Application of Effective Field Theory to Density Functional Theory for Finite Systems

DISSEPTION

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ABSTRACT

Density functional theory (DFT) is a tool of many-body physics whose popularity has grown over the years, primarily because it provides a useful balance between accuracy and computational cost, allowing large systems to be treated in a simple self-consistent manner. Effective field theory (EFT) is a framework which allows us to study the low-energy phenomena of a system in a systematic fashion. In this thesis, EFT methods are applied to DFT as part of a program to systematically go beyond mean-field approaches to medium and heavy nuclei. A system of fermions with short-range, natural interactions and an external confining potential (e.g., fermionic atoms in an optical trap) serves as a laboratory for studying DFT/EFT. An effective action formalism leads to a Kohn-Sham DFT by applying an inversion method order-by-order in the EFT expansion parameter. Results showing the convergence of Kohn-Sham calculations at zero temperature in the local density approximation (LDA) are compared to Thomas-Fermi calculations and to power-counting estimates. When conventional Kohn-Sham DFT for Coulomb systems is extended beyond the local density approximation, the kinetic energy density $\tau$ is sometimes included in energy functionals in addition to the fermion density. However, a local (semi-classical) expansion of $\tau$ is used to write the energy as a functional of the density alone, in contrast to the Skyrme approach. The difference is manifested in different single-particle equations, which in the Skyrme case include a spatially varying effective mass. The
EFT framework for DFT is generalized to reconcile these approaches. An effective action approach is used to illustrate how the exact Green’s function can be calculated in terms of the Kohn-Sham Green’s function. An example based on Skyrme energy functionals shows that single-particle Kohn-Sham spectra can be improved by adding sources used to construct the energy functional. Finally, spin-orbit interactions are incorporated in the formalism leading to an energy functional having the same form as that of the Skyrme functional. Gradient expansions in terms of the local Fermi momentum are also worked out, which will be of use in the immediate future.
This work is dedicated to my family
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CHAPTER 1

INTRODUCTION

Quantum Chromodynamics (QCD) is the fundamental theory for strong interactions. A proper description of nucleons and their interactions requires us to work in a framework consistent with QCD. We are interested in the low-energy regime of nuclear many-body physics where QCD is nonperturbative. At this energy scale, the quarks and gluons are no longer the relevant and efficient degrees of freedom (DOF). Instead, we have to deal with hadronic DOF, which means using an effective field theory (EFT) of QCD. In this thesis, we shall deal with non relativistic effective theory for a model system keeping in mind the theory of composite nucleons.

1.1 Challenges in Nuclear Structure

The conventional version of the two-nucleon interaction is characterized by a strong short-range repulsion, a long-range attraction, and strong spin, isospin and tensor components. As written in the RIA (Rare Isotope Accelerator) theory blue-book (2005),

Remarkably, although nuclei have been the object of intense study for the last 70 years, the ability to execute, theoretically, the conceptually simple task of “building” a nucleus up from its constituent parts, the protons and neutrons, has yet to be fully realized.
Hence, a lot needs to be done.

One of the major goals of modern nuclear structure theory is to compute bulk properties, such as the ground state energy, of medium to heavy nuclei in a systematic model-independent fashion that allows controlled extrapolations to regions far from the valley of stability. By controlled, we mean that there exists theoretical error bars. Thus, the challenge is to develop a systematic approach to the nuclear many-body problem, and in the process construct a robust microscopic framework that can describe bulk nuclear properties, nuclear excitations, and nuclear reactions. Understanding bulk properties of a wide range of nuclei (from stable ones to exotic forms such as neutron stars), their collective motion (manifested in fission, fusion), and large scale astrophysical phenomena (evolution of stars, effects of nuclear physics on nucleosynthesis) in a single framework is quite a challenge indeed. Reaction mechanisms from the standpoint of nuclear structure also needs to be studied. For heavier nuclei, these requirements call for the construction of a “universal microscopic energy density functional”. The following quote taken from the report of the NSAC subcommittee on nuclear theory says it all:

For heavy nuclei, a critical challenge is the quest for the universal energy density functional, which will describe properties of finite nuclei as well as extended asymmetric nuclear matter, as found in neutron stars. The quest is driven by new data of both terrestrial and cosmic origins, especially on nuclei far from stability, where new features, such as weak binding and altered interactions, make extrapolations of existing models (inspired by data on known nuclei) very unreliable.

