site Approximation (TCA(1))

A single-site approximation is the approximation which includes all the effects of electron scattering caused by a single impurity, but does not take account of effects such that an electron scattered by an impurity is appreciably influenced by other impurities before the first scattering is completed, except in an averaged way through the use of an effective medium.

Suppose \( W_i \) is the coherent potential associated with site \( i \); one get, for a single-site approximation,

\[
W = \sum_i W_i .
\] (3.23)
Considering the scattering from site \(i\), we can adapt Eq. (3.16) into
\[
W_1 = \tilde{V}_1 + \sum_{n=0}^{\infty} \Delta V_1 G_0 (\tilde{V}_1 G_0)^n \Delta V_1 ,
\]

it can be shown that this equation is equivalent to Eq. (2.15) for the ATA in Chapter 2.

The electron may be thought of as traveling with a self-consistent propagator (resolvent) that includes the coherent potential of all other sites except of its own. Hence we have
\[
W_1 = \tilde{V}_1 + \sum_{n=0}^{\infty} \Delta V_1 \hat{G}^{(i)} (\tilde{V}_1 \hat{G}^{(i)})^n \Delta V_1 ,
\tag{3.24}
\]

where
\[
\hat{G}^{(i)} = (G_0^{-1} - (\hat{W} - \tilde{W}_1))^{-1}
\tag{3.25}
\]
or
\[
\hat{W}^{(i)} = (G_0^{-1} - \hat{W}^{(i))})^{-1}
\tag{3.26}
\]

where
\[
\hat{W}^{(i)} = \hat{W} - \tilde{W}_1 .
\tag{3.27}
\]

Eqs. (3.24)-(3.27) can be used to find \(\hat{W}\), and \(\langle \hat{G} \rangle\) can then be found from
\[
\langle \hat{G} \rangle = (G_0^{-1} - \hat{W})^{-1}.
\]

Since
\[
\hat{W} = \tilde{V} + \Delta V (G_0^{-1} - \tilde{V})^{-1} \Delta V
\]
is equivalent to
\[
(G_0^{-1} - \hat{W})^{-1} = \langle (G_0^{-1} - \tilde{V})^{-1} \rangle,
\]
it follows that
\[
W_1 = \tilde{V}_1 + \Delta V_1 (\hat{G}^{(i)} - \tilde{V}_1)^{-1} \Delta V_1
\]
is equivalent to
\[
(\hat{G}^{(i)} - \tilde{W}_1)^{-1} = \langle (\hat{G}^{(i)} - \tilde{V}_1)^{-1} \rangle .
\]
By Eq. (3.25), the left and the right sides are equal to $\langle G \rangle$ and

$$\langle (G)^{-1} - (V_1 - W_1) \rangle^{-1}$$

respectively. So the TCA(1) is equivalent to

$$\langle G \rangle = \langle (G)^{-1} - (V_1 - W_1) \rangle^{-1}$$

which is just the form (2.28), with $G^0$ replaced by $\langle G \rangle$, as described in the following paragraph on page 20. This shows that the CPA and the TCA(1) are exactly equivalent to each other.

We now investigate what happens to CPA(n) when the consistency condition is applied. For example, consider the two-site CPA including nearest-neighbor pairs only (CPA(nn)). Considering those terms that do not include self-energy subgraphs, we see that CPA(nn) includes all the graphs that involve just two sites $i$ and $j$, say, for every nearest-neighbor pair $i,j$. But $i$ will have at least one other nearest neighbor $k$, say, and on application of the consistency condition, this requires including a large number of terms involving all three sites which are not included in CPA(nn); the same difficulty is found in any n-site CPA when $n \gg 2$. This gives the possibility of non-negative definiteness of $\text{Im} W$, and, hence, gives an indication why nonanalyticity is observed as mentioned in Chapter 2.

TCA(T) does satisfy the consistency condition regardless of whether a self-consistent resolvent is used, provided the family $T$ has certain properties (Specifically, inclusion of all subsets of any set in $T$). This does not, of course, require translational invariance, but we shall only be interested in translationally invariant choices of $T$. 
B.2.2 The Traveling Cluster Approximation (TCA)

We now introduce some terms which will be helpful in the formalism of the approximation.

For convenience, as will be seen later, we let x, y, and z instead of i, j, and k represent lattice sites or lattice displacement. Let U be a set of all sites in sample, S be the complementary set to S with respect to U, and \(S^*\) be the set of elements \(x^*\) which either are in S or satisfy the condition that the set consisting of \(x^*\) and the elements of S is in T.

\[ S^* = \{ x^* \mid x^* \cup S \in T \} \]

Let \(\tilde{S}\) be \(S^* \cap \overline{S}\); \(\tilde{S}\) is called the 'neighborhood' of S.

We have

\[ \langle G \rangle = (G^{-1}_0 - W)^{-1} \]

\[ W = \sum_{x,y} W_{xy}, \]

where \(W_{xy}\) is the part of the coherent potential which, in the expansion of \(W\), consists of all terms corresponding to those graphs with final site x and initial site y. We see that \(W_{xy}\) has the form (illustrated in Fig. (3.9)):

\[ W_{xy} = \tilde{V} \frac{\partial G}{\partial x_{xy}} + \Delta V \frac{G_{xy}}{x_{xy}} \Delta V_y, \]

**Fig. 3.9** The expansion of \(W_{xy}\).
where $\mathcal{G}_{xy}$ includes all possible sequences of vertices, consistent with the approximation, between $x$ and $y$. We see that there are four possibilities for $\mathcal{G}_{xy}$: the first one is that there are no intervening vertices and $x$ and $y$ are the same; the second one, that there is a factor $\tilde{V}_x$ on the left and after that $\mathcal{G}$ repeats itself; the third one, that there is a factor $\tilde{V}_z$ on the left and after that $\mathcal{G}$ repeats itself; and the last one, that there is a factor $\Delta V_z$ on the left and the remainder of the graph for $\mathcal{G}$ will depend not only on $x$ at the left hand side, but also on $z$. This is shown in Fig. (3.10).

![Figure 3.10](image)

**Fig. 3.10** The expansion of $\mathcal{G}_{xy}$.

In Fig. (3.10), we get the equation for $\mathcal{G}_{xy}$,

$$
\mathcal{G}_{xy} = \mathcal{G}_0 \left[ \tilde{G}_{xy} + \tilde{V}_x \tilde{G}_{xy} + \sum_{z \neq x} (\tilde{V}_z \tilde{G}_{xy} + \Delta V_z \tilde{G}_{xz,y}) \right] \quad (3.31)
$$

In the general case $\mathcal{G}$ will depend on a set of sites on both sides instead of an individual site as illustrated in Fig. (3.11).
In Fig.(3.11) includes all possibilities of vertices; there are five of them. From this figure, we get the self-consistent equation

\[
\mathcal{G}_{SS'} = G_0 \mathcal{G}_{SS'} + \sum_{x \in S} \mathcal{G}_{xSS} + \sum_{x' \in S'} \mathcal{G}_{x'SS'}
\]

\[+ \sum_{t''} \mathcal{X}_{xSS'} \mathcal{G}_{x't''t}
\]

(3.32)

We have the restriction for \(x\) for the last term as following; for \(S \subseteq S''\) (Fig.(3.11(e))) we must have \(S'' = S \cup x\), \(x\) represents \(\{x\}\) (the set consisting of \(x\)) here, whereas for \(S \supset S''\) (Fig.(3.11(f))) we must have \(S = S'' \cup x\), \(S'' \notin \Phi\) (null set).

All the relations obtained are exact. Now we are going to make an approximation. In an approximation we use a self-consistent resolvent instead of \(G_0\) because of the effect of self consistency as discussed in the case of a single-site approximation. If we define

\[
W^{(S)} = \sum_{\gamma \in \tilde{S}} W_{\gamma xy}
\]

(3.33)
and a self-consistent resolvent
\[ G^{(S)} = (G_0^{-1} - W^{(S)})^{-1}, \]  
we get
\[ G'_{SS'} = G^{(S)} \left[ \delta^{(S)}_{SS'} + \sum_{x \in S} \overline{\nu}_x G_{SS'} + \sum_{x \in S} \overline{\nu}_x G_{SS'} \right. \]
\[ + \left. \sum_{y \in S'} \Delta V_x \left\{ \Theta(x \in S) \Theta(S'' = S \cup x) + \Theta(x \in S') \Theta(S = S'' \cup x) \right\} \right]. \]  
We have the additional restriction for \( x \) for the last term as following: for \( S \subset S'' \) we must also have \( x \in S' \), whereas for \( S \supset S' \) we must also have \( x \in S'' \).

If we let \( \Theta(T) \) be a truth function, equal to 1 if the statement \( T \) in the brackets is true and equal to 0 otherwise, Eq. (3.35) can be written as
\[ G'_{SS'} = G^{(S)} \left[ \delta^{(S)}_{SS'} + \sum_{x \in S} \overline{\nu}_x G_{SS'} + \sum_{x \in S} \overline{\nu}_x G_{SS'} \right. \]
\[ + \left. \sum_{y \in S'} \Delta V_x \left\{ \Theta(x \in S) \Theta(S'' = S \cup x) + \Theta(x \in S') \Theta(S = S'' \cup x) \right\} \right]. \]  
If we define \( \nu_{SS'} \) for \( S, S' \neq \emptyset \), by
\[ \nu_{SS'} = \left( \sum_{x \in S} \overline{\nu}_x \right) \delta_{SS'} \left. + \sum_{x \in S} \overline{\nu}_x G_{SS'} + \sum_{x \in S} \overline{\nu}_x \right\} \Theta(x \in S) \Theta(S'' = S \cup x) \]
\[ + \Theta(x \in S') \Theta(S = S'' \cup x) \right\}, \]  
then we can rewrite Eq. (3.36) as
\[ G'_{SS'} = G^{(S)} \left[ \delta_{SS'} + \nu_{SS''} \right]. \]  
We can use these equations
\[ G = (G_0^{-1} - W)^{-1} \]  
\[ W = \sum W_{xy} \]  
\[ W_{xy} = \overline{\nu}_x G_{xy} + \Delta V_x G_{xy} \Delta V_y \]
by the effect of self consistency, Eq.(3.31) is changed to

\[ g_{xy} = g(x) \left[ \chi_{xy} + \sum_{z} \frac{\Delta V}{z} g_{zy} \right] \]  

(3.39)

where

\[ g(x) = \left( g^{-1} - \frac{w}{w_{xy}} \right) \]  

(3.40)

\[ w(s) = \frac{w}{w_{xy}} \sum_{x,y \in S} \]  

(3.33)

\[ g(s) = \left( g^{-1} - w(s) \right)^{-1} \]  

(3.34)

\[ v_{ss'} = \left( \sum_{x} \tilde{v}_{x} + \sum_{x} \tilde{v}_{x} \right) \delta_{ss'} + \varepsilon \Delta v_{x} \left\{ \theta(x \epsilon S') \theta(S' = S \cup x) \right\} \]  

(3.37)

\[ g_{ss'} = g(s) \left( \delta_{ss'} + \varepsilon v_{ss''} g_{ss''} \right) \]  

(3.38)

to find the mean resolvent \( \langle Q \rangle \). The iteration of these equations, with any choice of \( T \), has been proved to converge to a unique self-consistent solution analytic in the entire cut \( Z \)-plane. This completes our method for the formalism of the TCA.

Now we shall specialize our work to the case of a lattice with a separable potential, which includes the single-band model as a special case.

We consider, then, the case that \( V_{x} \) takes the form

\[ V_{x} = u_{x} v_{x} \tilde{u}_{x} \]  

(3.41)

where \( u_{x} \) is a normalized state vector localized near site \( x \), and \( V_{x} \) is a c-number taking the value \( V_{A} \) and \( V_{B} \) for species A and B respectively. Then we can write

\[ \tilde{v}_{x} = u_{x} v_{1} \tilde{u}_{x} \]  

\[ \tilde{\tilde{v}}_{x} = u_{x} v_{2} \tilde{u}_{x} \]  

\[ \Delta V_{x} = u_{x} v_{3} \tilde{u}_{x} \]  

(3.42)
where the parameters $V_1$, $V_2$, and $V_3$ are given by

$$V_1 = c_A V_A + c_B V_B,$$

$$V_2 = c_B V_A + c_A V_B,$$

$$V_3 = \sqrt{c_A c_B} (V_A - V_B).$$

From Eq. (3.30), we get

$$W_{xy} = u_x (V_1 \delta_{xy} + V_2^2 u_x \mathcal{G}_{xy} u_y) \bar{u}_y$$

$$= u_x (V_1 \delta_{xy} + V_3^2 g_{xy}) \bar{u}_y,$$

(3.43)

where $g_{xy} = \overline{u_x \mathcal{G}_{xy} u_y}$.

Since $g_{xy}$ is translationally invariant, it is a function of $x - y$; one has

$$g_{xy} = g(x - y).$$

We define $\mathcal{G}_{xy}$ by

$$W_{xy} = u_x \mathcal{G}_{xy} \bar{u}_y$$

(3.44)

by Eq. (3.43)

$$\mathcal{G}_{xy} = V_1 \delta_{xy} + V_3^2 g_{xy},$$

(3.45)

where we have

$$\mathcal{G}_{xy} = \mathcal{G}(x - y).$$

Here we deal with translational invariance; a translational equivalence or equivalence, for short, will play an important role in this case. We say a set $S_1$ is equivalent to a set $S_2$ if $S_1 = S_2 + x$, for some $x$. Each equivalence class of equivalent sets $S$ can be identified by one representative member $\mathfrak{S}$ of the class, and then any set $S$ in the
class can be written as \( S = \Xi + y \). Each set is specified uniquely by \( \Xi \) and \( y \). We use \( \Xi \) and \( y \) instead of \( S \) in order to take advantage of translational invariance, which will allow us to use a Fourier transform with respect to \( y \), thereby making the equation more tractable for actual calculation. If \( T \) is a translationally invariant set, then \( \widetilde{S} = \widetilde{\Xi} + y \).

From Eq. (3.37), we have

\[
\frac{V}{\Xi + y, \Xi' + y'} = \delta(\Xi + y, \Xi' + y') \left[ \frac{u}{z} \frac{V_z}{\Xi + y} + \frac{V_{\Xi + y}}{z} \frac{u}{z} \right] + \frac{\Theta(z \in \Xi + y)}{\Xi + y} = (\Xi + y) \cup z)
\]

(3.46)

\( \delta(\Xi + y, \Xi' + y') \) implies that we need \( \Xi = \Xi' \) and \( y = y' \) because each \( \Xi \) represents a different equivalence class. In order to take out the displacement \( y \), we let \( z = x + y \) and write

\[
\frac{V}{\Xi + y, \Xi' + y'} = \frac{\Xi'}{x + y} \frac{\Xi^y(y-y')}{x + y}
\]

(3.47)

with

\[
\frac{V}{x + y} = \left[ \int_{\Xi} \delta_{yy} \left\{ V_2 \Theta(x \in \Xi) + V_1 \Theta(x \in \Xi) \right\} 
+ V_3 \left\{ \Theta(x \in \Xi) \Theta(\Xi' + y' - y = \Xi \cup x) 
+ \Theta(x \in \Xi') \Theta(\Xi + y - y = \Xi \cup x) \right\} \right] \delta(\Xi + y, x + y).
\]

(3.48)

From Eq. (3.38), we get

\[
\bar{u}_{x+y} = \bar{u}_{x+y} \left\{ \int_{\Xi} \frac{G(\Xi + y)}{\Xi + y} u_{x+y} \delta_{yy} 
+ \frac{\bar{u}_{x+y}}{x + y} \left\{ \int_{\Xi} \frac{G(\Xi + y)}{\Xi + y} u_{x+y} \delta_{yy} \right\} \right\} u_{x+y}'
\]

\[
= \left\{ \int_{\Xi} (\Xi + y) \right\} u_{x+y}'.
\]

(3.49)
Substituting $V_{x+y, y'}$, from Eq. (3.47), into Eq. (3.49), we get
\[
\Gamma_{xx}^\pm (y, y') = \tilde{u}_{x+y} G_{x+y}^{(x+y)} u_{x+y} ' \delta_{yy'}
\]
\[
+ \sum_{\varepsilon \varepsilon'} \tilde{u}_{x+y} G_{x+y}^{(x+y)} u_{x+y} ' \delta_{yy'}
\]
\[
\times \sum_{\varepsilon'' \varepsilon'''} \Gamma_{xx}^{(x+y) \varepsilon'' \varepsilon'''} (y'' \varepsilon''') u_{x+y} ' u_{x+y} ' \delta_{yy'}.
\]
\[
(3.50)
\]

We define
\[
G^{(x)}_{xx^2} = \tilde{u} G^{(x)}_{xx^2} u_x '
\]
and
\[
\Gamma_{0xx}^\varepsilon (y) = \tilde{u}_{x+y} G_{x+y}^{(x+y)} u_{x+y} ' \delta_{yy^0}
\]
by Eq. (3.51),
\[
= G_{xx}^{(x)} \delta_{yy^0},
\]
and write Eq. (3.50) as
\[
\Gamma_{xx}^\varepsilon (y, y') = \Gamma_{0xx}^\varepsilon (y, y') + \sum_{\varepsilon'' \varepsilon'''} \sum_{y'' y'''} \Gamma_{0xx}^{(y'' \varepsilon'')} V_{xx^0}^{(y'' \varepsilon'')} \Gamma_{xx}^{(y'' \varepsilon''')} (y'' y''').
\]

Letting $y' = 0$, one gets
\[
\Gamma(y) = \Gamma_0(y) + \sum_{y'' y'''} \Gamma_0(y-y') V(y-y') \Gamma(y'),
\]
where a matrix notation is introduced with respect to the indices $x$ and $\varepsilon$. Note that in a given approximation both $\varepsilon$ and ultimately $x$ also will range over only a finite number of values, so that the matrices $\Gamma(y)$ and $V(y)$ will be of finite order.

The translational invariance of the problem now is seen in the way the variable $y$ appears in this equation. If we Fourier transform with respect to $y$, we obtain a simple algebraic equation for each value of the conjugate variable $k$. Using a caret to denote those Fourier transformed quantities, we get
\[
\Gamma_{xx}^{\varepsilon \varepsilon'} (y) = \frac{1}{\Delta \varepsilon} \int d \varepsilon \ e^{i \varepsilon \cdot y} \Gamma_{xx}^{\varepsilon \varepsilon'} (k),
\]
\[
\text{or} \quad \Gamma(y) = \frac{1}{\Delta} \int d \varepsilon \ e^{i \varepsilon \cdot y} \Gamma(k),
\]
where \( \mathcal{V} \) is the volume of the 1st Brillouin zone in k-space.