Meeting this challenge will require a better understanding of the dependence of the energy functional on density, on isovector pieces, and a systematic treatment of many-body correlations. In other words, we need to go beyond mean-field and develop a self-consistent nuclear density functional theory. Developing such a theory that
would treat excited states and giant resonances on the same footing is a further challenge. In addition, pairing plays a major role for neutron-rich nuclei (important for stellar nucleosynthesis). We need to have a “first-principle” derivation of the pairing interaction.

In order to address these challenges, we need to know more about effective nucleon-nucleon interactions. Effective low-momentum potentials \( V_{\text{lowk}} \) obtained from renormalisation group flow approach are a promising new development. This potential can be obtained from “realistic” potentials such as Argonne V18 or CD-Bonn, or from chiral EFT potentials.

We note that these potentials fail to reproduce the binding energy of even simple nuclei unless three-body interactions are taken into account. There is evidence that the three-body piece significantly affects the structure of nuclear levels and location of drip lines. For low-momentum potentials, it is also primarily responsible for saturation [97] contrary to conventional wisdom that the tensor force always plays the primary role in that matter. In this regard, one should note that the importance of different pieces of the interaction vary with the resolution of the potential, i.e., the momentum cutoff used. Incorporating correlations from the three-body piece is a major challenge.

1.2 Existing Methods

There are many approaches to nuclear structure calculations. The different methods are useful in different regimes, corresponding to light, medium or heavy nuclei. The following is a partial list of existing methods.

- Green’s function Monte Carlo is a numerical technique that has been used for nuclei having total number of nucleons \( A \) up to 12 as of now. This method has
a very high computational cost, scaling exponentially with $A$. However, this provides a benchmark for other calculations. Things may improve in the future with auxiliary field Monte Carlo, where quadratic spin and isospin operators are taken care of by introducing auxiliary fields. This method shows promise of handling nuclei upto $A \sim 100$. Coupled-cluster methods also have a lot of promise.

- Shell model calculations are used for nuclei with mass number upto $A \sim 60$. The computation time is not as bad as Monte Carlo, but is still significant. The “no-core” shell model approach (based on the application of effective-interactions within the context of the shell model and accounting for all the nucleons) can be used with EFT NN few body potentials.

- For $A > 60$, the usual employed method is mean-field type calculations. The semi-phenomenological Skyrme-Hartree-Fock approach successfully reproduces bulk properties of nuclei across the periodic table, but cannot produce reliable results for nuclei away from the valley of stability. In this thesis, we strive to generalize and systematize this approach.

There are two main areas that require improvement. One needs to get rid of model dependence and enforce a systematic approach that will provide us with reliable error estimates. These necessities indicate that an EFT calculational framework is a good candidate.

EFT provides the required framework to study low-energy phenomena with well-defined power counting and reliable error estimates. Although EFT has shown
promise in applications to few-body systems, there are formidable challenges in carrying out many-body calculations for larger finite systems. Density functional theory (DFT) on the other hand allows many-body systems to be treated in a simple self-consistent manner. Its framework retains the structure of a mean-field calculation while taking terms beyond Hartree-Fock (HF) into account. However, such correlation terms are either dealt with in the local density approximation (LDA) or with gradient terms developed empirically, thus infusing uncontrolled approximations into the framework. Thus, although DFT has the power to deal with large finite systems, it lacks the systematics of EFT. Dealing with a many-body problem by doing DFT in an EFT framework helps us to harness the advantages of both approaches. This is the line of attack we choose to address the many-body problem, and this forms the core of this thesis.