Hence from Eq. (3.53), we get the matrix equation

\[
\hat{\mathcal{J}}(k) = \hat{\mathcal{J}}_0(k) + \sum_{\gamma \in \mathcal{U}} e^{-ik \cdot \gamma} \hat{\gamma}(y),
\]

or

\[
\hat{\mathcal{J}}(k) = (\hat{\mathcal{J}}_0^{-1} - \hat{\gamma}(k))^{-1}.
\]

In Eq. (3.48), it turns out that \( \gamma_{x'x} = 0 \) unless \( x \in \mathcal{E} \) and \( x' \in \mathcal{F} \); in Eq. (3.49) and (3.52), there are no restrictions for \( x \) and \( x' \). However it can be shown that the subspace defined by \( x \in \mathcal{E} \) for each \( \mathcal{E} \) for \( \hat{\mathcal{J}}(k) \) and \( \hat{\mathcal{J}}_0(k) \) will not mix with each other as follows:

If \( \Lambda \) is defined as the projection on to the subspace \( \{ (x, \mathcal{E}) | x \in \mathcal{E} \} \), then what we need for the calculation of \( \mathcal{W} \) is only the part \( \Lambda \hat{\mathcal{J}}(k) \Lambda \) of \( \hat{\mathcal{J}}(k) \). But we have seen that \( \hat{\gamma}(k) \) satisfies \( \hat{\gamma}(k) = \Lambda \hat{\gamma}(k) \Lambda \), so that Eq. (3.54) gives

\[
\Lambda \hat{\mathcal{J}}(k) \Lambda = \Lambda \hat{\mathcal{J}}_0(k) \Lambda + \Lambda \hat{\mathcal{J}}_0(k) \hat{\gamma}(k) \hat{\mathcal{J}}(k) \Lambda
\]

\[
= \Lambda \hat{\mathcal{J}}_0(k) \Lambda + (\Lambda \hat{\mathcal{J}}_0(k) \Lambda) \hat{\gamma}(k) (\Lambda \hat{\mathcal{J}}(k) \Lambda).
\]

This completes our proof.

Hence we shall be interested only in the subspace defined by \( x \in \mathcal{E} \) for each \( \mathcal{E} \) for \( \hat{\mathcal{J}}(k) \) and \( \hat{\mathcal{J}}_0(k) \). In Eq. (3.44), the quantity we need, in order to find \( \mathcal{W} \) is

\[
\mathcal{E}(y) = V_1 \delta_{y,0} + V_2 g(y),
\]

where \( g(y) = \tilde{u}_y \delta_{y,0} \),

by Eq. (3.49),

\[
\Gamma_{00}(y).
\]
Taking the Fourier transform of Eqs. (3.57) and (3.58), we get

\[ \hat{\sigma}(k) = \sum_{y \in V} e^{-i k \cdot y} \sigma(y) = v_1 + y_2^2 \hat{g}(k), \quad (3.59) \]

\[ \hat{g}(k) = \sum_{y \in V} e^{-i k \cdot y} \rho_{00}(y) \]

\[ \equiv \hat{\rho}_{00}(k). \quad (3.60) \]

To find this quantity, we need (see Eq. (3.54)) \( \hat{V}_{xx}^* \) and \( \hat{V}_{0xx}^* \).

From Eqs. (3.52) and (3.55) we see that \( \hat{V}_{0xx}^* \) is independent of \( k \):

\[ \hat{V}_{0xx}^* = G^{(\varepsilon)}_{xx} \rho_{xx}. \quad \text{We now need to obtain a working expression for} \ G^{(\varepsilon)} \).

Letting \( S = \varepsilon \) in Eq. (3.51), one gets

\[ G^{(\varepsilon)}_{xx'} = \hat{u}_x G^{(\varepsilon)} u_{x'}, \]

by Eq. (3.34),

\[ = \hat{u}_x G_0 u_{x'} + \hat{u}_x G^{(\varepsilon)} G^{(\varepsilon)} u_{x'}, \]

substituting

\[ \hat{u}^{(\varepsilon)} = \sum_{y,z \in \mathbb{Z}^d} \hat{u}_{yz}, \]

and, by Eq. (3.44),

\[ \hat{u}_{yz} = \hat{u}_y G^{(\varepsilon)} \hat{u}_z, \]

we get

\[ G^{(\varepsilon)}_{xx'} = G_{0xx'} + \sum_{y,z \in \mathbb{Z}^d} \hat{u}_x G_0 u_y G^{(\varepsilon)}_{yz} \hat{u}_z G^{(\varepsilon)} u_{x'}, \]

\[ = G_{0xx'} + \sum_{y,z \in \mathbb{Z}^d} G_{0xy} G^{(\varepsilon)}_{yz} G^{(\varepsilon)}_{zx'}. \quad (3.61) \]

Let \( P \) be a projection operator on to \( \Xi^* \), and let the symbol \( \Xi^* \) under any matrix denote the projection of the matrix on to the subspace \( x \in \Xi^* \).
Let $A$ and $B$ be any two matrices, we have

\[ APB = A \cdot B. \]  

(3.62)

From Eq. (3.61), we get

\[ G(\varepsilon) = G_0 + G_0(1-P)G(1-P)G(\varepsilon). \]  

(3.63)

We have

\[ G(\varepsilon) = (G_0^{-1} - \mathcal{W}(\varepsilon))^{-1}; \]

$\mathcal{W}(\varepsilon)$ is not translationally invariant since it is tied to $\varepsilon$; from Eq. (3.33), it will have an infinite number of terms. To avoid this we shall change to the form

\[ G(\varepsilon) = (G_0^{-1} - \mathcal{W}(\varepsilon) + \mathcal{W})^{-1} \]

\[ = (G^{-1} - (\mathcal{W}(\varepsilon) - \mathcal{W}))^{-1} \]

\[ = G + G(\mathcal{W}(\varepsilon) - \mathcal{W})G(\varepsilon), \]  

(3.64)

where use has been made of Eq. (3.28) and, for convenience, the notation $G$ is used for $\langle G \rangle$ from now on. Eq. (3.63) gives

\[ \mathcal{W}(\varepsilon) = (1-P)G(1-P), \]

hence Eq. (3.64) can be written as

\[ G(\varepsilon) = G + G \left\{ (1-P)G(1-P) - G \right\} G(\varepsilon) \]

\[ = G - GPGG(\varepsilon) - GPG(\varepsilon) + GPGPG(\varepsilon), \]  

(3.65)

or, since we are interested only in the subspace $\varepsilon$,

\[ G(\varepsilon) = G - GPG(\varepsilon) - GPG(\varepsilon) + GPGPG(\varepsilon), \]

by Eq. (3.62),

\[ = G - G \mathcal{W}G(\varepsilon) - G \mathcal{W}G(\varepsilon) + G \mathcal{W}G(\varepsilon). \]  

(3.66)
Now we are going to separate $G^{*}$ from $G$ in order to find $G^{*}$ in Eq.(3.66). Operating $G$ on both sides of Eq.(3.65), and, then, projecting them on to $\xi^{*}$, we get

$$\tilde{G}^{*}(\xi) = \frac{G^{*}}{G} - \frac{G^{*} G G^{*}}{G} - \frac{G^{*} G G^{*}}{G} + \frac{G^{*} G G^{*}}{G}.$$ 

By using Eq.(3.62), we solve for $\tilde{G}^{*}(\xi)$ and substituting into Eq.(3.66), we get an equation for $\tilde{G}^{*}(\xi)$ involving only the finite matrices $G$, $G^{*}$ and $G G^{*}$, all of which can be obtained either by use of the Fourier transform of $G$, or in the single-band model as we shall see, through the defining equations (Eqs.(2.6), (3.44)) for $G$.

$$\tilde{G}(\xi) = \frac{G}{G} - \frac{G G^{*}}{G} - \frac{G G^{*}}{G} + \frac{G G^{*}}{G}.$$ 

(3.67)

Operating with $(1 + \delta G) G^{-1}$ on both sides, we get

$$(1 + \delta G) G^{-1} \tilde{G}(\xi) = (1 + \delta G) - \frac{G G^{*}}{G} - \frac{G G^{*}}{G} + \frac{G G^{*}}{G} - (1 + \delta G) G^{-1} G^{*}$$

from which

$$\tilde{G}(\xi) = \left[(1 + \delta G) G^{-1}(1 + \delta G) - \frac{G G^{*}}{G} - \frac{G G^{*}}{G}\right]^{-1}. \quad (3.68)$$

Matrix operations in space $\xi^{*}$ must be done in configuration space whereas those in space $U$ can be done by using a Fourier transform, or by using an equation relating $\tilde{G}$ and $G$ as follows:

$$G = \tilde{G} + \tilde{G}^{*} G^{\dagger},$$

which becomes, in the case of a separable potential,

$$G_{xy} = \tilde{x} \tilde{u} G_{xy} = G_{0xy} + \sum G_{0xz} \tilde{z} \tilde{G}_{zy}. $$
In matrix form, this is
\[
G = G_0 + G_0 \mathcal{Q} = G_0 + G \mathcal{Q} G_0 ,
\]
which gives
\[
\mathcal{Q} G = G_0^{-1} G - 1 \quad (3.69)
\]
and
\[
G \mathcal{Q} = G_0^{-1} - 1 . \quad (3.70)
\]
Eqs. (3.69) and (3.70), furthermore, can be used to obtain
\[
\mathcal{Q} G \mathcal{Q} = G_0^{-1} G \mathcal{Q} - \mathcal{Q}
\]
\[
= G_0^{-1} (G_0^{-1} - 1) - \mathcal{Q}
\]
\[
= G_0^{-1} G_0^{-1} - G_0^{-1} - \mathcal{Q} . \quad (3.71)
\]
Substituting \( 1 + \mathcal{Q} G, 1 + G \mathcal{Q}, \mathcal{Q} G \mathcal{Q}, \) from Eqs. (3.69)-(3.71), into Eq. (3.68), one gets
\[
(G (\mathcal{Q})^{-1} = G_0^{-1} G (\mathcal{Q})^{-1} G_0^{-1} - G_0^{-1} G_0^{-1} + G_0^{-1} . \quad (3.72)
\]
But we have
\[
G_0^{-1} = Z - H_0 , \quad (3.73)
\]
where \( Z = ZI , \quad \sum_{x,y} u_x (Z \mathcal{Q} y - H_{0xy}) u_y . \)

We can thus change Eq. (3.72) in such a way that it involves \( H_0 G, \)
\( G H_0 , \) and \( H_0 CH_0 ; \) these terms involve sums over \( U , \) but since only elements in \( \mathcal{Q} \) are being calculated, and since \( H_0 \) typically has matrix elements only between adjacent or at most nearby sites, these sums over \( U \) reduce to a small number of terms.

By use of Eq. (3.73), Eq. (3.72) can be written as
\[
(G (\mathcal{Q})^{-1} = (Z \mathcal{Q} - H_0 G) (\mathcal{Q})^{-1} (Z \mathcal{Q} - G H_0) - Z^2 G
\]
\[
+ Z G H_0 + Z H_0 G - H_0 G H_0 + Z - H_0 .
\]
We can simplify Eq.(3.74) by projecting some parts into $I^*$; this will help reduce the size of matrices in our calculation as will be seen below.

Let $P$ be the projection operator on to $K^*$, that is $P = 1 - P$.

For any two matrices $A$ and $B$, we have

$$AB = APB + APB\tag{3.62}$$

by Eq.(3.62),

$$= A \cdot B + APB\ .\tag{3.75}$$

Hence from Eq.(3.74), by using Eq.(3.75), we get

$$\begin{align*}
(G^0)^{-1} &= (H_0G + H_0^s \bar P)(G)^{-1}(G - H_0 + G \bar P H_0) \\
&- H_0^s \bar H_0 - H_0^s \bar G \bar P H_0 + Z - H_0 \\
&= (H_0 \bar G + H_0 \bar P)(G)^{-1}(G - H_0 + G \bar P H_0) \\
&- H_0 \bar G \bar H_0 - H_0 \bar G \bar P \bar H_0 - H_0 \bar \bar P \bar G \bar H_0 + Z - H_0 \\
&= H_0 \bar P \bar G \bar (G)^{-1} \bar G \bar P \bar H_0 + Z - H_0 .\tag{3.76}
\end{align*}$$

We can see that this form is better than that in Eq.(3.74); because of the effect of $\bar P$, terms corresponding to the subspace $K^*$ in some of the matrix products can be eliminated. This reduces our calculation as mentioned before.

From Eq.(3.32), now, we get

$$\begin{align*}
\varphi_{\xi \xi'}^0 &= G_{\xi \xi'}(\xi) \xi' \tag{3.77},
\end{align*}$$

where $G_{\xi \xi'}(\xi)$, of any rank $n$, can be found from Eq.(3.76).

Now we are going to find $\varphi_{\xi \xi}(k)$, which we need in Eq.(3.50):

$$\varphi_{\xi \xi}(k) = \sum_{\gamma \in U} e^{-i \gamma \cdot \tilde y} \varphi_{\xi \xi}(y) .\tag{3.78}$$
Letting \( y' = 0 \) in Eq. (3.48), and substituting \( V_{xx}^{'y}(y) \) into Eq. (3.78), we get

\[
\hat{V}_{xx}^{'y}(k) = \sum_{\epsilon \in \Omega} e^{-i\mathbf{k} \cdot \mathbf{r}} \left[ \mathcal{D} \left( \mathbf{k} \right) \right]_{\epsilon} \left\{ V_2 \Theta(\epsilon, \epsilon_x) + V_1 \Theta(\epsilon, \epsilon_x') \right\} + V_3 \left\{ \Theta(\epsilon, \epsilon_x') \Theta(\epsilon - y = \epsilon \cup x) \right. \\
+ \left. \Theta(\epsilon', \epsilon_x') \Theta(\epsilon + y = \epsilon' \cup x') \right\} \left[ \delta_{\epsilon', \epsilon_x+y} \right.
\]

\[
= \sum_{\epsilon \in \Omega} \sum_{\epsilon'} e^{-i\mathbf{k} \cdot \mathbf{r}} \left[ \mathcal{D} \left( \mathbf{k} \right) \right]_{\epsilon} \left\{ V_2 \Theta(\epsilon, \epsilon_x) + V_1 \Theta(\epsilon, \epsilon_x') \right\} \\
+ V_3 e^{-i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x'})} \left\{ \Theta(\epsilon, \epsilon_x') \Theta(\epsilon' - x' + x = \epsilon \cup x) \right. \\
+ \left. \Theta(\epsilon', \epsilon_x') \Theta(\epsilon + x' - x = \epsilon' \cup x') \right\}.
\]  

(3.79)

Now we complete what we need in order to solve for \( \hat{g}(k) \) in Eq. (3.59). The procedure of the method for the approximation can be summarized as follows:

Start with \( \hat{g}(k) \) by best guess or as the result of previous iterations. Calculate

\[
\hat{G}(k) = \left[ Z - \hat{H}_0(k) - \hat{g}(k) \right]^{-1},
\]

where

\[
k \in \Omega = \text{1st Brillouin zone} = \frac{(2\pi)^d}{V},
\]

where \( d \) and \( V \) are dimension of space and volume of a cell in configuration space respectively. Calculate the necessary matrix elements of \( \hat{G} \) from

\[
G_{xx'} = G(x-x')
\]

\[
= \frac{1}{V} \int_{\Omega} e^{-i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x'})} \hat{G}(k) \mathrm{dk},
\]

and \( \left( \hat{g}^{(\Omega)} \right)^{-1} \) by using Eq. (3.76). Calculate \( \hat{g}^{-1} \) from Eq. (3.77), and \( \hat{v} \) from Eq. (3.79). Then we get
\hat{\eta}(k) = \left( J_0^{-1} - \hat{\gamma}(k) \right)^{-1},

from which we can find, from Eqs. (3.59) and (3.60),

\hat{\varphi}(k) = v_1 + v_2 \hat{\gamma}_{00}(k).

This completes the cycle of the procedure. The block diagram of this is shown in Appendix C.
CHAPTER IV

METHOD OF CALCULATION FOR THE NEAREST-NEIGHBOR APPROXIMATION (TCA(nn))

In this chapter the method of calculation for the nearest-neighbor approximation (TCA(nn)) for both two-dimensional and three-dimensional systems will be given. The definition of TCA was given in section B.2 of the last chapter; for the nearest-neighbor approximation, T is a family of two classes of sets, namely sets consisting of a single site and sets consisting of a nearest-neighbor pair, \( T = \{ \{ i \}, \{ i, j \} \mid i, j \text{ adjacent to } i \} \).

In this calculation we suppose the lattice spacing is 1, and shall be interested only in the nn interaction; we restrict to single-band tight-binding approximation. We also suppose the hopping integrals are completely independent of alloy composition (i.e., no off diagonal disorder), and let them be \( h \).