The Skyrme-Hartree-Fock approach can be considered as a form of nuclear DFT. It has had many phenomenological successes in reproducing bulk properties of nuclei across the periodic table [76, 107, 78, 79, 80, 81] and, generalized to include the effects of pairing correlations, continues to be a major tool for analyzing the nuclear structure of medium and heavy nuclei. The form of the Skyrme interaction was originally motivated as an expansion of an effective interaction (G-matrix) in the medium [82]. Negele and Vautherin made the connection concrete with the density matrix expansion method [83], but there has been little further development since their work. Many unresolved questions remain, which become acute as one attempts to reliably extrapolate away from well-calibrated nuclei and to connect to modern treatments of the few-nucleon problem. We need to understand the origin of the functionals and what are the expansion parameters. Questions like how we can estimate uncertainties
in the predictions, and whether correlations are adequately taken care of, are central before we can hope to reliably predict bulk properties of unstable nuclei. We turn to effective field theory to address these questions, using a DFT rather than a G-matrix approach as in Ref. [84].

EFT offers a systematic approach for describing low-energy nuclear physics that can provide a framework for nuclear DFT. In this thesis, we take the first steps towards systematically going beyond models by applying EFT methods to Kohn-Sham DFT. We approach this problem in the low energy regime for a model system of dilute fermions in an external confining potential. We carry out a perturbation theory not in the underlying potential, but by forming a dilute expansion parameter using the hierarchy of scales in our model system. The EFT describing our model system is analogous to pionless EFT. Ultimately we are interested in calculating self-bound systems like nuclei, with spin- and isospin-dependent interactions and long-range forces (e.g., pion exchange) in a systematic fashion, and this work serves as a starting point.

1.3 Thesis Organization

We start off in chapter two by reviewing, in some detail, the fundamentals of DFT. In chapter three, we give a more modest introduction to the concept of an effective theory and proceed to define EFT. We also work out examples to illustrate the methodology and end the chapter by reviewing a basic EFT calculation carried out at finite density, the infinite dilute Fermi gas. This calculation sets the stage for the present work, that aims at treating a finite system in a systematic manner.
In chapter four, we carry out the merger of the computational power of DFT with the organizational advantages of EFT using an effective action formalism. This provides us with the tool we need to address the many-body problem for a finite system. Dilute fermions with spin-independent contact interactions in an optical trap serve as our theoretical laboratory. The calculations are done in the local density approximation (LDA). My specific contribution to the work in this chapter was to carry out an independent numerical calculation using a matrix diagonalization approach to solve the single-particle Kohn-Sham equations self-consistently in both Mathematica and C programming languages. This chapter is based on Ref. [42].

In chapter five, we take a step beyond LDA. We extend the framework by incorporating a source coupled to the kinetic energy density operator in the action. We find the ground-state energy functional and single-particle equations for this dilute system to be of the same form as those in Skyrme Hartree-Fock calculations without the spin-orbit term. We observe however that the inclusion of the kinetic energy density does not have a significant impact on bulk observables like the ground-state energy and density profile, even though it is a step beyond LDA. However, it has a tremendous effect on the single-particle spectra. This chapter is based on Ref. [94].

In chapter six, we investigate the accuracy of the single-particle Kohn-Sham spectra by relating the Kohn-Sham Green’s function to the exact one. We find the Kohn-Sham spectra to coincide with the exact spectra at the HF level, indicating that incorporating the kinetic energy density in the formalism had its merits apart from yielding a Skyrme look-alike energy functional. This chapter is based on Ref. [95].

In chapter seven, we take the next step by incorporating spin-orbit in the formalism, resulting in an energy functional that has the same form as that of the Skyrme
functional. We lay out the basic formalism and analytical results without going into numerics. Work is in progress to see how bulk properties as well as single-particle spectra get affected.

We conclude in chapter eight, with a brief discussion on areas for future work. The appendices are worked out in great detail and serve to fill the gaps in the chapters and review techniques and definitions that have been used and are relevant for future work. In particular, appendix D discusses various ways of carrying out semiclassical expansions and derives an expression for the local Fermi momentum as a functional of the density, its gradients and the kinetic energy density. This will prove to be useful in going beyond LDA, and will be pursued in future work. In general, mastering techniques of semiclassical expansion will help us deal with the evaluation of Feynman diagrams (that contribute to energy) with long-range forces as an expansion in density and its gradients.
CHAPTER 2

DENSITY FUNCTIONAL THEORY

Calculations of bulk observables for medium to heavy nuclei typically rely on non-relativistic (Skyrme) or covariant (QHD) mean-field models. These nuclear mean-field approaches can be viewed as approximate implementations of Kohn-Sham density functional theory [51, 52, 53]. In this chapter, we review the current status of this method. This is necessary before we can take a step towards achieving the goal of systematically constructing a universal energy functional for nuclei. Our strategy is to embed the Skyrme approach in a more systematic framework.

2.1 What is Density Functional Theory?

Traditional wavefunction methods can be applied with sufficient accuracy and reasonable computational cost to systems consisting of a relatively small number of particles only. Density functional theory (DFT) [1, 2, 4, 5, 6] provides a calculational framework that greatly extends the range of many-body calculations in finite systems. In DFT, the particle density function $\rho(\mathbf{x})$ plays a central role rather than the many-body wave function. We will be working with the most commonly used version of DFT, called Kohn-Sham (KS) DFT. KS DFT is a formally rigorous way of approaching any interacting problem. Its basic idea is to shuffle parts of the interaction
into the non-interacting part. This new non-interacting part is called the KS system. This shuffling is done in such a way that the density calculated from the KS system is exactly the same as that of the original system, and the non-local kinetic term is treated exactly.

2.1.1 Motivation

The primary motivation behind an alternative approach to the many-body system problem is the computational cost, which scales in an exponential fashion in the wavefunction approach. For a classical system with \( A \) interacting particles, there are \( 6A \) degrees of freedom (DOF). For a quantum system, ignoring symmetries and spin, there are \( 3A \) DOF since specifying the wave function at any time fixes it at a later time through the evolution equation. In order to meet a prescribed computational accuracy, if we need \( p \) parameters per DOF, then the total number of parameters needed to describe the system would be \( M = p^{3A} \). If we assume that \( p \approx 3 \), then \( \ln M = CA, C = 3 \ln 3 \). Thus \( M \) scales exponentially with \( A \). If we take \( A = 100 \), we get an \( M \) so huge that present day computers cannot minimise a quantity (e.g., a variational energy) in a space of such high dimensions [1]. Nuclear interactions have complicated spin-isospin dependence and important many-body forces, which makes things worse. No wonder that wavefunction methods like Green’s function Monte Carlo (GFMC) when applied to nuclear systems can only deal with \( A \) around 12 at present [7]. In DFT, the computing time \( T \) rises much more moderately with the number of particles, currently \( T \sim A^\alpha \) with \( \alpha \approx 2 - 3 \) for Coulomb systems. There is ongoing progress towards making this scaling linear [1]. There is also the issue of “Van Vleck Catastrophe”, according to which the many-body wavefunction is not a
legitimate scientific concept when $A \approx 10^3$ in the sense that the wave function cannot be calculated and recorded with sufficient accuracy [1]. Therefore an alternative method that is stable for large $A$ systems is needed. Apart from having a reasonable time complexity, DFT provides a computationally simple framework where the basic equation can be solved in a self-consistent manner. This framework retains the structure of the Hartree calculation, but is much more powerful because it is formally exact, unlike Hartree or Hartree-Fock, which are approximations. Low momentum potentials ($V_{\text{lowk}}$) give additional argument in favour of such an approach to nuclear systems since they show that one can get reasonable results even at the Hartree-Fock order with a proper choice of Hamiltonian [97]. This is in contrast to conventional wisdom for nuclear matter, which claims that it must be highly nonperturbative.

Apart from the computational standpoint, there is also the matter of dealing with quantities that are more physically intuitive. The basic variable in DFT is the density, which is a real observable and appeals to us more from that standpoint. We know that in treating situations where the number of particles $A$ is constrained and relatively small, such as atomic nuclei, it is preferable to use it as the free variable rather than the chemical potential $\mu$. Similarly one might think of interactions as imposing strong constraints on the density distribution $\rho(x)$, so that it is preferable to use it as a natural variable instead of the external potential.

The utility of DFT heavily depends on the exactness of the exchange-correlation piece. A major research effort is directed at the determination of this nontrivial piece for a given interaction, and approximations are abundant. This is a major limitation of DFT. In the DFT framework, we can calculate bulk energy and densities, but not
single-particle energies or matrix elements of arbitrary operators. Thus, DFT has the
disadvantage of having a limited set of accessible observables.