The basic idea of calculation is to find \( \hat{\gamma}^{00}_{00}(k) \) in order to calculate \( \hat{\gamma}(k) \), which we need, from Eqs. (3.59) and (3.60)

\[
\hat{\gamma}(k) = \gamma_1 + \gamma_2 \hat{\gamma}^{00}_{00}(k) .
\] (4.1)

\( \hat{\gamma}^{00}_{00}(k) \) can be found from Eq. (3.56)

\[
\hat{\gamma}^{00}_{00}(k) = (\hat{\Gamma}^{-1} - \hat{\gamma}(k))^{-1} ,
\] (4.2)

where \( \hat{\Gamma}^{-1} \) and \( \hat{\gamma}(k) \) can be found from Eq. (3.77) and Eq. (3.79) respectively.
A. Two-Dimensional System

For this case, there are three distinct equivalence classes, each represented by a characteristic set: the single site sets, the vertical nn pairs, and the horizontal nn pairs. We have

\[
\begin{align*}
\Sigma_1^+ & = \begin{pmatrix} 0 & 0 & \ldots \end{pmatrix} \\
\Gamma_1 & = (G(\varepsilon_1))^{-1} \\
\Gamma_2 & = (G(\varepsilon_2))^{-1} \\
\Gamma_3 & = (G(\varepsilon_3))^{-1} \\
\Gamma_0^{-1} & = \begin{pmatrix} 0 & \ldots & 0 \end{pmatrix}
\end{align*}
\]

where, from Eq.(3.76),

\[
(G(\varepsilon))^{-1} = H_0^{-1} \overline{\text{PG}} (G)^{-1} \overline{\text{GP}} H_0 - H_0^{-1} \overline{\text{PG}} \overline{\text{PH}} H_0 + Z - H_0. \tag{4.5}
\]

\[
\hat{\psi}(k) = \hat{\psi}(k^1, k^2) = \begin{pmatrix} \psi(x, x) + \psi(x, x) \end{pmatrix} + \begin{pmatrix} \psi(x, x) \end{pmatrix} + \begin{pmatrix} \psi(x, x) \end{pmatrix} + \begin{pmatrix} \psi(x, x) \end{pmatrix}
\]

A. Two-Dimensional System

For this case, there are three distinct equivalence classes, each represented by a characteristic set: the single site sets, the vertical nn pairs, and the horizontal nn pairs. We have

\[
\begin{align*}
\varepsilon_0 &= \{ (0, 0) \}, \\
\varepsilon_0^+ &= \{ (0, 0), (\pm 1, 0), (0, \pm 1) \}
\end{align*}
\]

\[
\varepsilon_1 = \{ (0, 0), (1, 0) \} = \varepsilon_1^+ \\
\varepsilon_2 = \{ (0, 0), (0, 1) \} = \varepsilon_2^+
\]

where, from Eq.(3.76),

\[
(G(\varepsilon))^{-1} = H_0^{-1} \overline{\text{PG}} (G)^{-1} \overline{\text{GP}} H_0 - H_0^{-1} \overline{\text{PG}} \overline{\text{PH}} H_0 + Z - H_0. \tag{4.5}
\]
where it will be recalled (see page 40) that

$$\mathcal{E}^n = \{ x \mid \{x \} \cup \mathcal{E} \subseteq T \},$$

$$\widetilde{\mathcal{E}} = \mathcal{E}^+ \cap \overline{\mathcal{E}} \quad (\overline{\mathcal{E}} = \text{complement of } \mathcal{E}).$$

In this case both $\widetilde{\mathcal{E}}_1$ and $\widetilde{\mathcal{E}}_2$ are the null set.

First we shall find $\hat{\mathcal{V}}(k)$ from Eq.(4.4). This equation shows that the first part contributes to only the diagonal elements of $\hat{\mathcal{V}}(k)$. For the second part, we shall find only the first term because the second one can be found from the Hermitian properties of $\hat{\mathcal{V}}(k)$ ($\hat{\mathcal{V}}(k) = \hat{\mathcal{V}}^+(k)$); this means that we shall be interested in $\mathcal{E} = \mathcal{E}_0 = \{(0,0)\}$ only. Table (4.1) will help us find the contribution of the second part.

<table>
<thead>
<tr>
<th>$x$</th>
<th>$\mathcal{E} \cup x$</th>
<th>$\mathcal{E} \cup x - x$</th>
<th>$\mathcal{E}'$</th>
<th>$x'$</th>
<th>$x' - x$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(-1,0)</td>
<td>{(-1,0),(0,0)}</td>
<td>{(0,0),(1,0)}</td>
<td>{(0,0),(1,0)}</td>
<td>(0,0)</td>
<td>(1,0)</td>
</tr>
<tr>
<td>(1,0)</td>
<td>{(1,0),(0,0)}</td>
<td>{(0,0),(-1,0)}</td>
<td>{(1,0),(0,0)}</td>
<td>(1,0)</td>
<td>(0,0)</td>
</tr>
<tr>
<td>(0,-1)</td>
<td>{(-1,0),(0,0)}</td>
<td>{(0,0),(0,1)}</td>
<td>{(0,0),(0,1)}</td>
<td>(0,0)</td>
<td>(0,1)</td>
</tr>
<tr>
<td>(0,1)</td>
<td>{(0,1),(0,0)}</td>
<td>{(0,0),(0,-1)}</td>
<td>{(0,1),(0,0)}</td>
<td>(0,1)</td>
<td>(0,0)</td>
</tr>
</tbody>
</table>

Table 4.1 Solutions of $\mathcal{E}' - x' = \mathcal{E} \cup x - x$ for the two-dimensional system, for $\mathcal{E} = \mathcal{E}_0$.

In Table (4.1), we need consider only values of $x$ in $\mathcal{E}$. Eq.(4.4) shows that we also need $\mathcal{E}' - x' = \mathcal{E} \cup x - x$; there are only two possibilities of $\mathcal{E}'$, namely $\mathcal{E}'_1$ and $\mathcal{E}'_2$. From this we can find the corresponding $\mathcal{E}'$ and $x'$ to $x$ as shown in Table (4.1). For compactness in writing tables and matrices, we shall use the notation $\mathbf{i}$ for $-i$ hereafter. Using the results of Table (4.1), we can now obtain $\hat{\mathcal{V}}(k)$:
\[ \Xi'_1 = \Xi_1 \]
\[ \Xi'_2 = \Xi_2 \]
\[ \Xi'_3 = \Xi_3 \]

\[
\hat{V}(k) =
\begin{bmatrix}
  v_2 & 0 & 0 & 0 & 0 & 0 & 0 & (0,0) \\
  0 & v_1 & 0 & 0 & 0 & v_3^a & 0 & (1,0) \\
  0 & 0 & v_1 & 0 & 0 & 0 & v_3 & (0,0) \\
  0 & 0 & 0 & v_1 & 0 & 0 & v_3^b & (0,1) \\
  0 & 0 & 0 & 0 & v_1 & 0 & 0 & (0,1) \\
  0 & v_3^c & 0 & 0 & 0 & v_2 & 0 & (0,0) \\
  0 & 0 & v_3 & 0 & 0 & 0 & v_2 & (1,0) \\
  0 & 0 & 0 & v_3^d & 0 & 0 & 0 & v_2 & (0,1) \\
  0 & 0 & 0 & 0 & v_3 & 0 & 0 & (0,0) \\
\end{bmatrix}
\]

where \( a, b, c, \) and \( d \) are equal to \( e^{-ik_1}, e^{-ik_2}, e^{ik_1}, \) and \( e^{ik_2} \) respectively.

Now we are going to find \( \hat{G}(\Xi) \) by use of Eq.\((4.5)\). Because of a translational invariance, we can write

\[
\mathcal{G}_{x,x'} = \mathcal{G}_{x-x'}
\]

\[ = \mathcal{G}_y, \]

where \( y = x-x' \), and because of a rotational and reflectional symmetry, we get

\[
\mathcal{G}_y = \mathcal{G}(y_1, y_2)
\]

\[ = \mathcal{G} |y_1|, |y_2| \]

\[ = \mathcal{G} |y_2|, |y_1| \]

in matrices, from now on, we shall let \[ |y_1| \quad |y_2| \] symbolize \( \mathcal{G}(y_1, y_2) \) and
First we deal with the case

\[ \mathcal{E}_0 = \{(0,0)\} \]

\[ \mathcal{E}^\star_0 = \{(0,0), (\pm 1,0), (0, \pm 1)\} \]

Consider \( H_0 \) in Eq. (4.5), the number of rows we need is only the number of elements in set \( \mathcal{E}^\star_0 \) because of the effect of \( P \), whereas the number of columns is the total number of nearest neighbors of any of those elements, excluding those elements themselves because of the effect of \( \tilde{P} \) as mentioned in Chapter 3; these are shown in Fig. (4.1) as dots and crosses respectively.

Fig. 4.1 Two sets of sites needed in calculating \( (\Omega^{(E_0)}_x - 1)^{-1} \).

Dots represent \( \mathcal{E}^\star_0 \), and crosses, the sites in \( \mathcal{E}^\star_0 \) connected to \( \mathcal{E}_0 \) by matrix elements of \( H_0 \).

We have

\[
\begin{array}{cccccccc}
(2,0)(1,1)(1,1)(0,2)(0,2)(1,1)(1,1)(2,0) & \times' \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\
0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\
\end{array}
\]

\[
H_0 \mathcal{PG}/h =\]

\[
\begin{array}{cccccccc}
(0,0) \\
(\bar{1},0) \\
(1,0) \\
(0,\bar{1}) \\
(0,1) \\
\end{array}
\]
where we let $A_1$, $A_2$, $A_3$, and $A_4$ represent, respectively, the 2nd, 3rd, 4th, and 5th rows of $H_0^\perp G/h$. Next we have

$$(0,0)(1,0)(0,1)(0,1) (0,0)(1,0)(0,1)$$

$$(0,0)(1,0)(0,1) (0,0) (0,0) (0,1) (0,1) (0,1) (0,1)$$
From Eqs. (4.7) and (4.8), we get

$$H_{0 \overline{PG}} (Q)^{-1} G_{PH_0} / h^2$$

\[
\begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & A_1 G_F^{-1} A_1 & A_1 G_F^{-1} A_2 & A_1 G_F^{-1} A_3 & A_1 G_F^{-1} A_4 \\
0 & A_2 G_F^{-1} A_1 & A_2 G_F^{-1} A_2 & A_2 G_F^{-1} A_3 & A_2 G_F^{-1} A_4 \\
0 & A_3 G_F^{-1} A_1 & A_3 G_F^{-1} A_2 & A_3 G_F^{-1} A_3 & A_3 G_F^{-1} A_4 \\
0 & A_4 G_F^{-1} A_1 & A_4 G_F^{-1} A_2 & A_4 G_F^{-1} A_3 & A_4 G_F^{-1} A_4
\end{bmatrix}
\]

(4.9)

We also need to calculate \( H_{0 \overline{PGPH_0}} \):

$$H_{0 \overline{PGPH_0}} / h^2$$

\[
\begin{bmatrix}
(\bar{2}, 0)(\bar{1}, 1)(\bar{1}, 1)(0, \bar{2})(0, 2)(1, \bar{1})(1, 1)(2, 0) \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & (0, 0) \\
1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & (1, 0) \\
0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & (1, 0) \\
0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & (0, \bar{1}) \\
0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & (0, 1)
\end{bmatrix}
\]

\[
\begin{bmatrix}
00 & 11 & 11 & 22 & 22 & 31 & 31 & 40 & 0 & 1 & 0 & 0 & 0 \\
11 & 00 & 02 & 11 & 13 & 20 & 22 & 31 & 0 & 1 & 0 & 1 & 0 \\
11 & 02 & 00 & 13 & 11 & 22 & 20 & 31 & 0 & 1 & 0 & 0 & 1 \\
22 & 11 & 13 & 00 & 04 & 11 & 13 & 22 & 0 & 0 & 0 & 1 & 0 \\
22 & 13 & 11 & 04 & 00 & 13 & 11 & 22 & 0 & 0 & 0 & 0 & 1 \\
31 & 20 & 22 & 11 & 13 & 00 & 02 & 11 & 0 & 0 & 1 & 1 & 0 \\
31 & 22 & 20 & 13 & 11 & 02 & 00 & 11 & 0 & 0 & 1 & 0 & 1 \\
40 & 31 & 31 & 22 & 22 & 11 & 11 & 00 & 0 & 0 & 1 & 0 & 0
\end{bmatrix}
\]
It will be seen from the relation between $A_1$, $A_2$, $A_3$, and $A_4$ in Eq.(4.7), and from the symmetry properties of $(Q^{-1})_F$ (Eq.(4.8)), that the expression (4.9) has the same symmetry as (4.10). In particular,

$$A_1^{-1} F A_1^{-1} = A_2^{-1} F A_2^{-1} = A_3^{-1} F A_3^{-1} = A_4^{-1} F A_4^{-1},$$

$$A_2^{-1} F A_1^{-1} = A_1^{-1} F A_2^{-1} = A_3^{-1} F A_4^{-1} = A_4^{-1} F A_3^{-1},$$

etc.

so that we need to calculate only three elements $A_1^{-1} F A_1^{-1}$, $A_2^{-1} F A_1^{-1}$, and $A_3^{-1} F A_1^{-1}$.

We get, then, from Eqs.(4.9) and (4.10),

$$\left( G^{-1} \sigma_0^L \right)^{-1} = \begin{pmatrix} Z & -h & -h & -h & -h \\ -h & E_1' & E_2 & E_3 & E_3 \\ -h & E_2 & E_1' & E_3 & E_3 \\ -h & E_3 & E_3 & E_1 & E_2 \\ -h & E_3 & E_3 & E_2 & E_1 \end{pmatrix} + Z - \frac{Z}{2}$$

$$= \begin{pmatrix} \left( G^{-1} \sigma_0^L \right)^{-1} \\ \left( G^{-1} \sigma_0^L \right)^{-1} \\ \left( G^{-1} \sigma_0^L \right)^{-1} \\ \left( G^{-1} \sigma_0^L \right)^{-1} \\ \left( G^{-1} \sigma_0^L \right)^{-1} \end{pmatrix}, \quad (4.11)$$
where
\[ E_1' = h^2(A_1G_F^{-1}A_1^{\text{tr}} - P_1) + Z, \]
\[ E_2 = h^2(A_2G_F^{-1}A_1^{\text{tr}} - P_2), \]
\[ E_3 = h^2(A_3G_F^{-1}A_1^{\text{tr}} - P_3). \]

We now do the corresponding calculation for the case
\[ \mathcal{E}_1 = \{(0,0),(1,0)\} = \mathcal{E}_1^4; \]
note that \( ) \) has a different significance, depending on the choice of \( \mathcal{E} \).

We have
\[
\begin{array}{c|cccccc|ccc|cc}
\hline
& (1,0) & (0,1) & (0,1) & (1,1) & (2,0) \\
\hline
0 & 1 & 1 & 0 & 0 & 0 & (0,0) & 10 & 20 & (1,0) \\
0 & 0 & 0 & 1 & 1 & 1 & (1,0) & 01 & 11 & (0,1) \\
& 01 & 11 & (0,1) & 11 & 01 & (1,1) & 11 & 01 & (1,1) \\
& 20 & 10 & (2,0) & \\
\hline
\end{array}
\]
\[
\begin{align*}
H_{0PG/h} &= \begin{vmatrix}
3(01) & 2(11)+(02) \\
2(11)+(02) & 3(01)
\end{vmatrix} \\
&= \begin{vmatrix}
3(01) & 2(11)+(02) \\
2(11)+(02) & 3(01)
\end{vmatrix}.
\end{align*}
\]

Letting
\[
L = (3(01) \quad 2(11)+(02))
\]
and
\[
M = (2(11)+(02) \quad 3(01)),
\]
and
\[
(G)^{-1} = \begin{vmatrix}
00 & 01 \\
01 & 00
\end{vmatrix} \equiv G_S^{-1},
\]
we get, from Eqs. (4.13) and (4.14),
\[
H_{0PG} \frac{(G)^{-1}}{h^2} = \begin{vmatrix}
g_S^{-1}L^{\text{tr}} & g_S^{-1}M^{\text{tr}} \\
g_S^{-1}M^{\text{tr}} & g_S^{-1}M^{\text{tr}}
\end{vmatrix}.
\]
Likewise,

\[
\frac{\hbar^2}{\mathbf{H}_0^{\text{PGPH}_0}} = \begin{bmatrix}
1 & 1 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 1 & 1 \\
0 & 0 & 0 & 1 & 2 & 1 \\
0 & 1 & 0 & 1 & 0 & 1 \\
0 & 1 & 0 & 1 & 0 & 1 \\
0 & 1 & 0 & 1 & 0 & 1 \\
\end{bmatrix}
\begin{bmatrix}
0 & 11 & 21 & 11 & 0 & 0 \\
1 & 0 & 1 & 0 & 1 & 0 \\
1 & 0 & 1 & 0 & 1 & 0 \\
1 & 0 & 1 & 0 & 1 & 0 \\
1 & 0 & 1 & 0 & 1 & 0 \\
1 & 0 & 1 & 0 & 1 & 0 \\
\end{bmatrix}
\]

\[
(0,0)(1,0)
\]

\[
\mathbf{H}_0^{\text{PGPH}_0} = \begin{bmatrix}
1 & 1 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 1 & 1 \\
0 & 0 & 0 & 1 & 2 & 1 \\
0 & 1 & 0 & 1 & 0 & 1 \\
0 & 1 & 0 & 1 & 0 & 1 \\
0 & 1 & 0 & 1 & 0 & 1 \\
\end{bmatrix}
\begin{bmatrix}
1 & 0 \\
0 & 1 \\
0 & 1 \\
0 & 1 \\
0 & 1 \\
0 & 1 \\
\end{bmatrix}
\]

\[
(\xi_1)^{-1} = \mathbf{H}_0^{\text{PGPH}_0} (\xi)^{-1} - \mathbf{H}_0^{\text{PGPH}_0} + Z - \mathbf{H}_0
\]

\[
(\xi_1)^{-1} = \begin{bmatrix}
E_4 & E_5 \\
E_5 & E_4'
\end{bmatrix}
\]

\[
E_4' = \hbar^2 (L G_{L}^{-1} L_{1}^{\text{tr}} - P_1) + Z
\]

\[
E_5' = \hbar^2 (L G_{S}^{-1} M_{1}^{\text{tr}} - P_5) - h
\]

For the case \(\xi_2\), the calculation is exactly identical to that for \(\xi_1\), to which it is related by reflectional symmetry.

We are now ready to consider \(\hat{f}(k)\), of which we need to calculate only one element, \(\hat{f}_{00}(k)\).
From Eqs. (4.2), (4.3), (4.6), (4.11), and (4.17), we get

\[
\hat{A}(k) = \begin{pmatrix}
Z-V_2 & -h & -h & -h & 0 & 0 & 0 & 0 & -1 \\
-h & E_1 & E_2 & E_3 & E_3 & -V_3^a & 0 & 0 \\
-h & E_2 & E_1 & E_3 & E_3 & 0 & -V_3 & 0 & 0 \\
-h & E_3 & E_3 & E_1 & E_2 & 0 & 0 & -V_3^b & 0 \\
-h & E_3 & E_3 & E_2 & E_1 & 0 & 0 & 0 & -V_3 \\
0 & -V_3^c & 0 & 0 & 0 & E_4 & E_5 & 0 & 0 \\
0 & 0 & -V_3 & 0 & 0 & E_5 & E_4 & 0 & 0 \\
0 & 0 & 0 & -V_3^d & 0 & 0 & E_4 & E_5 \\
0 & 0 & 0 & 0 & -V_3 & 0 & 0 & E_5 & E_4
\end{pmatrix},
\]

where

\[a = e^{-ik_1}, \]
\[b = e^{-ik_2}, \]
\[c = e^{ik_1}, \]
\[d = e^{ik_2}, \]

\[E_1 = E'_1 - V_1, \]
\[E_4 = E'_4 - V_2, \]

and where \(E'_1, E_2, E_3, E'_4, E_5\) are given by Eqs. (4.12) and (4.18).

The actual calculation of \(\hat{A}_{00}(k)\) can be simplified by the use of symmetry properties for diagonal blocks, and between \(k_1\) and \(k_2\), and \(k_1\) and \(-k_1\), (i = 1, 2).
If we write

\[
\begin{array}{cccccc}
0 & 1 & 2 & 3 & 4 & 1 & 2 & 3 & 4 \\
0 & & & & & 0 & 0 & 0 & 0 \\
1 & & & & & -V_3a & 0 & 0 & 0 \\
2 & & & & & 0 & -V_3 & 0 & 0 \\
3 & & \begin{array}{c} A \end{array} & & & 0 & 0 & -V_3b & 0 \\
4 & & & & & 0 & 0 & 0 & -V_3 \\
\end{array}
\]

and express \( \hat{\rho}^{(k)} \) as the ratio of two determinants:

\[
\hat{\rho}^{(k)} = \frac{N}{D},
\]

where \( N \) is the determinant with the first row and column omitted, and \( D \) is the full determinant. Thus

\[
N = (A_{1234}(1234)B_{12}(12)C_{34}(34)) \]

\[
-4V_3^2A_{123}(123)B_{12}(12)C_{33} + 2V_3^4A_{12}(12)B_{12}(12)
+ 4V_3^4A_{13}(13)B_{11}C_{33} - 4V_3^8A_{11}B_{11} + V_3^8
+ 2V_3(-A_{124}(124)B_{12}(12)C_{34}
+ 2V_3^2A_{14}(14)B_{11}C_{34} - V_3^4A_{34}C_{34})(\cos k_1 + \cos k_2)
+ 4V_3^4A_{24}(24)B_{12}C_{34}\cos k_1 \cos k_2,
\]

where \( A_{1234}(1234) \) is the determinant of the submatrix of \( A \) with rows 1, 2, 3, 4 and columns 1, 2, 3, 4, etc. For \( D \) we include the 1st row and
column, by the replacements:

\[ A_{(1234)(1234)} \rightarrow A_{(01234)(01234)} \]

\[ A_{(123)(123)} \rightarrow A_{(0123)(0123)} \]

e etc.

B. Three-Dimensional System

The general procedure for this case is similar to that for two-dimensional system; hence we shall not discuss it in as much detail.

For this case, following the pattern of Eqs. (4.2)-(4.5), we have

\[ (k) = (k_1, k_2, k_3) \]

\[ \Xi_0 = \{(0,0,0), (1,0,0), (0,1,0), (0,0,1)\} \]

\[ \Xi_1 = \{(0,0,0), (1,0,0)\} \]

\[ \Xi_2 = \{(0,0,0), (0,1,0)\} \]

\[ \Xi_3 = \{(0,0,0), (0,0,1)\} \]

<table>
<thead>
<tr>
<th>( x )</th>
<th>( \Xi \cup x )</th>
<th>( \Xi \cup x - x )</th>
<th>( \Xi' )</th>
<th>( x' )</th>
<th>( x' - x )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1,0,0)</td>
<td>{(1,0,0),(0,0,0)}</td>
<td>{(0,0,0),(1,0,0)}</td>
<td>{(0,0,0),(1,0,0)}</td>
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</tr>
<tr>
<td>(0,0,1)</td>
<td>{(0,0,1),(0,0,0)}</td>
<td>{(0,0,0),(0,0,1)}</td>
<td>{(0,0,0),(0,0,1)}</td>
<td>(0,0,0)</td>
<td>(0,0,1)</td>
</tr>
<tr>
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<td>{(0,0,1),(0,0,0)}</td>
<td>{(0,0,0),(0,0,1)}</td>
<td>{(0,0,1),(0,0,0)}</td>
<td>(0,0,1)</td>
<td>(0,0,0)</td>
</tr>
</tbody>
</table>

Table 4.2 Solutions of \( \Xi' - x' = \Xi \cup x - x \) for the three-dimensional system, for \( \Xi = \Xi_0 \).
By Eq.(4.4) and the help of Table(4.2), we get

\[ \hat{V}(k) = \]

| \( v_2 \) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | (000) |
| \( v_1 \) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | (100) |
| \( v_3 \) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | (010) |
| \( v_1 \) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | (010) |
| \( v_3 \) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | (001) |

\[ \text{where } a, b, c, d, f, g \text{ are equal to } e^{-ik_1}, e^{-ik_2}, e^{-ik_3}, e^{ik_1}, e^{ik_2}, \]

and \( e^{ik_3} \) respectively.

Now we are going to find \((G(x^2))^{-1}\) by use of Eq.(4.5). We have

\[ G_{x,x'} = G_{x-x'} = G_y = G(y_1, y_2, y_3) \]

\[ = \frac{G}{\sqrt{|y_1||y_j||y_k|}} \]

Where \( |y_1|, |y_j|, \text{ and } |y_k| \) represent the three number \( |y_1|, |y_2|, \text{ and } |y_3| \).
in any convenient order.

As before, we shall let \( y_i \) symbolize \( G(y_i) \) and \( n(y_i) \) symbolize \( nG(y_i) \), where \( n \) is a positive integer.

First we deal with the case

\[
\Sigma_0 = \{(0,0,0)\}
\]

\[
\Sigma^* = \{(0,0,0), (\pm 1, 0, 0), (0, \pm 1, 0), (0, 0, \pm 1)\}
\]

We have

\[
H_0 \overline{pG}/h =
\]

\[
\begin{array}{ccccccc}
\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\
0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\
1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\
0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0
\
0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0
\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0
\end{array}
\]
\[
\begin{array}{cccccccc}
(000) & (100) & (100) & (0\bar{1}0) & (010) & (00\bar{1}) & (001) \\
\hline
200 & 300 & 100 & 210 & 210 & 201 & 201 & (200) \\
110 & 210 & 010 & 120 & 100 & 111 & 111 & (1\bar{1}0) \\
110 & 210 & 010 & 100 & 120 & 111 & 111 & (1\bar{1}\bar{1}) \\
101 & 201 & 001 & 111 & 111 & 102 & 100 & (101) \\
101 & 201 & 001 & 111 & 111 & 100 & 102 & (10\bar{1}) \\
200 & 100 & 300 & 210 & 210 & 201 & 201 & (200) \\
110 & 010 & 210 & 100 & 120 & 111 & 111 & (1\bar{1}0) \\
110 & 010 & 210 & 120 & 100 & 111 & 111 & (1\bar{1}\bar{1}) \\
101 & 001 & 201 & 111 & 111 & 102 & 100 & (10\bar{1}) \\
101 & 001 & 201 & 111 & 111 & 100 & 102 & (10\bar{1}\bar{1}) \\
o20 & 120 & 120 & 030 & 010 & 021 & 021 & (020) \\
o11 & 111 & 111 & 021 & 001 & 012 & 010 & (011) \\
o11 & 111 & 111 & 021 & 001 & 010 & 012 & (01\bar{1}) \\
o20 & 120 & 120 & 010 & 030 & 021 & 021 & (020) \\
o11 & 111 & 111 & 001 & 021 & 012 & 010 & (0\bar{1}1) \\
o11 & 111 & 111 & 001 & 021 & 010 & 012 & (0\bar{1}\bar{1}) \\
o02 & 102 & 102 & 012 & 012 & 003 & 001 & (002) \\
o02 & 102 & 102 & 012 & 012 & 001 & 003 & (002) \\
\end{array}
\]
where

\[ a_1 = G_{200} + 4G_{110} \]
\[ a_2 = 5G_{100} \]
\[ a_3 = G_{300} + 4G_{120} \]
\[ a_4 = G_{100} + 2G_{111} + 2G_{120} . \]

This can be written

\[
H_{FG/h}^0 = \begin{pmatrix}
0 \\
B_1 \\
B_2 \\
B_3 \\
B_4 \\
B_5 \\
B_6 \\
\end{pmatrix},
\]

(4.20)

where we let \( B_1, B_2, B_3, B_4, B_5, \) and \( B_6 \) represent, respectively, the \( 2^{\text{nd}}, 3^{\text{rd}}, 4^{\text{th}}, 5^{\text{th}}, \) and \( 6^{\text{th}} \) rows of \( H_{FG/h}^0 \). We have

\[
(G)^{-1} = \begin{pmatrix}
(000) & (\overline{0}10) & (100) & (0\overline{1}0) & (010) & (00\overline{1}) & (001) \\
000 & 100 & 100 & 100 & 100 & 100 & 100 \\
100 & 000 & 200 & 110 & 110 & 110 & 110 \\
100 & 200 & 000 & 110 & 110 & 110 & 110 \\
100 & 110 & 110 & 000 & 200 & 110 & 110 \equiv G_F^{-1}. (4.21) \\
100 & 110 & 110 & 200 & 000 & 110 & 110 \\
100 & 110 & 110 & 110 & 000 & 200 & (00\overline{1}) \\
100 & 110 & 110 & 110 & 110 & 200 & 000 & (001) \\
\end{pmatrix}
\]
From Eqs. (4.20) and (4.21), then, we get

\[
H_0 \Phi G (G)^{-1} \Phi G h^2 =
\]

\[
\begin{bmatrix}
0 & 0 & \ldots & 0 \\
0 & B_1 G_F B_1^{-1} B_2 G_F B_2^{-1} & \ldots & B_1 G_F B_6^{-1} B_6 \\
0 & B_2 G_F B_1^{-1} B_2^{-1} B_2 & \ldots & B_2 G_F B_6^{-1} B_6 \\
\vdots & \vdots & \ddots & \vdots \\
0 & B_6 G_F B_1^{-1} B_6^{-1} B_2 & \ldots & B_6 G_F B_6^{-1} B_6 \\
\end{bmatrix}
\]

(4.22)

We also need to calculate \( H_0 \Phi G \Phi h^2 \):

\[
\begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & (000) \\
0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & (100) \\
1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & (100) \\
0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & (010) \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & (010) \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & (001) \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & (001)
\end{bmatrix}
\]
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<th>110</th>
<th>101</th>
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<td>101</td>
<td>101</td>
<td>112</td>
<td>112</td>
<td></td>
</tr>
</tbody>
</table>

| 101 | 011 | 011 | 000 | 002 | 301 | 211 | 211 | 200 | 202 | 121 | 110 | 112 | 121 | 110 | 112 | 101 | 103 |
| 101 | 011 | 011 | 002 | 000 | 301 | 211 | 211 | 202 | 200 | 121 | 112 | 110 | 121 | 112 | 110 | 103 | 101 |

| 400 | 310 | 310 | 301 | 301 | 000 | 110 | 110 | 101 | 101 | 220 | 211 | 211 | 220 | 211 | 211 | 202 | 202 |
| 310 | 220 | 200 | 211 | 211 | 110 | 000 | 020 | 011 | 011 | 130 | 121 | 121 | 110 | 101 | 101 | 112 | 112 |
| 310 | 200 | 220 | 211 | 211 | 110 | 020 | 000 | 011 | 011 | 110 | 101 | 101 | 130 | 121 | 121 | 112 | 112 |

| 301 | 211 | 211 | 200 | 202 | 101 | 011 | 011 | 000 | 002 | 121 | 110 | 112 | 121 | 110 | 112 | 101 | 103 |
| 301 | 211 | 211 | 202 | 200 | 101 | 011 | 011 | 002 | 000 | 121 | 112 | 110 | 121 | 112 | 110 | 103 | 101 |

| 220 | 110 | 130 | 121 | 121 | 220 | 130 | 110 | 121 | 121 | 000 | 011 | 011 | 040 | 031 | 031 | 022 | 022 |
| 211 | 101 | 121 | 110 | 112 | 211 | 121 | 101 | 110 | 112 | 011 | 000 | 002 | 031 | 020 | 022 | 011 | 013 |
| 211 | 101 | 121 | 112 | 110 | 211 | 121 | 101 | 112 | 110 | 011 | 002 | 000 | 031 | 022 | 020 | 013 | 011 |

| 220 | 130 | 110 | 121 | 121 | 220 | 110 | 130 | 121 | 121 | 040 | 031 | 031 | 000 | 011 | 011 | 022 | 022 |
| 211 | 121 | 101 | 110 | 112 | 211 | 101 | 121 | 110 | 112 | 031 | 020 | 022 | 011 | 000 | 002 | 001 | 013 |
| 211 | 121 | 101 | 112 | 110 | 211 | 101 | 121 | 112 | 110 | 031 | 022 | 020 | 011 | 002 | 000 | 013 | 011 |

| 202 | 111 | 112 | 101 | 103 | 202 | 112 | 112 | 101 | 103 | 022 | 011 | 013 | 022 | 011 | 013 | 000 | 004 |
| 202 | 112 | 112 | 103 | 101 | 202 | 112 | 112 | 103 | 101 | 022 | 013 | 011 | 022 | 013 | 011 | 004 | 002 |
\[
\begin{array}{cccccccc}
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\
0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
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0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\
\end{array}
\]

\[
\begin{array}{cccccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & P_1 & P_2 & P_3 & P_3 & P_3 & P_3 & P_3 \\
0 & P_2 & P_1 & P_3 & P_3 & P_3 & P_3 & P_3 \\
0 & P_3 & P_3 & P_3 & P_3 & P_3 & P_3 & P_3 \\
0 & P_3 & P_3 & P_2 & P_1 & P_3 & P_3 & P_3 \\
0 & P_3 & P_3 & P_3 & P_3 & P_3 & P_1 & P_2 \\
0 & P_3 & P_3 & P_3 & P_2 & P_3 & P_1 & P_2 \\
0 & P_3 & P_3 & P_3 & P_3 & P_3 & P_1 & P_2 \\
\end{array}
\]

\[
H_0 \Pi_0 \Pi H_0 / \hbar^2 = \begin{array}{cccccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & P_3 & P_3 & P_3 & P_3 & P_3 & P_3 & P_3 \\
0 & P_3 & P_3 & P_2 & P_1 & P_3 & P_3 & P_3 \\
0 & P_3 & P_3 & P_3 & P_3 & P_3 & P_1 & P_2 \\
0 & P_3 & P_3 & P_3 & P_2 & P_1 & P_2 & P_1 \\
\end{array}
\]
where

\[ P_1 = 5G_{000} + 16G_{110} + 4G_{200} \]
\[ P_2 = 8G_{130} + 8G_{112} + 4G_{200} + 4G_{220} + G_{400} \]
\[ P_3 = 2G_{220} + G_{000} + 8G_{110} + 2G_{130} + 10G_{112} + 2G_{200} \]

It will be seen from the relation between \( B_1, B_2, B_3, B_4, B_5, \) and \( B_6 \) in Eq. (4.20), and from the symmetry properties of \( (G^{-1}) \) (Eq. (4.21)), that the expression \( (4.22) \) has the same symmetry as \( (4.23) \). Hence we need to calculate only three elements \( B_1 G_F^{-1} B_1^{tr}, B_2 G_F^{-1} B_1^{tr}, \) and \( B_3 G_F^{-1} B_1^{tr} \).

We get, from Eqs. (4.22) and (4.23),

\[ (G^{(\mathbf{s}^0)})^{-1} = H_0^{-1} G (G^{-1})^{-1} G^{-1} - H_0^{-1} G^{-1} (G^{-1})^{-1} G^{-1} + Z - H_0 \]

\[
\begin{vmatrix} 
Z & -h & -h & -h & -h & -h & -h \\
-h & E_1' & E_2 & E_3 & E_3 & E_3 & E_3 \\
-h & E_2 & E_1' & E_3 & E_3 & E_3 & E_3 \\
-h & E_3 & E_3 & E_1' & E_2 & E_3 & E_3 \\
-h & E_3 & E_3 & E_2 & E_1' & E_3 & E_3 \\
-h & E_3 & E_3 & E_3 & E_3 & E_2 & E_1' \\
-h & E_3 & E_3 & E_3 & E_3 & E_3 & E_1 \\
\end{vmatrix}

(4.25)

where

\[ E_1' = h^2 (B_1 G_F^{-1} B_1^{tr} - P_1) + Z \]
\[ E_2 = h^2 (B_2 G_F^{-1} B_1^{tr} - P_2) \]
\[ E_3 = h^2 (B_3 G_F^{-1} B_1^{tr} - P_3) \]

(4.26)
We now do the corresponding calculation for the case

\[ \varepsilon = \{ (0,0,0),(1,0,0) \} = \varepsilon^* \]

\[
\begin{array}{cccccccccc}
100 & 001 & 010 & 010 & 001 & 200 & 110 & 110 & 101 & 101 \\
110 & 010 & 000 & 110 & 101 & 100 & 110 & 110 & 101 & 101 \\
000 & 010 & 110 & 010 & 001 & 110 & 010 & 010 & 001 & 110 \\
010 & 110 & 000 & 010 & 001 & 010 & 101 & 010 & 001 & 101 \\
200 & 100 & 110 & 100 & 110 & 100 & 110 & 100 & 110 & 100 \\
110 & 010 & 110 & 010 & 001 & 110 & 010 & 010 & 001 & 110 \\
001 & 101 & 001 & 011 & 001 & 011 & 001 & 011 & 001 & 011 \\
011 & 101 & 011 & 001 & 011 & 001 & 011 & 001 & 011 & 001 \\
200 & 100 & 110 & 100 & 110 & 100 & 110 & 100 & 110 & 100 \\
110 & 010 & 110 & 010 & 001 & 110 & 010 & 010 & 001 & 110 \\
001 & 101 & 001 & 011 & 001 & 011 & 001 & 011 & 001 & 011 \\
011 & 101 & 011 & 001 & 011 & 001 & 011 & 001 & 011 & 001 \\
\end{array}
\]

\[
= \begin{vmatrix}
5(100) & (200) + 4(110) \\
(200) + 4(110) & 5(100)
\end{vmatrix}.
\]  

(4.27)