2.1.2 DFT Formulation

The first theorem of Hohenberg and Kohn (HK) states that the ground state
density \( \rho(\mathbf{x}) \) of a bound system of interacting particles in some external potential
\( v(\mathbf{x}) \) determines this potential uniquely up to an additive constant [2].

This means that the knowledge of the ground state density for any system uniquely
determines the system. In the case of a degenerate ground state, the lemma refers to
\textit{any} ground state density. The interesting question that arises is whether \textit{any} well-
behaved positive function \( \rho(\mathbf{x}) \), which integrates to a positive integer \( A \), is a possible
ground state density corresponding to some external potential \( v(\mathbf{x}) \). The class of
density functions which meet the above requirement are termed as V-representables
(VR). For a single particle, any normalised density \( \rho(\mathbf{x}) \) is a VR. On the other hand,
it has been shown by an example which involves degenerate ground states, that there
do exist well-behaved densities which are \textit{not} VR [3]. This topic of \( \nu \)-representability
is currently under study, but this issue has not hampered the practical application of
DFT so far.

HK showed that the ground state energy can be obtained from a functional of
the local density alone in general. According to HK, for a system with an external
potential \( v(\mathbf{x}) \), there exists an energy functional \( E[\rho(\mathbf{x})] \) which when minimised gives
the ground state energy when evaluated at the exact ground state density, which is
constrained by the requirement that \( \int d^3\mathbf{x} \rho(\mathbf{x}) = A \), the total number of particles.
We note that this is a variational approach and the minimal principle is formulated
in terms of trial densities rather than trial wavefunctions. The energy functional is
given by:

\[ E[\rho(x)] = F_{HK}[\rho(x)] + \int d^3x \rho(x)v(x), \quad (2.1) \]

Varying the above keeping the total number of particles \( A \) constant, we get

\[ \frac{\delta}{\delta \rho(x)} \left( E[\rho(y)] - \mu \int d^3y \rho(y) \right) = 0, \quad (2.2) \]

where \( \mu \) is the Lagrange multiplier. This leads to

\[ \frac{\delta F_{HK}}{\delta \rho(x)} + v(x) = \mu. \quad (2.3) \]

We can always enforce a constant particle number by hand, and work with \( \mu = 0 \)
as long as the system does not exhibit pairing. \( F_{HK}[\rho(x)] \) is called the HK free
energy, and is universal in the sense that it has no explicit knowledge of the potential
\( v(x) \). This is the second theorem of HK. At this stage, let us focus on central, spin-
independent potentials only. \( F_{HK}[\rho(x)] \) can be decomposed as follows [4]:

\[ F_{HK}[\rho(x)] = T_s[\rho(x)] + \frac{1}{2} \int \int d^3x d^3y \rho(x) V(x,y) \rho(y) + E_{xc}[\rho(x)]. \quad (2.4) \]

The first term is the noninteracting kinetic energy, and the second term is the classical
energy term or Hartree term and is also referred to as \( E_H[\rho(x)] \). For a Coulomb
interaction, it is the energy of a charge distribution. The final piece is the exchange-
correlation term which can be splitted into the exchange and the correlation pieces,

\[ E_{xc}[\rho(x)] = E_x[\rho(x)] + E_c[\rho(x)]. \quad (2.5) \]

This piece captures the rest of the many-body physics. For a one-particle system,
\( E_x[\rho(x)] = -E_H[\rho(x)] \) and \( E_c[\rho(x)] = 0 \). The correlation piece is always less than or
equal to zero in general [104], and this serves as a check.
The most rudimentary form of DFT is the Thomas-Fermi (TF) theory where the noninteracting functional is evaluated within the local density approximation (LDA). Note that for a uniform system, TF theory as applied to the noninteracting part is not an approximation. Kohn and Sham [4] introduced a method involving auxiliary orbits by which the kinetic term could be treated exactly. This has the huge advantage of treating a leading source of non-locality in the energy functional in an exact manner. This is why the KS framework is generally superior to the Thomas-Fermi approximation, and has formed the basis of modern DFT [1, 4, 5, 104, 105].