Letting

\[ L = (5(100) (200) + 4(110)) \]

and

\[ M = ((200) + 4(110) 5(100)) \],

and

\[ (G)^{-1} = \begin{vmatrix}
000 & 100 \\
100 & 000
\end{vmatrix} = G_S^{-1} \],

(4.28)

we get, from Eqs. (4.27) and (4.28),

\[
H_{0PG} (G)^{-1} G_{PH_0}/h^2 = \begin{vmatrix}
L G_S^{-1} L_{tr} & L G_S^{-1} M_{tr} \\
M G_S^{-1} L_{tr} & M G_S^{-1} M_{tr}
\end{vmatrix}.
\]  

(4.29)
Likewise,

\[
\tilde{H}_0 \frac{\tilde{G} \tilde{F} \tilde{P} H_0}{h^2} =
\]

\[
\begin{array}{cccccccccccc}
1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
\end{array}
\]

\[
\begin{array}{cccccccccccc}
0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 1 \\
1 & 1 & 0 & 2 & 0 & 0 & 0 & 2 & 1 & 0 & 1 & 1 \\
1 & 2 & 0 & 1 & 0 & 1 & 1 & 1 & 1 & 1 & 0 & 0 \\
1 & 2 & 0 & 1 & 0 & 1 & 1 & 1 & 1 & 1 & 0 & 2 \\
1 & 2 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 0 \\
1 & 2 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\
1 & 2 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 2 \\
1 & 2 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 \\
\end{array}
\]

\[
\begin{array}{cccccccccccc}
(\tilde{H}_0) & 1 & 0 \\
(\tilde{O}_0) & 1 & 0 \\
(\tilde{O}_0) & 1 & 0 \\
(\tilde{O}_0) & 1 & 0 \\
(\tilde{O}_0) & 1 & 0 \\
(\tilde{O}_0) & 1 & 0 \\
(\tilde{O}_0) & 1 & 0 \\
(\tilde{O}_0) & 1 & 0 \\
(\tilde{O}_0) & 1 & 0 \\
\end{array}
\]

\[
\begin{array}{cccccccccccc}
1 & 0 \\
0 & 1 \\
0 & 1 \\
0 & 1 \\
0 & 1 \\
0 & 1 \\
0 & 1 \\
0 & 1 \\
0 & 1 \\
\end{array}
\]

\[
= \begin{vmatrix}
P_5 & P_4 \\
P_4 & P_5 \\
\end{vmatrix}
\]

(4.30)

where

\[
P_5 = 5G_{000} + 16G_{110} + 4G_{200} = P_1
\]

\[
P_4 = 4G_{100} + 12G_{120} + 8G_{111} + G_{300}.
\]

We get, then, from Eqs. (4.29) and (4.30)

\[
(G\vec{\Sigma}_{\perp})^{-1} - \frac{H_0 \tilde{G} \tilde{F} \tilde{P} H_0}{h^2} = \frac{1}{h_0} [G_{0}^{-1} \tilde{G} \tilde{P} \tilde{H}_0 + Z - \tilde{H}_0]
\]

\[
= \begin{vmatrix}
E^' & E_5 \\
E_5 & E^' \\
\end{vmatrix}
\]

(4.31)
where

\[ E'_4 = h^2 (L_G L_{-1}^T r - P_1) + Z \]
\[ E_5 = h^2 (L_G L_{-1}^T r - P_5) - h \]

(4.32)

For the case \( \varepsilon_2 \) and \( \varepsilon_3 \), the calculation is exactly identical to that for \( \varepsilon_1 \), to which it is related by reflectional symmetry.

We are now ready to consider \( \hat{\Gamma}(k) \), of which we need to calculate only one element, \( \hat{\rho}^{00}(k) \).

From Eqs. (4.2), (4.3), (4.19), (4.25), and (4.31), we get

\[
\hat{\rho}(k) =
\begin{vmatrix}
Z-V_2 & -h & -h & -h & -h & -h & 0 & 0 & 0 & 0 & -1
-h & E_1 & E_2 & E_3 & E_3 & E_3 & E_3 & -V_{3a} & 0 & 0 & 0 & 0
-h & E_2 & E_1 & E_3 & E_3 & E_3 & E_3 & 0 & -V_3 & 0 & 0 & 0 & 0
-h & E_3 & E_3 & E_1 & E_2 & E_3 & E_3 & 0 & 0 & -V_{3b} & 0 & 0 & 0 & 0
-h & E_3 & E_3 & E_3 & E_2 & E_1 & E_3 & 0 & 0 & 0 & -V_3 & 0 & 0 & 0
-h & E_3 & E_3 & E_3 & E_3 & E_1 & E_2 & 0 & 0 & 0 & 0 & -V_{3c} & 0
-h & E_3 & E_3 & E_3 & E_3 & E_2 & E_1 & 0 & 0 & 0 & 0 & 0 & -V_3
\end{vmatrix}
\]
where
\[ a = e^{-i k_1}, \quad b = e^{-i k_2}, \quad c = e^{-i k_3} \]
\[ d = e^{i k_1}, \quad f = e^{i k_2}, \quad g = e^{i k_3} \]
\[ E_1 = E_1' - V_1 \]
\[ E_4 = E_4' - V_2 \]

and where \( E_1', E_2, E_3, E_4, E_5 \) are given by Eqs. (4.26) and (4.32).

The actual calculation of \( \hat{\mathbf{p}}_{00}(k) \) can be simplified by the use of symmetry properties for diagonal blocks, and among \( k_1, k_2 \) and \( k_3 \), and \( k_i \) and \( -k_i \) (\( i = 1, 2, 3 \)).

If we write
\[ \hat{\mathbf{p}}(k)^{-1} = \]

\[
\begin{array}{cccccccc}
0 & 1 & 2 & 3 & 4 & 5 & 6 & 0 & 1 & 2 & 3 & 4 & 5 & 6 \\
0 & & & & & & & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & & & & & & & -V_3a & 0 & 0 & 0 & 0 & 0 \\
2 & & & & & & & 0 & -V_3 & 0 & 0 & 0 & 0 \\
3 & & & & & & & 0 & 0 & -V_3b & 0 & 0 & 0 \\
4 & & & & & & & 0 & 0 & 0 & -V_3 & 0 & 0 \\
5 & & & & & & & 0 & 0 & 0 & 0 & -V_3c & 0 \\
6 & & & & & & & 0 & 0 & 0 & 0 & 0 & -V_3 \\
\end{array}
\]

\[
\begin{array}{cccccccc}
0 & -V_3d & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & -V_3 & 0 & 0 & 0 & 0 & 0 \\
2 & 0 & 0 & 0 & -V_3 & 0 & 0 & 0 & 0 \\
3 & 0 & 0 & 0 & 0 & -V_3f & 0 & 0 & 0 \\
4 & 0 & 0 & 0 & 0 & 0 & -V_3 & 0 & 0 \\
5 & 0 & 0 & 0 & 0 & 0 & 0 & -V_3g & 0 \\
6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -V_3 \\
\end{array}
\]

\[
\begin{array}{cccccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{array}
\]

\[
\begin{array}{cccccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{array}
\]

\[
\begin{array}{cccccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{array}
\]
and express $\hat{r}_{00}^{00}(k)$ as the ratio of two determinants:

$$\hat{r}_{00}^{00}(k) = \frac{N}{D_e}$$

where $N$ is the determinant with the first row and column omitted, and $D_e$ is the full determinant. Thus


$$- 6V^2_A(12345)(12345)B(12)(12)C(34)(34)D_{55}$$

$$+ 12V^4_A(1235)(1235)B(12)(12)C_{33}D_{55}$$

$$- 8V^6_A(135)(135)B_{11}C_{33}D_{55}$$

$$+ 3V^4_A(1234)(1234)B(12)(12)C(34)(34)$$

$$- 12V^6_A(123)(123)B(12)(12)C_{33}$$

$$+ 12V^8_A(13)(13)B_{11}C_{33} + 3V^8_A(12)(12)B(12)(12)$$

$$- 6V^{10}_A(11B_{11} + V^{12}_A)$$

$$+ 2V^2_3(-A(12346)(12345)B(12)(12)C(34)(34)D_{56}$$

$$+ 4V^2_3(1235)(1236)B(12)(12)C_{33}D_{56}$$

$$- 4V^4_3(135)(136)B_{11}C_{33}D_{56}$$

$$- 2V^4_3(123)(124)B(12)(12)C_{43} + 4V^6_3(13)(23)B_{21}C_{33}$$

$$- V^8_3A_{12}B_{21}(\cos k_1 + \cos k_2 + \cos k_3)$$

$$+ 4V^4_3(1236)(1245)B(12)(12)C_{43}D_{56}$$

$$- 2V^2_3(135)(146)B_{11}C_{43}D_{65}$$

$$+ V^4_3(13)(24)B_{21}C_{43}(\cos k_1\cos k_2 + \cos k_1\cos k_3 + \cos k_2\cos k_3)$$

$$- 8V^6_3(135)(246)B_{21}C_{43}D_{65}\cos k_1\cos k_2\cos k_3$$.
where $A_{(123456)(123456)}$ is the determinant of the submatrix of $A$ with rows 1, 2, 3, 4, 5, 6 and columns 1, 2, 3, 4, 5, 6, etc. For $D_e$ we include the 1st row and column, by the replacements:

$$A_{(123456)(123456)} \rightarrow A_{(0123456)(0123456)}$$

$$A_{(123)(123)} \rightarrow A_{(0123)(0123)}$$

etc.

This completes the derivations needed to proceed with a numerical calculation of the nearest neighbor TCA for the two-dimensional and three-dimensional single-band models.

From the result we got, we see that in order to calculate $\hat{G}(k)$, some matrix elements of $G$ need to be calculated. Fourier transformation will play an important role in this part. Consider a one-dimensional case, we have

$$A_{(123456)(123456)} = A_{(0123456)(0123456)}$$

$$A_{(123)(123)} = A_{(0123)(0123)}$$

etc.

For a tight-binding approximation, we have

$$\hat{H}_0(k) = \sum_{x} e^{-i(x'-x)k} h_0(x'-x), \quad (4.33)$$

for a tight-binding approximation, we have

$$H_0(x'-x) = h(\delta_{x,x+1} + \delta_{x',x-1}).$$

From Eq. (4.33), we get

$$\hat{H}_0(k) = \sum_{x} e^{-ik} h(\delta_{x,1} + \delta_{x,-1})$$

$$= 2\hbar \cos k, \quad (4.34)$$

where we let $x'$ and $x$ be $n$ and $0$ respectively.

We have, for the 1st Brillouin zone,

$$G_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} \hat{G}(k) e^{ik} dk$$

$$= \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{e^{ik}}{(z - \hat{G}(k) - \hat{H}_0(k))} dk.$$
substituting \( \hat{R}_0(k) \) from Eq.(4.34), yields

\[
\begin{align*}
G_n &= \frac{1}{\pi} \int_0^{\pi} \frac{\sin k}{(Z - \hat{\Omega}(k) - 2h \cos k)} \cos nk \, dk \\
&= \frac{1}{\pi} \int_0^{\pi} \cos nk \, dk \\
&\quad \text{because } \sin nk \text{ is an odd function of } k.
\end{align*}
\]

For convenience, we let \( h = 1/2 \), hence

\[
G_n = \frac{1}{\pi} \int_0^{\pi} \frac{\cos nk \, dk}{(Z - \hat{\Omega}(k) - \cos k)}.
\]

For the two-dimensional and three-dimensional cases, we have

\[
G_{mn} = \frac{1}{\pi^2} \int_0^{\pi} \int_0^{\pi} \frac{\cos k_1 \cos k_2 \cos k_3 \, dk_1 \, dk_2 \, dk_3}{(Z - \hat{\Omega}(k_1, k_2) - \cos k_1 - \cos k_2)}
\quad \text{(4.35)}
\]

and

\[
G_{1mn} = \frac{1}{\pi^3} \int_0^{\pi} \int_0^{\pi} \int_0^{\pi} \frac{\cos k_1 \cos k_2 \cos k_3 \, dk_1 \, dk_2 \, dk_3}{(Z - \hat{\Omega}(k_1, k_2, k_3) - \cos k_1 - \cos k_2 - \cos k_3)}
\quad \text{(4.36)}
\]

respectively.
CHAPTER V
RESULTS, DISCUSSION AND CONCLUSION

The results in this chapter are due to a single-band calculation, with nn interaction, and site diagonal disorder only, although the formalism given in Chapter 3 is generally applicable if there are no site-site correlations.

A. Results and Discussion

For convenience, we can fix $V^B = 0$; this gives $V_3 = \sqrt{V_1 V_2}$. The effect is just to shift the energy by $-V^B$. We shall experiment both the TCA(1), which is exactly equivalent to the CPA, and the TCA(nn) in order to compare the results; the formalism for writing the computer program for the TCA(1) is given in Appendix A. We see in Appendix B (see, especially, Eqs. (B.1) and (B.2)) that in calculating necessary matrix elements of $G$, we can have difficulties in integrating when the denominator gets small. To avoid this problem, we shall use a linear approximation for such a denominator within each integration cell, and call this method of integration the 'cellular method'; the formalism of this method for the two- and three-dimensional systems is given in Appendix B. Computer programs with some explanation are given in Appendix C.

We remind the reader that when $V^A > 2nh$, where $n$ is the number of nearest neighbors at any lattice site and $h$ the hopping integral in a tight binding approximation, the spectrum of $H$ splits into two subbands. This occurs, loosely, because the greatest width either subband can
obtain is 2nh, and in fact this width is reached only in the limit of low concentrations of either A or B atoms.

In both two-dimensional and three-dimensional lattices, we allowed $c_A$ to approach zero and compared the results with perfect lattices as shown in Figs. (5.1) and (5.2). They show the results as expected, both the CPA and the TCA(nn) gave almost exactly the same results as the perfect lattices give.

For two-dimensional alloys, we study two cases, $V^A < 2nh$ and $V^A > 2nh$. In Fig. (5.3), we show results for the case $V^A < 2nh$; the band is not yet split, although a minority subband is beginning to emerge. The curves of the CPA are comparable with those of the TCA(nn) for the over-all band shape; however the latter spreads over a slightly larger range of energies than that predicted by the CPA. This is because the states near the limits of the allowed spectrum in the TCA(nn) are associated with pairs which are beyond the scope of a single-site approximation. In addition there is some structure for the case of the TCA(nn), which does not appear in the case of the CPA. In Fig. (5.4), we show results for the case $V^A > 2nh$, so that the subbands are well separated. It is of interest to study the formation of the satellite levels as a function of concentration. As the concentration of impurity is decreased, the minority band narrows and finally emerges from the satellite states. Fig. (5.4(c)) shows the minority band with a three peaked structure. Physically, the central peak is due to isolated impurities, while the two satellite peaks arise from the bonding and antibonding levels of a nearest-neighbor impurity pair cluster. \[37\] This three peaked behavior also appears in the minority band in Fig. (5.6). The CPA cannot show this structure.
For three-dimensional alloys, we used the same values of the parameters as R. Alben et al. and compared our results with theirs, which are exact for a sample of $19 \times 20 \times 21$ sites, with site-diagonal disorder. In order to compare our results, we must scale the energy a factor of three and shift it by $-V^A/2$, and also multiply the density by three, since they used $h = 1/6$ and $V^A = -V^B$, whereas we used $h = 1/2$ and $V^B = 0$. In Fig. (5.5), the TCA(nn) gives the result quite well when compared with the exact results. We would like to note here that the difference between the TCA(nn) and the CPA has a strong resemblance to that shown in Fig. (5.3). In Fig. (5.6), there is a three-peaked structure in the minority band. Although the TCA(nn) cannot give the substructure, in the satellite levels, which is beyond the scope of the nearest-neighbor approximation, it does give the central peak in good agreement with the exact results.

We would like to note here that the agreement between the machine calculations and the CPA results is better in higher-than in lower-dimensional systems since the CPA is a mean-field theory and corrections to it are expected to scale as $1/n$, where $n$ is the number of nearest neighbor. 18
Fig. 5.1 Density of states for a two-dimensional lattice. Broken curve shows calculated density of states of a perfect crystal. Solid curve shows density of states of an alloy with $V^A = 3.8$, $V^B = 0$, $c_A = .0001$, $c_B = .9999$; CPA and TCA(nn) give the same curve.
Fig. 5.2 Density of states for a three-dimensional lattice. Broken curve shows density of states of a perfect crystal. Solid curve shows density of states for an alloy with $V_A = 3.8, V_B = 0$, $c_A = .0001, c_B = .9999$; CPA and TCA(nn) give the same curve.
Fig. 5.3  Density of states for a two-dimension alloy with $V^A = 1.75$, $V^B = 0$, $c_A = .25$ and $c_B = .75$; solid curve from TCA(nn) and broken curve from CPA.
Fig. 5.4 Density of states in the B-subband for a two-dimensional alloy with $V^A = 20$, $V^B = 0$; solid curves from TCA(nn) and broken curves from CPA. (a) $c_A = .285$, $c_B = .715$. (b) $c_A = .499$, $c_B = .501$. (c) $c_A = .713$, $c_B = .287$. 

Fig. 5.5  Density of states for a three-dimensional alloy with $V_A = .4$, $V_B = -.4$, $c_A = .16$, $c_B = .84$; solid curve for exact results.\textsuperscript{36} (a) Broken curve from TCA(nn). (b) Broken curve from CPA.
Fig. 5.6 Density of states for a three-dimensional alloy with $V_A = .75$, $V_B = -.75$, $c_A = .1$, $c_B = .9$; solid curve for exact results. (a) Broken curve from TCA(nn). (b) Broken curve from CPA.
B. Conclusion

Recently, the coherent potential approximation (CPA) has been shown to be in many ways the best single-site approximation for disordered alloys. However, being a single-site approximation, it is incapable of describing effects due to multi-site scattering processes and correlations. Many authors have attempted to generalize the CPA by including pair and cluster scattering; Nickel and Krumhansl gave the first logical n-site generalization of the CPA (CPA(n)). In 1973, Nickel and Butler discovered through numerical computations that these n-site approximations gave a nonanalytic mean resolvent in many cases of strong disorder; branch cuts in particular were found which made it impossible to define a single solution of the self-consistent equation. This makes the approximations unacceptable, since physical quantities, such as the density of states, cannot then be uniquely determined.