The KS system is simply a fictitious system of non-interacting particles, chosen to have the same density as the physical system. The procedure at zero temperature for a closed shell configuration boils down to solving the single particle Schrödinger equation for the lowest \(A\) occupied states (including degeneracies) as shown below:

\[
[-\frac{\nabla^2}{2M} + v_s(x)]\psi_a(x) = \varepsilon_a \psi_a(x) 
\]

(2.6)

where

\[
\rho(x) = \sum_a |\psi_a(x)|^2 \theta(\varepsilon_F - \varepsilon_a), 
\]

(2.7)

and \(a\) denotes the quantum numbers labelling the states and \(\varepsilon_F\) denotes the Fermi energy. The effective local background potential is given by

\[
v_s(x) = v(x) + \int d^3y V(x, y) \rho(y) + v_{xc}(x) 
\]

(2.8)

where \(v_{xc}(x)\) is the exchange-correlation potential and is given by:

\[
v_{xc}(x) = \frac{\delta E_{xc}}{\delta \rho(x)}. 
\]

(2.9)

Note that we need \(\rho(x)\) to find \(v_{xc}(x)\), and we get the full \(\rho(x)\) only after solving the single particle Schrödinger equation. This is the trademark of problems requiring
self-consistent solutions. The KS potential is itself a functional of the orbitals, so we have a self-consistent problem that is solvable by iteration. Another advantage of this procedure is that solving the Schrödinger equation with local potentials for eigenvalues is relatively simple and fast. Although this procedure is very similar to the self-consistent Hartree approximation, it incorporates all correlations if the correct KS functional is used.

The energy of the KS system is just the sum of the eigenvalues \( \varepsilon_a \).

\[
E_{KS} = \sum_a \varepsilon_a = T_s[\rho] + \int d^3x v_s(x)\rho(x). \tag{2.10}
\]

Using this with Eq. (2.1), Eq. (2.4) and Eq. (2.8), the total ground-state energy becomes:

\[
E = \sum_a \varepsilon_a + E_{xc}[\rho(x)] - \int d^3x v_{xc}(x)\rho(x) - \frac{1}{2} \int \int d^3x \, d^3y \, \rho(x) V(x,y) \rho(y). \tag{2.11}
\]

The effective single-particle potential \( v_s(x) \) is a unique fictitious external potential, which leads for non-interacting particles to the same physical density \( \rho(x) \) as that of the interacting system in the external potential \( v(x) \). Thus if the density is accurately known, we can construct \( v_s(x) \) and hence \( v_{xc}(x) \) [8]. With the exact \( E_{xc} \), the KS formalism includes in principle all the many-body effects.

### 2.1.3 Local Density Approximation (LDA)

The utility of DFT rests on finding a good approximation for \( E_{xc} \) [1, 5, 105, 104]. The first step in DFT was to introduce \( F_{HK}[\rho(x)] \), which is the difference between the ground state energy and the external potential energy, or the sum of the interaction energy and the kinetic energy of the particles. The second step is to introduce a practical approximation of the energy functional \( E_{xc}[\rho(x)] \). The simplest approximation
is the LDA, which takes the exchange-correlation energy-density at each point in the system to be equal to its known value (which is calculated numerically) for a uniform interacting system (comprising of the same particles) of the same density [5]. For the Coulomb problem, $E_{xc}(\rho(\mathbf{x}))$ is approximated by a fit to Monte Carlo results for the energy of a uniform electron gas as a function of density. The exchange-correlation functional takes the following analytic form:

$$E_{xc}^{LDA}[\rho] = \int d^3x \rho(\mathbf{x}) \epsilon_{xc}(\rho(\mathbf{x})).$$