In 1974, Mills proposed an approximation to deal with the problem of analyticity. In this approximation, the graphs of the corrected cumulant expansion are partially summed in such a way that the Herglotz property of the mean resolvent can be analysed easily at each stage, and the proper modified graphs combined in such a way as to preserve this property in any desired level of approximation. Because of the fact that a single graph in this approximation may involve a sequence of clusters traveling arbitrarily large distances through the sample, such a specific approximation is called a 'Traveling Cluster Approximation (TCA).' He also proved that, for this approximation, the solution exists, and is unique and analytic. It was shown that the CPA and the single-site TCA are exactly equivalent to each other.
The aim of this work is to apply the TCA in the level of nearest-neighbor approximation (TCA(nn)) to both two-dimensional and three-dimensional alloys in the single-band approximation, and to compare the results with those of the CPA and with exact results for 19 x 20 x 21 site alloys with site diagonal disorder.

It showed that the TCA(nn) gives quite satisfactory results when compared with exact calculations. It gives substructure which does not appear in the results of the CPA, and also gives better band edges of the spectrum.

The results presented in this paper are due to a single-band calculation, with nn interaction, and site diagonal disorder only, and the level of nearest-neighbor approximation. We hope that this kind of approximation is able to achieve more realistic calculations without impossible complexity. Such calculations might include many-band models, with not only nn interaction, or higher levels of approximation, such as the next nearest-neighbor approximation for example. A more serious problem, which has not yet been solved, is to include effects of site-site correlation, and off diagonal disorder (beyond what can be reduced to equivalent diagonal disorder).
APPENDIX A

SINGLE-SITE TRAVELING CLUSTER APPROXIMATION (TCA(1))

We are going to derive the equations for the coherent potential for the TCA(1) in the single-band approximation, which are used in computer programs S2SP and S3SP.

In the TCA(1), \( \mathbf{W} \) is a site-diagonal matrix,
\[
\mathbf{W} = \Sigma \mathbf{W}_x
\]
and Eq.(3.30) reduces to
\[
\mathbf{W}_x = \mathbf{\bar{V}}_x + \Delta \mathbf{V}_x \mathbf{\mathcal{G}}_{xx} \Delta \mathbf{V}_x .
\]

From Eq.(3.36), we get
\[
\mathbf{G}_{xx} = \mathbf{G}(x)(1 + \mathbf{\bar{V}}_x \mathbf{G}_{xx})
\]
or
\[
\mathbf{G}_{xx} = \left( (\mathbf{G}(x))^{-1} - \mathbf{\bar{V}}_x \right)^{-1}
\]
\[
= \left( \mathbf{G}_0^{-1} - \mathbf{W}(x) - \mathbf{\bar{V}}_x \right)^{-1}
\]
\[
= \left( \mathbf{G}_0^{-1} - \mathbf{W} + \mathbf{W}_x - \mathbf{\bar{V}}_x \right)^{-1}
\]
\[
= \left( \mathbf{G}^{-1} + \mathbf{W}_x - \mathbf{\bar{V}}_x \right)^{-1}
\]

where, for convenience, the notation \( \mathbf{G} \) is used for \( \langle \mathbf{G} \rangle \). Eq.(A.2) gives
\[
\mathbf{W}_x = \mathbf{\bar{V}}_x + \Delta \mathbf{V}_x \left( \mathbf{G}^{-1} + \mathbf{W}_x - \mathbf{\bar{V}}_x \right)^{-1} \Delta \mathbf{V}_x
\]
\[
\mathbf{u}_x \mathbf{W}_x \mathbf{u}_x = \mathbf{U}(\mathbf{\bar{V}}_x + \Delta \mathbf{V}_x \left( \mathbf{G}^{-1} + \mathbf{W}_x - \mathbf{\bar{V}}_x \right)^{-1} \Delta \mathbf{V}_x \mathbf{u}_x ,
\]
where \( \mathbf{u}_x \) is a normalized state vector localized near site \( x \) (see Eq.(3.41)).
Letting

\[ S = \tilde{u} W u, \]

and considering the two-dimensional case, from Eq.(A.3), we get

\[ S = \tilde{u} \tilde{V} u + \tilde{u} A V (G + G(\tilde{V}_{x} - \tilde{W}_{x})G \]
\[ + G(\tilde{V}_{x} - \tilde{W}_{x})G(\tilde{V}_{x} - \tilde{W}_{x})G + \ldots \) A V \]
\[ \]
\[ \text{by Eq.(3.42)} \]
\[ = V_{1} + \tilde{u} A V G A V u + \tilde{u} A V G(\tilde{V}_{x} - \tilde{W}_{x})G A V u \]
\[ + \tilde{u} A V G(\tilde{V}_{x} - \tilde{W}_{x})G(\tilde{V}_{x} - \tilde{W}_{x})G A V u + \ldots \]
\[ \text{by Eq.(3.42)} \]
\[ = V_{1} + V_{3}^{2} G_{00}(1 - (V_{2} - S)G_{00})^{-1} \]
\[ = V_{1} + V_{3}^{2}(G_{00}^{-1} + S - V_{2}), \]  \hspace{1cm} (A.4)

for the three-dimensional case, we get

\[ S = V_{1} + V_{3}^{2}(G_{00}^{-1} + S - V_{2}). \]  \hspace{1cm} (A.5)

Eqs.(A.4) and (A.5) are used, respectively, in computer programs S2SP and S3SP in Appendix C.
APPENDIX B

CELLULAR METHOD

From Eqs. (4.35) and (4.36), we have

\[ G_{mn} = \frac{1}{\eta} \int_{\theta} \int_{\phi} \frac{\cos mk_1 \cos n k_2 \, dk_1 \, dk_2}{(Z - \tilde{G}(k) - \cos k_1 - \cos k_2)} \]  

\[ \text{(B.1)} \]

and

\[ G_{1mn} = \frac{1}{\eta} \int_{\theta} \int_{\phi} \int_{\phi} \frac{\cos l k_1 \cos mk_2 \cos nk_3 \, dk_1 \, dk_2 \, dk_3}{(Z - \tilde{G}(k) - \cos k_1 - \cos k_2 - \cos k_3)} \]

\[ \text{(B.2)} \]

where \( (k) = (k_1, k_2) \) or \( (k_1, k_2, k_3) \) in Eq. (B.1) or Eq. (B.2) respectively.

\( \tilde{G} \) in these equations is an unknown function of \( k \), so that makes us not be able to use an analytical method to find \( G_{mn}, G_{1mn} \). By use of a numerical method we are faced with a problem that the denominator can become very small, so that the integrand is rapidly varying, which requires an impractically fine grid for numerical integration. We therefore use a linear approximation to the denominator and then integrate exactly over each integration cell. This permits accurate results with a much coarse grid. We first deal with the case that the numerator = 1, and then, at the end of this appendix, with the complication of having cosines in the numerator, which, however, are smoothly varying since \( l, m, n \) are not too large.
A. Two-Dimensional Case

Letting

\[
I = \frac{1}{\eta^2} \int_{0}^{\eta} \int_{0}^{\eta} f \, dk_1 dk_2.
\]

Now we are going to divide the denominator of the integrand into cells and find the integral for each cell; after that we express \( I \) as the sum of those terms. We have four corners for each cell but we have only three coefficients \( p, q, \) and \( r \) which are defined by a linear fit,

\[
f = p + q k_1 + r k_2.
\]

It proves most convenient to divide each cell into two triangles, as shown in Fig.(B.1), and, then each triangle will contribute to \( I_1 \) and \( I_2 \), where \( I_1 + I_2 = I \).

![Fig. B.1 Linear fit for \( f \) for the two-dimensional case.](image)

Let \( \Delta k_1 \) and \( \Delta k_2 \) be 1, hence the integral of the shaded triangle is

\[
i_1 = \frac{1}{\eta^2} \left( \frac{d k_2}{\eta} \right) \left( \frac{d k_1}{p + q k_1 + r k_2} \right),
\]

where \( p = f(i,j), q = f(i+1,j) - f(i,j), \) and \( r = f(i+1,j+1) - f(i+1,j). \)
We get

\[ i_1 = \frac{1}{r^2q} \left( \frac{1}{r} \left\{ \frac{1}{r} \left( (p + q + r) \ln(p + q + r) - (p + q + r) \right) \\
- \frac{1}{s} \left( (p + q + r) \ln(p + q + r) - (p + q + r) \right) \\
- plnp \right\} \right) \\
= \frac{1}{n} \left( \frac{1}{sr} f(i+1,j+1) \ln f(i+1,j+1) - \frac{1}{qr} f(i+1,j) \ln f(i+1,j) \\
+ \frac{1}{sq} f(i,j) \ln f(i,j) \right), \]

where we substitute \( p, q, r \) in terms of \( f \) at the corners, and let \( s = q + r \).

In the same way we do for another triangle of the cell. After that we sum over cells, we get the final result

\[ I = \frac{1}{n} \sum \left[ \frac{1}{sr} f(i+1,j+1) \ln f(i+1,j+1) \\
- \frac{1}{qr} f(i+1,j) \ln f(i+1,j) + \frac{1}{sq} f(i,j) \ln f(i,j) \\
+ \frac{1}{sr} f(i+1,j+1) \ln f(i+1,j+1) \\
- \frac{1}{qr} f(i+1,j+1) \ln f(i+1,j+1) \\
+ \frac{1}{sr} f(i+1,j+1) \ln f(i+1,j+1) \right], \quad (B.3) \]

or

\[ = \frac{1}{n} \sum f(i,j) \ln f(i,j) \left( \frac{1}{s_{i-1,j-1}} \right) \\
- \frac{1}{q_{i-1,j}} + \frac{1}{s_{i,j}} + \frac{1}{s_{i-1,j-1}} \\
- \frac{1}{r_{i-1,j}} + \frac{1}{s_{i,j}} \right), \quad (B.4) \]
where, and we define new notation,

\[ s_{i-1,j-1} = f(i,j) - f(i-1,j-1) = 1/a_{ij} \]
\[ r_{i-1,j-1} = f(i,j) - f(i,j-1) = 1/b_{ij} \]
\[ q_{i-1,j} = f(i,j) - f(i-1,j) = 1/c_{ij} \]
\[ r_{i-1,j} = f(i,j+1) - f(i,j) = 1/d_{ij} \]
\[ s_{ij} = f(i+1,j+1) - f(i,j) = 1/e_{ij} \]
\[ q_{ij} = f(i+1,j) - f(i,j) = 1/g_{ij} \]

we get, for new notation,

\[ I = \frac{1}{N^2} \sum_{i,j} f(i,j) \ln f(i,j) \left[ a_{ij} (b_{ij} + c_{ij}) \right. \]
\[ \left. + g_{ij} (e_{ij} - b_{ij}) + d_{ij} (e_{ij} - c_{ij}) \right] \tag{B.5} \]

**B. Three-Dimensional Case**

The method in section A is also applied here; in this case we divide the denominator of the integrand into cubical cell, divide each cubical cell into six tetrahedrons about the main diagonal, and make a linear fit for \( f \), within each tetrahedron.

\[ f = a + bk_1 + ck_2 + dk_3 \]

we consider a tetrahedron because of having four coefficients, as shown in Fig.(B.2), instead of a triangle.
Fig. B.2 Linear fit for $f$ for the three-dimensional case.

Letting

$$I = \frac{1}{\eta^3} \int_0^1 \int_0^1 \int_0^1 \frac{dk_1 dk_2 dk_3}{f}. $$

Let $\Delta k_1$, $\Delta k_2$ and $\Delta k_3$ be 1; what we want is the integral, see Eq. (B.2), in the form

$$I = \frac{1}{\eta^3} \int_0^1 \int_0^1 \int_0^1 \frac{dk_3}{k_3} \frac{dk_2}{k_2} \frac{dk_1}{k_1} (a + bk_1 + ck_2 + dk_3).$$

The result depends on $f^2 \Delta f$ evaluated at the corners. In the same way we do for the remaining tetrahedrons of the cells. After that we sum over cells, we get

$$I = \frac{1}{2\eta^3} f^2(i,j,k) \Delta f(i,j,k) \left[ a_1 (d_1 + c_1)(e_1 - b_2) 
+ h_1 (c_1 + b_1)(e_1 - d_2) + a_2 (b_1 - e_2)(c_2 + d_2) 
+ h_2 (b_2 + c_2)(d_1 - e_2) + a_3 (b_1 + d_1)(e_1 - c_2) 
+ a_4 (b_2 + d_2)(c_1 - e_2) \right],$$

(B.6)
where

\[ a_1 = \frac{1}{f(i,j,k) - f(i,j-1,k-1)} \]
\[ a_2 = \frac{1}{f(i,j+1,k+1) - f(i,j,k)} \]
\[ a_3 = \frac{1}{f(i,j,k) - f(i-1,j,k-1)} \]
\[ a_4 = \frac{1}{f(i+1,j,k+1) - f(i,j,k)} \]
\[ b_1 = \frac{1}{f(i,j,k) - f(i-1,j,k)} \]
\[ b_2 = \frac{1}{f(i+1,j,k) - f(i,j,k)} \]
\[ c_1 = \frac{1}{f(i,j,k) - f(i,j-1,k)} \]
\[ c_2 = \frac{1}{f(i,j+1,k) - f(i,j,k)} \]
\[ d_1 = \frac{1}{f(i,j,k) - f(i,j,k-1)} \]
\[ d_2 = \frac{1}{f(i,j,k+1) - f(i,j,k)} \]
\[ e_1 = \frac{1}{f(i,j,k) - f(i-1,j,k-1)} \]
\[ e_2 = \frac{1}{f(i+1,j+1,k+1) - f(i,j,k)} \]
\[ h_1 = \frac{1}{f(i,j,k) - f(i-1,j-1,k)} \]
\[ h_2 = \frac{1}{f(i+1,j+1,k) - f(i,j,k)} . \]

In the case with the complication of having cosines in the numerator, we shall make replacement such as

\[
\int \frac{\cos nk}{f} \, dk = \int \frac{dk}{f/(\cos nk + 2)} - \int \frac{2dk}{f}
\]

in order to avoid problems with singularities arising from the zeroes of \( \cos nk \), and make a linear fit for \( f/(\cos nk + 2) \) for the first integral in the right-hand side.

Eqs. (B.5) and (B.6) are used, respectively, in computer programs SPP2 and SPP3 in Appendix C.
APPENDIX C

COMPUTER PROGRAM

The basic idea of calculation is to find \( \hat{\rho}^{00}(k) \) in order to calculate \( \hat{G}(k) \), which we need, from Eqs. (3.59) and (3.60)

\[
\hat{G}(k) = v_1 + v_2 \hat{\rho}^{00}(k).
\] (C.1)

\( \hat{\rho}^{00}(k) \) can be found from Eq. (3.56)

\[
\hat{\rho}^{00}(k) = (\hat{\rho}_0^{-1} - \hat{\nu}(k))^{-1},
\] (C.2)

where \( \hat{\rho}_0^{-1} \) and \( \hat{\nu}(k) \) can be found from Eq. (3.77) and Eq. (3.79) respectively.

In order to find \( \hat{\rho}_0^{-1} \) we need some matrix elements of \( G \). These matrix elements can be found from Eqs. (4.35) and (4.36) for the two-dimensional and three-dimensional cases respectively,

\[
G_{mn} = \frac{1}{\eta^2} \int \int \frac{\cos k_1 \cos k_2 dk_1 dk_2}{(Z - \hat{G}(k_1, k_2) - \cos k_1 - \cos k_2)}
\] (C.3)

\[
G_{1mn} = \frac{1}{\eta^2} \int \int \frac{\cos k_1 \cos k_2 \cos k_3 dk_1 dk_2 dk_3}{(Z - \hat{G}(k_1, k_2, k_3) - \cos k_1 - \cos k_2 - \cos k_3)}
\] (C.4)

the cellular method in Appendix B will take care for this calculation.

The procedure of the method is summarized by block diagram as shown in Fig. (C.1).
Fig. C.1 Block diagram of the procedure for calculating $G_d$:

$T = \text{true}, F = \text{false}$.
In Fig. (C.1), we start with
\[ \hat{\mathcal{G}}(k) = \mathcal{G}_{\text{init.}} = V_1 - V_2. \]
\( \hat{\mathcal{G}}(k) \) is the inverse of the denominator of the integrand in Eq. (C.3) or (C.4). Calculate the necessary matrix elements of \( \mathcal{G} \) from Eq. (C.3) or Eq. (C.4) and find \( \hat{\mathcal{G}}(k) \) by Eqs. (C.1) and (C.2). Calculate \( \mathcal{G}_d \) (= \( G_{00} \) or \( G_{000} \) for the two-dimensional or the three-dimensional case respectively) and compare with the old one. If we do not get the criterion we set, we shall calculate needed matrix elements of \( \mathcal{G} \) with new \( \hat{\mathcal{G}}(k) \); the procedure will repeat until we get the criterion.

In computer programs, we used an array of \( Z \) (E in block diagram) for each calculation in order to save time consuming of the machine. We use SPEAKEASY LANGUAGE\(^{39,40} \) for all programs.

Some explanation for computer programs is given as following.

In these programs the notation \( V \) is used for \( V_3 \).

PROGRAM CPP2

This is a control program for the two-dimensional case. It calls for stored parameters \( V_1, V_2, Z \) (E in block diagram), \( P_0 \) (maximum number of cycle of the procedure which we set), and \( dk \) (\( Ak \) in block diagram). It divides \( Z \) into NB groups, each group containing an array of \( Z \)-values (line 5). It uses program NN2P (nearest-neighbor approximation) to run for an array of \( Z \) for each time. It compares \( G_{00} \)'s from program NN2P with the previous ones (line 22), and selects \( G_{00} \)'s (line 32) which meet the criterion (line 24), and lets the remaining ones and corresponding \( Z \) (line 38) be run by program NN2P. The procedure continues, if there are still some \( G_{00} \) which do not meet the criterion, until \( P \) reaches \( P_0 \), where \( P \) is the number of cycle of procedure. It will tabulate the order
of $Z(I)$, $Z$, $G_{00}$, del (line 22) and corresponding $P$ when $G_{00}$ meet the
criterion (PZ). After that it will repeat again for another group of $Z$
until all groups are done.

This program can call program S2SP (single-site approximation) by
changing four lines, as follows:

- line 6 change NN2P to S2SP
- line 20 change NN2P to S2SP
- line 39 add $S = SN(LL)$
- line 43 add $S = SN$.

**PROGRAM NN2P**

This program calculates $G_{00}$ with the help of program SPP2. Because
of the limit of number of lines for each program, this one has another
part (NN22P). It follows the calculation given in section A in Chapter 4.

To avoid the singularity of $GK/cosnk$ (see Eqs. (C.3) and (C.4), we
use $GK/(cosnk + 2)$ instead of $GK/cosnk$ where $GK$ is the denominator of the
integrand, and, after integration by the cellular method (program SPP2),
have correcting terms as shown, for example, in lines 10 and 11.

**PROGRAM SPP2**

This is a special program for the cellular method. Line 8 is the term
in the brackets in Eq. (B.5) in Appendix B with $a$, $g$, $e$ and $d$ are replaced
by $D$, shiftrig(C), $H$ and shiftdow(B) respectively. The command 'shift'
plays an important role in this program.

Each coefficient in Eq. (B.5) is concerned with the relationship
between $f(i,j)$ and its neighbor. Hence in order to carry on the calculation
by array instead of each element we need the method to shift the column
or the row of the array. The command 'shift' can take care of this.

For example, we use the command 'shiftup' in line 3.

"SHIFTUP(X,N) shifts the elements of X up. The elements of X are shifted N rows. The vacated rows are filled with zeroes. If a second argument is not present, it is assumed to be 1."

**PROGRAM S2SP**

This program is for a single-site approximation; its detail is shown in Appendix A.

**PROGRAM CPP3**

This control program is for the three-dimensional case. The purpose of this program for program NN3P is the same as that of program CPP2 for NN2P. However, this program is more complicated in selecting and keeping converging $G_{000}$. In this case we have four array-parameters, instead of three as in CPP2, namely $Z$, $k_1$, $k_2$, and $k_3$.

This program can call program S3SP (single-site approximation) by changing four lines as follows:

- line 6 change NN3P to S3SP
- line 20 change NN3P to S3SP
- line 38 add $S = SN(L1)$
- line 42 add $S = SN$.

**PROGRAM NN3P**

This program calculates $G_{000}$ with the help of program SPP3. For the same reason as in program NN2P, it has two other parts NN33P and NN333P. It follows the calculation given in section B in Chapter 4.
PROGRAM SPP3

This is a special program for the cellular method. Lines 19 and 21 are the term in the brackets in Eq.(B.6) in Appendix B.

PROGRAM S3SP

This program is for a single-site approximation; its detail is shown in Appendix A.

The method we always use is how to arrange both a one-dimensional and a two-dimensional array into the form we want.

For example, in line 18 of program CPP2, we have ints(1,NZ*NK). This is one-dimensional array which starts with 1 and ends with NZ*NK by increasing by 1 at each time. Line 18 changes this one-dimensional array to a two-dimensional one with NZ rows and NK columns; the elements in the first row are the first NK elements in the original array etc.

If we want the original array, we just write

\[ B = AlD(NZ*NK:A), \]

where A is defined by the equation in line 18.
1. PROGRAM CPP2

2. SIGNIFIC(8); DOMAIN COMPLEX

3. GET(DXP); X1=DXP(1); X2=DXP(2); NX=DXP(3); NZ0=DXP(4)

4. GET(DNNP); V1=DNNP(1); V2=DNNP(2); NK=DNNP(3); P0=DNNP(4)

5. ZG=GRID(X1, X2, (X2-X1)/NX); NB=WHOLE(NX/NZ0)+1

6. N=0; KEPT NN2P; KEPT SPP2

7. LCP: I=INTS(N*NZ0+1, MIN(NX+1, (N+1)*NZ0))

8. Z=A1D(:ZG(1))

9. IF(N.NE.0) GOTO LCP1

10. VV=V1*V2; VV2=VV*VV; VV3=VV**3; VV4=VV2*VV2

11. DK=1/(NK-1); K=GRID(0, 1, DK); CO=DK*DK

12. K=K*ACOS(-1)

13. CK=COS(K); C2K=2*CK*CK-1

14. C3K=CK*(2*C2K-1); C4K=2*C2K*C2K-1

15. LCP1: NZ=NOELS(Z)

16. NNZ=2*NZ

17. ZS=Z; NZS=NZ; IN=INTZ(1, NZ); NLL=0

18. A=A2D(NZ, NK: INTS(1, NZ*NK))

19. P=1

20. LCP2: NN2P

21. NNZ=NZ

22. DEL=G00N/G00-1

23. DEE= |DEL|

24. LOO=(A1D(:DEE).LT.1E-5)

25. NO=SUM(LOO)
26. IF(P.EQ.P0) GOTO LCP3
27. IF(NO.EQ.0) GOTO LCP7
28. LCP3: L1=LOC(.NOT.LOO)
29. IF(NO.EQ.0) GOTO LCP5
30. LO=LOC(L00)
31. LCP4: LL(NLL+1)=IN(L0)
32. PZ(NLL+1)=(NO:)P;GG(NLL+1)=GOON(LO);DELL(NLL+1)=DEL(L0)
33. NLL=NLL+N0
34. IF(NLL.EQ.NZS) GOTO LCP9
35. IF(P.LT.P0) GOTO LCP6
36. LCP5: LO=L1;NO=NZS-NLL;P=1E50
37. GOTO LCP4
38. LCP6:  Z=Z(L1);GOO=GOON(L1);IN=IN(L1)
39. GK=GK(A1D(:A(L1,)),)
40. NZ=NZ-N0
41. M1=A2D(NZ*NK,NK:);M2=A2D(NZ,NK:)
42. GOTO LCP8
43. LCP7:  GOO=GOON
44. LCP8:  FREEIF(GOON,L00,L0,L1)
45. FREEIF(SN)
46. P=P+1
47. GOTO LCP2
48. LCP9:  RL=RANKER(LL)
49. Z=ZS;GOO=GG(RL);DEL=DELL(RL);PZ=PZ(RL)
50. FREEIF(GG,GOON,LL,L00,L0,L1)
51. FREEIF(II,YY)
52. FREE IF(SN)
53. TABULATE(I,Z,G00,DEL,PZ)
54. N=N+1
55. IF(N.LT.NB) GOTO LCP
1. PROGRAM NN2P
2. IF(NNZ.EQ.NZ) GOTO LNN
3. M1=A2D(NZ*NK,NK:);M2=A2D(NZ,NK:)
4. YY=M1+1;YY(INTS(NK,NK*NZ,NK),)=0
5. LNN: IF(P.NE.1) GOTO LNN1
6. GK=A1D(NZ*NK:Z+M2-CK)+M1-V1+.11-CK
7. F=GK
8. KEPT SPP2;SPP2
9. G00=GC
10. LNN1: F=GK/(CK+2);SPP2
11. G01=GC-2*G00
12. F=1/(A1D(:M2+CK+2))*F;SPP2
13. G11=GC-4*(G00+G01)
14. F=GK/(C2K+2);SPP2
15. G02=GC-2*G00
16. F=1/(A1D(:M2+CK+2))*F;SPP2
17. G12=GC-4*G00-2*(G01+G02)
18. F=1/(A1D(:M2+C2K+2))*GK/(C2K+2);SPP2
19. G22=GC-4*(G00+G02)
20. F=GK/(C3K+2);SPP2
21. G03=GC-2*G00
22. F=1/(A1D(:M2+CK+2))*F;SPP2
23. G13=GC-4*G00-2*(G01+G03)
24. F=GK/(C4K+2);SPP2
25. G04=GC-2*G00
26. FREE(GK,GC)
27. \( F = 2G_{11} + G_{02}; L = 3G_{01}; M = G_{03} + 2G_{12}; H = G_{01} + 2G_{12} \)
28. \( P_{11} = 3G_{00} + 2(2G_{11} + G_{02}) \)
29. \( P_{12} = G_{04} + 2(2G_{13} + G_{02} + G_{22}) \)
30. \( P_{13} = G_{00} + 2(G_{11} + G_{22} + G_{02} + G_{13}) \)
31. \( P_{22} = G_{03} + 2(3G_{12} + G_{01}) \)
32. \( G_{002} = G_{00} - G_{02} ; G_{020} = G_{00} + G_{02} ; G_{11P} = G_{11} * G_{11} ; G_{01P} = G_{01} * G_{01} ; G_{00P} = G_{00} * G_{00} \)
33. \( G_{002P} = G_{002} * G_{002} \)
34. \( \text{DET1} = G_{002P} * (G_{020} - 2G_{11}) * (G_{00} * (G_{020} + 2G_{11}) - 4G_{01P}) \)
35. \( A_A = G_{002P} * (G_{020} * G_{020} - 4G_{11P}) \)
36. \( B_B = -G_{01P} * G_{002} * (G_{00} * (G_{00} - 2G_{11}) + G_{02} * (2G_{11} - G_{02})) \)
37. \( C_C = G_{002} * (G_{00P} * G_{020} - 2G_{00} * G_{11P}) + G_{01P} * (4G_{11} - 3G_{00} - G_{02}) \)
38. \( D_D = -G_{002} * (G_{00} * G_{02} * G_{020} - 2G_{00} * G_{11P}) + G_{01P} * (4G_{11} - 3G_{02} - G_{00}) \)
39. \( \text{EE} = -G_{002} * (G_{00} * G_{11} * G_{002} - G_{01P} * G_{002}) \)
40. \( \text{AAA} = F * (A_A * F + 2B_B * (L + M + 2H)) \)
41. \( B_BB = 2H * (H * (C_C + D_D) + 2 * E_E * (M + L)) \)
42. \( M_L = M * M + L * L \)
43. \( E_{51} = (0.25 * (A_A * L * C_C + 2L * D_D * M + B_B B B)) / \text{DET1} - P_{11} / 4 + Z - V1 \)
44. \( E_{52} = (0.25 * (A_A * M * D_D + 2L * C_C * M + B_B B B)) / \text{DET1} - P_{12} / 4 \)
45. \( E_{53} = (0.25 * (A_A + E_E * M_L + 2L * (E_E * M + H * (C_C + D_D)) + 2H * (2 * E_E * H + M * (C_C + D_D)))) / \text{DET1} - P_{13} / 4 \)
46. \( \text{DET2} = G_{00P} * G_{01P} \)
47. \( Q = 2G_{11} + G_{02} ; Q_P = Q * Q ; Z_2 = Z - V2 \)
48. \( E_{21} = (0.25 * (3G_{01P} * (3G_{00} - 2Q) + G_{00} * Q_P)) / \text{DET2} - P_{11} / 4 + Z_2 \)
49. \( E_{22} = (0.25 * (G_{01} * (3 * (2Q * G_{00} - 3G_{01P}) - Q_P))) / \text{DET2} - P_{22} / 4 - 0.5 \)
50. \( E_{512} = E_{51} - E_{52} ; E_{521} = E_{51} + E_{52} ; E_{513} = E_{51} - E_{53} ; E_{531} = E_{51} + E_{53} ; E_{21P} = E_{21} * E_{21} \)
51. \( E_{22P} = E_{22} * E_{22} ; E_{51P} = E_{51} * E_{51} ; E_{52P} = E_{52} * E_{52} ; E_{53P} = E_{53} * E_{53} \)
52. \[ E_{512P} = E_{512} \times E_{512}; TE_{53} = 2 \times E_{53} \]

53. \[ \text{FREE} (F, L, M, H, P11, P12, P13, P22, G002, G020, G11P, G01P, G00P, G002P, \text{DET1}) \]

54. \[ \text{FREE} (AA, BB, CC, DD, EE, AAA, BBB, ML, DET2, Q, QP) \]

55. \[ \text{FREE} (G01, G02, G03, G04, G11, G12, G13, G22) \]

56. \[ MA_{11} = E_{512P} \times (E_{521} \times (Z2 \times E_{521} - 1) - TE_{53} \times (TE_{53} \times Z2 - 1)) \]

57. \[ MA_{1} = E_{512P} \times (E_{521} - TE_{53}) \times (E_{521} + TE_{53}) \]

58. \[ MA_{22} = E_{512} \times (E_{513} \times (2 \times Z2 \times E_{531} - 1) - E_{512} \times (Z2 \times E_{51} - .25)) \]

59. \[ MA_{2} = E_{512} \times (E_{513} \times E_{531} \times 2 - E_{51} \times E_{512}) \]

60. \[ MA_{33} = E_{512} \times (Z2 \times (E_{52} \times E_{521} - 2 \times E_{53P}) + E_{53} \times .75 \times E_{52} - .25 \times E_{51}) \]

61. \[ \text{KEPT} \ NN22P; NN22P \]

62. \[ \text{RETURN} \]
1. PROGRAM NN22P
2. MA3=E512*(E52*E521-2*E53)
3. MA4=E512*(Z2*E521-.5)
4. MA5=E513*(Z2*E531-.5)
5. MA6=Z2*(E51*E52-E53)-.25*(E521-TE53)
6. MA7=(E52-E53)*(Z2*(E52+E53)-.5)
7. D=E21P-E22P;D1=E51P-E52P;TVV=2*VV;FVV=2*TVV;FVV2=4*VV2
8. AA0=D*D;AA1=-FVV*D*E21;AA2=2*VV2*D;AA3=FVV2*E21P
9. AA4=-4*VV3*E21;AA5=D*E22
10. AA6=2*E21*E22*VV;AA7=-VV2*E22;AA8=FVV2*E22P
11. A0=AA0*MA1+AA1*MA2+AA2*D1+AA3*(E51P-E53P)+AA4*E51+VV4
15. A2=AA8*(E52P-E53P)
18. FREE(E512P,TE53,MA11,MA1,MA22,MA2,MA33,MA3,MA4,MA5,MA6,MA7,D,D1,TVV,FVV,FVV2)
19. FREE(AA0,AA1,AA2,AA3,AA4,AA5,AA6,AA7,AA8,AA11)
23. FREE(B0,B2,NU,DE,A11)
24. F=GK
25. SPP2
26. \texttt{GOON=GC}

27. \texttt{FREE(GC,F)}

28. \texttt{RETURN}
1. PROGRAM SPP2
2. C=SHIFTLEF(1/(F-SHIFTRIG(F)))
3. D=SHIFTUP(F)
4. B=YY/(D-F)
5. D=YY/(SHIFTLEF(D)-F)
6. D(:,NK)=0
7. H=SHIFTDOW(SHIFTRIG(D))
8. T=SHIFTRIG(C)*(H-B)+SHIFTDOW(B)*(H-C)+D*(B+C)
9. FREE(B,C,D,H)
10. GC=CO*A1D (:SUMROWS(A2D(NZ,NK:SUMROWS(F*LOG(F)*T))))
11. FREE(T)
12. RETURN
1. PROGRAM S2SP

2. IF(NNZ.EQ.NZ) GOTO LNN

3. M1=A2D(NZ*NK,NK:);M2=A2D(NZ,NK:)

4. YY=M1+1;YY(INTS(NK,NK*NZ,NK),)=0

5. LNN: IF(P.NE.1) GOTO LNN1

6. S=V1-.1I

7. GK=A1D(NZ*NK:Z+M2-CK)+M1-S-CK

8. F=GK;SPP2

9. G0O=GC


11. SN=V1+VV/(1/G0O+S-V2)

12. F=GK;SPP2

13. G00N=GC

14. RETURN
1. PROGRAM CPP3

2. SIGNIFIC(8); DOMAIN COMPLEX

3. GET(DXP); X1=DXP(1); X2=DXP(2); NX=DXP(3); NZO=DXP(4)

4. GET(DNNP); V1=DNNP(1); V2=DNNP(2); NK=DNNP(3); P0=DNNP(4)

5. ZG=GRID(X1,X2,(X2-X1)/NX); NB=WHOLE(NX/NZO)+1

6. N=0; KETP NN3P; KETP SPP3

7. LCP: I=INTS(N*NZO+1,MIN(NX+1,(N+1)*NZO))

8. Z=ALD(:ZG(I))

9. IF(N.NE.0) GOTO LCP1

10. VV=V1*V2; VV2=VV*VV; VV3=VV**3; VV4=VV2*VV2; VV5=VV**5; VV6=VV3*VV3

11. DK=1/(NK-1); K=GRID(0,1,DK); CO=DK*DK*DK/2

12. K=K*ACOS(-1)

13. CK=COS(K); C2K=2*CK*CK-1; C3K=CK*(2*C2K-1); C4K=2*C2K*C2K-1

14. LCP1: NZ=COELS(Z)

15. NNZ=2*NZ

16. ZS=Z; NZS=NZ; IN=INTS(1,NZ); NLL=0

17. A=A2D(NZ,NK:INTS(1,NZ*NK))

18. B=A2D(NZ,NK*NK:INTS(1,NZ*NK*NK))

19. P=1

20. LCP2: NN3P

21. NNZ=NZ

22. DEL=G000N/G000-1; DEE=|DEL|

23. LOO=(ALD(:DEE).LT.1E-5)

24. NO=SUM(LOO)

25. IF(P.EQ.P0) GOTO LCP3

26. IF(NO.EQ.0) GOTO LCP7
27. LCP3: \( L_1 = \text{LOC}(\text{NOT.} \ L_0) \)

28. IF(\( \text{NO} \ . \text{EQ.} \ 0 \)) GOTO LCP5

29. \( L_0 = \text{LOC}(\ L_0) \)

30. LCP4: \( L_L(\text{NLL}+1) = \text{IN}(L_0) \)

31. \( PZ(\text{NLL}+1) = (\text{NO:} + P) ; \text{GG}(\text{NLL}+1) = \text{GOON}(L_0) ; \text{DELL}(\text{NLL}+1) = \text{DEL}(L_0) \)

32. \( \text{NLL} = \text{NLL} + \text{NO} \)

33. IF(\( \text{NLL} \ . \text{EQ.} \text{NZS} \)) GOTO LCP9

34. IF(\( P < \text{LT.} \text{PO} \)) GOTO LCP6

35. LCP5: \( L_0 = L_1 ; \text{NO} = \text{NZS} - \text{NLL} ; P = 1E50 \)

36. GOTO LCP4

37. LCP6: \( Z = Z(L_1) ; \text{GOOO} = \text{GOON}(L_1) ; \text{IN} = \text{IN}(L_1) \)

38. \( \text{GK} = \text{CK} \left( \text{AUD}(:,B(L_1)) \right) \)

39. \( \text{NZ} = \text{NZ} - \text{NO} \)

40. \( \text{M1} = \text{AUD}(\text{NZ*NK*NK},\NK::) ; \text{M2} = \text{AUD}(\text{NZ*NK},\NK::) ; \text{M3} = \text{AUD}(\text{NZ},\NK::) \)

41. GOTO LCP8

42. LCP7: \( \text{GOOO} = \text{GOON} \)

43. LCP8: FREEIF(\( \text{GOON},L_00,L_0,L_1 \))

44. FREEIF(\( \text{SN} \))

45. \( P = P + 1 \)

46. GOTO LCP2

47. LCP9: \( RL = \text{RANKER}(L_L) \)

48. \( Z = Z_S ; \text{GOOO} = \text{GC}(RL) ; \text{DEL} = \text{DELL}(RL) ; PZ = PZ(RL) \)

49. FREEIF(\( \text{GG}, \text{GOON}, L_L, L_00, L_0, L_1 \))

50. FREEIF(\( \text{SN} \))

51. TABULATE(\( I,Z,GO00,DEL,PZ \))
52. \( N = N + 1 \)

53. IF \( N \lt NB \) GOTO LCP
1. PROGRAM NN3P
2. IF(NNZ.EQ.NZ) GOTO LNN
3. M1=A2D(NZ*NK*NK,NK:);M2=A2D(NZ*NK,NK:);M3=A2D(NK,NK:)
4. Y=M1+1
5. YYY=Y;YYY(INTS(1,1+NZ*NK*NK-NK,NK),)=0
6. YY=A2D(NZ,NK*NK:)+1
7. YY=A1D(SHIFTRIG(YY,NK))
8. Y(INTS(NK+1,NK*(NZ*NK-1)+1,NK),)=0;Y=YY*Y
9. LNN: IF(P.NE.1) GOTO LNN1
11. F=GK
12. SPP3
13. G000=GC
14. LNN1: F=GK/(CK+2);SPP3
15. GS=2*G000
16. G001=GC-GS
17. F=1/(A1D(:M2+CK+2))*F;SPP3
18. G110=GC-4*(G000+G001)
19. F=1/(A1D(: (A1D(:M3+CK+2)+M2)))*F;SPP3
20. G111=GC-6*G110-12*G001-8*G000
21. F+CK/(C2K+2);SPP3
22. G002=GC-GS
23. F=1/(A1D(:M2+CK+2))*F;SPP3
24. G021=GC-2*(G001+G002)-4*G000
25. F=1/(A1D(: (A1D(:M3+CK+2)+M2)))*F;SPP3
26. $G_{112} = G - 2 \ast G_{110} - 4 \ast (G_{021} + G_{002}) - 8 \ast (G_{001} + G_{000})$

27. $F = G_k / (C_3 + 2)\text{; SPP3}$

28. $G_{003} = G - G_S$

29. $F = 1 / (A_1 \ast D(M_2 + C_2 + 2)) \ast F\text{; SPP3}$

30. $G_{130} = G - 2 \ast (G_{001} + G_{003}) - 4 \ast G_{000}$

31. $F = G_k / (C_4 + 2)\text{; SPP3}$

32. $G_00 = G - G_S$

33. FREE(GS)

34. $F = 1 / (A_1 \ast D(M_2 + C_2 + 2)) \ast G_k / (C_2 + 2)\text{; SPP3}$

35. $G_{022} = G - 4 \ast (G_{000} + G_{002})$

36. FREE(GK,GC,F)

37. $P_{11} = 5 \ast G_{000} + 4 \ast (4 \ast G_{110} + G_{002})$

38. $P_{12} = 4 \ast (G_{002} + G_{022} + 2 \ast (G_{112} + G_{130})) + G_{004}$

39. $P_{13} = G_{000} + 2 \ast (G_{002} + G_{130} + G_{022} + 4 \ast G_{110} + G_{112})$

40. $P_{22} = G_{003} + 4 \ast (G_{001} + 2 \ast G_{111} + 3 \ast G_{021})$

41. $H = G_{002} + 4 \ast G_{110}; H = G_{003} + 4 \ast G_{021}; F = G_{001} + 2 \ast (G_{021} + G_{111})$

42. $U_{51} = .5 \ast \text{TRANS}(A_2D(7, NZ: H, 5 \ast G_{001}, H, F, F, F))$

43. $U_{52} = .5 \ast \text{TRANS}(A_2D(7, NZ: H, H, 5 \ast G_{001}, F, F, F))$

44. $U_{53} = .5 \ast \text{TRANS}(A_2D(7, NZ: H, F, F, 5 \ast G_{001}, H, F, F))$

45. $J = 0$

46. LNN3: $J = J + 1$

47. $G_{FF} = A_1 \ast D(: G_{001} (J), G_{110} (J), G_{110} (J), G_{000} (J), G_{001} (J), G_{110} (J), G_{110} (J), G_{002} (J))$

48. $G_{FFF} = A_1 \ast D(: G_{000} (J), G_{001} (J), G_{110} (J), G_{110} (J), G_{110} (J), G_{110} (J), G_{000} (J), G_{001} (J))$
49. \( \text{GFFFF} = A1D(:, \text{G110}(J), \text{G110}(J), \text{G110}(J), \text{G110}(J), \text{G002}(J), \text{G000}(J)) \)

50. \( \text{GF} = \text{SMAT}(7: \text{G000}(J), \text{G001}(J), \text{G000}(J), \text{G001}(J), \text{G002}(J), \text{G000}(J), \text{GFF}, \text{GFFF}, \text{GFFFF}) \)

51. \( \text{E511}(J) = \text{VEC}(7: \text{U51}(J))/\text{GF} \times \text{VEC}(7: \text{U51}(J)) \)

52. \( \text{E521}(J) = \text{VEC}(7: \text{U51}(J))/\text{GF} \times \text{VEC}(7: \text{U52}(J)) \)

53. \( \text{E531}(J) = \text{VEC}(7: \text{U51}(J))/\text{GF} \times \text{VEC}(7: \text{U53}(J)) \)

54. IF(J.LT.NZ) GOTO LNN3

55. \( \text{E51} = \text{E511} - \text{P11}/4 + Z - V1 \)

56. \( \text{E52} = \text{E521} - \text{P12}/4 \)

57. \( \text{E53} = \text{E531} - \text{P13}/4 \)

58. \( \text{DET1} = \text{G000} \times \text{G000} - \text{G001} \times \text{G001} \)

59. \( \text{GP} = \text{G002} + 4 \times \text{G110} \)

60. \( Z2 = Z - V2 \)

61. \( \text{E21} = 0.25 \times \left( \frac{(5 \times \text{G001} \times \text{G001} \times (5 \times \text{G000} - 2 \times \text{GP}) + \text{G000} \times \text{GP} \times \text{GP}}{\text{DET1} - \text{P11}} \right) + Z2 \)

62. \( \text{E22} = 0.25 \times (\text{G001} \times (5 \times (2 \times \text{GP} \times \text{G000} - 5 \times \text{G001} \times \text{G001}) - \text{GP} \times \text{GP})/\text{DET1} - \text{P22}) - 0.5 \)

63. FREE(E511, E521, E531)

64. FREEIF(P11, P12, P13, P22, H, HH, F, GF, GFF, GFFF, GFFFF)

65. \( \text{E512} = \text{E51} - \text{E52}; \text{E521} = \text{E51} + \text{E52}; \text{E513} = \text{E51} - \text{E53}; \text{E531} = \text{E51} + \text{E53}; \text{E21P} = \text{E21} \times \text{E21} \)

66. \( \text{E22P} = \text{E22} \times \text{E22}; \text{E51P} = \text{E51} \times \text{E51}; \text{E52P} = \text{E52} \times \text{E52}; \text{E53P} = \text{E53} \times \text{E53}; \text{E512P} = \text{E512} \times \text{E512} \)

67. \( \text{E55P} = \text{E521} - 2 \times \text{E53}; \text{E555P} = \text{E555} \times \text{E555}; \text{E523} = \text{E52} - \text{E53}; \text{E523P} = \text{E523} \times \text{E523} \)

68. FREEIF(G001, G002, G003, G004, G021, G022, G110, G112, G130, G111)

69. \( \text{MA11} = \text{E512P} \times \text{E512} \times \text{E555P} \times (Z2 \times (\text{E521} + 4 \times \text{E53}) - 1.5) \)

70. KEPT NN33P; NN33P

71. RETURN
1. PROGRAM NN33P

2. MA1=E512P*E512*E555P*(E521+4*E53)

3. MA22=-.5*E512P*E555*(Z2*E555*(3*E51+E52-4*E53)+(.5-Z2*E521)*(5*E51 +E52-6*E53))


5. MA33=-.5*E512P*E555*(Z2*E555*(E51+3*E52-4*E53)+(.5-Z2*E521)*(E51+5 *E52-6*E53))


7. MA44=E513*E512*((2*E51+E52-3*E53)*(Z2*E521-.5)-Z2*E555P)

8. MA4=E513*E512*(E521*(2*E51+E52-3*E53)-E555P)

9. E521P=E521+E521;E513P=E513*E513

10. MA=E521P*E521*E52-6*E53*(E521-E53)

11. MA55=.5*E512*((Z2*E521-.5)*MA-Z2*E555P*E555)

12. MA5=.5*E512*(MA*E521-E555P*E555)

13. MAA=(2*E53-E52)*(2*E53+E52)-E52*E531-E51*E53

14. MA66=E512*(-E523)*(Z2*MAA+.5*(2*E52-3*E53+E51))

15. MA6=E512*(-E523)*MAA


17. MA7 =E512P*(E521P-4*E53P)

18. MA88=E513P*(Z2*(E531+E53)-.75)

19. MA8=E513P*(E531+E53)


21. MA9=.5*E513*(E531*(E521+E52-3*E53)-E513P)


23. MA10=.5*E523*((E52+E53)*(E521+E51-3*E53)-E523P)

24. MA1111=E523P*(Z2*(E52+2*E53)-.75)
25. \( MA_{11} = E_{523}P \times (E_{52} + 2 \times E_{53}) \)
26. \( MA_{1212} = E_{512} \times (Z_2 \times (E_{51} \times E_{52} - 2 \times E_{53}) - 0.25 \times (3 \times E_{51} + E_{52} - 4 \times E_{53})) \)
27. \( MA_{12} = E_{512} \times (E_{51} \times E_{52} - 2 \times E_{53}) \)
28. \( MA_{1313} = E_{512} \times (Z_2 \times (E_{52} \times E_{52} - 2 \times E_{53}) + E_{53} \times 0.75 \times E_{52} - 0.25 \times E_{51}) \)
29. \( MA_{13} = E_{512} \times (E_{52} \times E_{52} - 2 \times E_{53}) \)
30. \( D = E_{21P} - E_{22P}; D_1 = E_{51P} - E_{52P}; D_2 = E_{51P} - E_{53P}; DP = D \times D \)
31. \( AA_{0} = DP \times D; AA_{1} = -6 \times VV \times DP \times E_{21} \)
32. \( AA_{2} = 12 \times VV_2 \times D \times E_{21}; AA_{3} = -8 \times VV_3 \times E_{21} \times E_{21} \)
33. \( AA_{4} = 3 \times VV_2 \times DP; AA_{5} = -12 \times VV_3 \times D \times E_{21}; AA_{6} = 12 \times VV_4 \times E_{21} \times E_{21} \)
34. \( AA_{7} = 3 \times VV_4 \times D; AA_{8} = -6 \times VV_5 \times E_{21} \)
35. \( AA_{9} = -2 \times VV \times DP \times E_{22}; AA_{10} = 8 \times VV_2 \times D \times E_{21} \times E_{22} \)
36. \( AA_{11} = -8 \times VV_3 \times E_{21} \times E_{21} \)
37. \( AA_{12} = -4 \times VV_3 \times D \times E_{22} \)
38. \( AA_{13} = 8 \times VV_4 \times E_{22} \times E_{21}; AA_{14} = -2 \times VV_5 \times E_{22} \)
39. \( AA_{15} = 4 \times VV_2 \times D \times E_{22}; AA_{16} = -8 \times VV_3 \times E_{21} \times E_{22} \)
40. \( AA_{17} = 4 \times VV_4 \times E_{22}; AA_{18} = -8 \times VV_3 \times E_{22} \times E_{22} \)
41. \( AO_{1} = AA_{6} \times D_2 + AA_{7} \times D_1 + AA_{8} \times E_{51} + VV_6 \)
42. \( AO = AA_{0} \times MA_{11} + AA_{1} \times MA_{22} + AA_{2} \times MA_{44} + AA_{3} \times MA_{88} + AA_{4} \times MA_{77} + AA_{5} \times MA_{1212} + A0_{1} \)
43. \( B0_{1} = AA_{6} \times E_{513} \times (Z_2 \times E_{53} - 0.5) + AA_{7} \times E_{512} \times (Z_2 \times E_{52} - 0.5) + AA_{8} \times (Z_2 \times E_{51} - 0.25) + VV_6 \times Z_2 \)
44. \( B0 = AA_{0} \times MA_{11} + AA_{1} \times MA_{22} + AA_{2} \times MA_{44} + AA_{3} \times MA_{88} + AA_{4} \times MA_{77} + AA_{5} \times MA_{1212} + B0_{1} \)
45. \( A1 = AA_{9} \times MA_{33} + AA_{10} \times MA_{55} + AA_{11} \times MA_{99} + AA_{12} \times MA_{13} + AA_{13} \times (E_{51} \times E_{52} - E_{53}) \) + AA_{14} \times E_{52} \)
46. \( B0_{2} = AA_{13} \times (Z_2 \times (E_{51} \times E_{52} - E_{53}) - 0.25 \times (E_{52} - 2 \times E_{53})) + AA_{14} \times (Z_2 \times E_{52} - 0.25) \)
47. \( B1 = AA_{9} \times MA_{33} + AA_{10} \times MA_{55} + AA_{11} \times MA_{99} + AA_{12} \times MA_{13} + B0_{2} \)
48. \[ A_2 = AA_{15} \times MA_6 + AA_{16} \times MA_{10} + AA_{17} \times E_{523} \times (E_{52} + E_{53}) \]

49. \[ B_2 = AA_{15} \times MA_{66} + AA_{16} \times MA_{1010} + AA_{17} \times E_{523} \times (Z_2 \times (E_{52} + E_{53}) - .5) \]

50. \[ A_3 = AA_{18} \times MA_{11} \]

51. \[ B_3 = AA_{18} \times MA_{1111} \]

52. KEPT NN333P; NN333P

53. RETURN
1. PROGRAM NN333P
2. AB3=A3/B3
3. A11=A0-AB3*B0
4. A22=A1-AB3*B1
5. A33=A2-AB3*B2
   E53P,E512P)
7. FREE(E555,E555P,MA11,MA1,MA22,MA2,MA33,MA3,MA44,MA4,MA55,MA5,MA66,
   MA6,MA77)
8. FREE(MA7,MA88,MA8,MA99,MA9,MA1010,MA10,MA1111,MA111,MA1212,MA12,
   B01,B02,A01)
9. FREE(D,D1,D2,DP AA0,,AA1,AA2,AA3,AA4,AA5,AA6,AA7,AA8,AA9,AA10,
   AA11,AA12,AA13)
10. FREE(AA14,AA15,AA16,AA17,AA18,A0,A1,A2,A3)
11. N1=NZ*NK*NK;N2=NZ*NK
12. NU=(A1D(N1:A1D(N2:A22+A33*(M3+CK)))+A1D(N2:A33+M3)*M2+CK)))*
   (M1+CK)
   (M2+CK))+NU
14. DE=A1D(N2:B1+B2*(M3+CK))
   *(M1+CK)
17. FREE(B0,B1,B2,B3,AA1,AA2,AA3)
19. FREE(NU,DE,AB3)
20. F=GK; SPP3
21. G000N=GC
22. FREE(GC, F)
23. RETURN
1. PROGRAM SPP3
2. C1=SHIFTDOW(F)
3. A1=YYY*SHIFTRIG(SHIFTLEF(1/(F-SHIFTRIG(C1))))
4. A2=SHIFTLEF(SHIFTUP(A1))
5. C1=YYY/(F-C1)
6. C2=SHIFTUP(C1)
7. D1=SHIFTRIG(1/(SHIFTLEF(F)-F))
8. D2=SHIFTLEF(D1)
9. B1=SHIFTDOW(F,NK)
10. A3=YY*SHIFTRIG(SHIFTLEF(1/(F-SHIFTRIG(B1))))
11. A4=SHIFTLEF(SHIFTUP(A3,NK))
12. B1=YY/(F-B1)
13. B2=SHIFTUP(B1,NK)
14. H1=SHIFTDOW(F,NK+1)
15. E1=Y*SHIFTRIG(SHIFTLEF(1/(F-SHIFTRIG(H1))))
16. E2=SHIFTLEF(SHIFTUP(E1,NK+1))
17. H1=Y/(F-H1)
18. H2=SHIFTUP(H1,NK+1)
20. FREE(A1,A2,A3)
22. FREE(A4,B1,B2,C1,C2,D1,D2,E1,E2,H1,H2)
23. GC=CO*A1D(:SUMROWS(A2D(NZ,NK):SUMROWS(A2D(NZ*NK,NK):SUMROWS(F*F*LOG(F)*T)))))
24. FREE(T)
25. RETURN
1. PROGRAM S3SP
2. IF(NNZ.EQ.NZ) GO TO LNN
3. M1=A2D(NZ*NK*NK,NK:); M2=A2D(NZ*NK,NK:); M3=A2D(NZ,NK:)
4. Y=M1+1
5. YYY=Y; YYY(INTS(1,1+NZ*NK*NK-NK,NK),)=0
6. YY=A2D(NZ,NK*NK:)+1
7. YY=A1D(SHIFTRIG(YY,NK))
8. Y(INTS(NK+1,NK*(NZ*NK-1)+1,NK),)=0; Y=YY*Y
9. LNN: IF(P.NE.1) GO TO LNN1
10. S=V1-.1I
12. F=GK; SPP3
13. GO00=GC
14. LNN1: GK=A1D(NZ*NK*NK:A1D(NZ*NK:Z-V1-VV/(1/GO00+S-V2)+M3-CK)
 +M2-CK)+M1-CK
15. SN=V1+VV/(1/GO00+S-V2)
16. F=GK/SPP3
17. GO00N=GC
18. RETURN
BIBLIOGRAPHY

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