The energy per particle $\epsilon_{xc}(\rho(\mathbf{x}))$ is known for the uniform electron gas exactly in the limit of high density, and can be computed accurately at densities of interest using Monte-Carlo techniques. LDA is accurate at high densities when the characteristic scale over which the fermion density changes is small compared to the Fermi wavelength $\lambda_F(\mathbf{x}) \sim [\rho(\mathbf{x})]^{-1/3} \sim k_F^{-1}$. One of the advantages of LDA is the fact that it is size consistent. Configuration interaction (CI) calculations (in which a trial wavefunction is formed as a linear combination of products of HF orbitals), although much more controlled than LDA, do not respect this property, apart from the fact that they can deal with small systems only. The simplest example of an LDA is the Thomas-Fermi (TF) approximation to the kinetic energy. Purely from dimensional analysis, one can say that $T_{kin}^{LDA}[\rho(\mathbf{x})] = C_{TF} \int d^3x [\rho(\mathbf{x})]^{5/3}$, where $C_{TF} = \frac{3}{10}(3\pi^2)^{2/3}$. The coefficient follows from the fact that the average kinetic energy of system of non-interacting fermions with spin-multiplicity $\nu = 2$ is given by $\frac{3}{5} \epsilon_F$.

The LDA has given good results for many atomic, molecular and crystalline interacting electron systems, even though the density of these systems are not slowly varying. This is because LDA satisfies a sum-rule which expresses the normalisation of the exchange-correlation hole [1, 5].

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2.2 Beyond the Local Density Approximation

2.2.1 Sum Rule

The exchange-correlation (xc) hole density describes how the presence of a particle at point $\mathbf{x}$ depletes the total density of the other particles at the point $\mathbf{y}$. The physical xc hole is given by [1]

$$n_{xc}(\mathbf{x}, \mathbf{y}) = n_2(\mathbf{x}, \mathbf{y}) - \rho(\mathbf{y}) ,$$

where $n_2(\mathbf{x}, \mathbf{y})$ is the conditional density at $\mathbf{y}$ given that one particle is at $\mathbf{x}$. If one particle is definitely at $\mathbf{x}$, then it is missing from the rest of the system, so that

$$\int d^3y \, n_2(\mathbf{x}, \mathbf{y}) = A - 1 .$$

The xc hole density $n_{xc}(\mathbf{x}, \mathbf{y})$ therefore describes a “hole” dug into the density $\rho(\mathbf{y})$ by the presence of a particle at $\mathbf{x}$. The xc hole is normalised, the condition being

$$\int d^3y \, n_{xc}(\mathbf{x}, \mathbf{y}) = -1 .$$

This is known as the “sum-rule”, and it reflects the screening of the particle at $\mathbf{x}$ [1]. To define the average xc hole, one introduces a fictitious Hamiltonian $\hat{H}_\lambda$ where $0 \leq \lambda \leq 1$, which differs from the physical Hamiltonian as follows:

$$\hat{V}(\mathbf{x}, \mathbf{y}) \rightarrow \lambda \hat{V}(\mathbf{x}, \mathbf{y}), \hat{\varphi}(\mathbf{x}) \rightarrow \hat{\varphi}_\lambda(\mathbf{x}) .$$

The fictitious $\hat{\varphi}_\lambda(\mathbf{x})$ is so chosen that for each $\lambda$ in the interval $[0, 1]$ the corresponding density equals the physical density $\rho(\mathbf{x})$. The KS system corresponds to $\lambda = 0$, and the fully interacting system is given by $\lambda = 1$. The interaction vanishes in the KS system and $\hat{\varphi}_{\lambda=0}(\mathbf{x}) \rightarrow \hat{\varphi}_s(\mathbf{x})$. The coupling constant averaged xc hole density is then defined by

$$n_{xc}^{av}(\mathbf{x}, \mathbf{y}) = \int_0^1 d\lambda \, n_{xc}(\mathbf{x}, \mathbf{y}; \lambda) .$$
The HK free energy has an exact expression given by

\[ F_{HK}[\rho] = T_s[\rho] + \int_0^1 d\lambda \frac{\partial F_{HK}}{\partial \lambda}, \]

where the \( \lambda \) dependence of \( F_{HK} \) is implicit. This is easy to see since for the KS system, \( F_{HK}(\lambda = 0) = T_s \). From Eq. (2.1), we see that

\[ \frac{\partial F_{HK}}{\partial \lambda} = \frac{\partial E_\lambda}{\partial \lambda} - \int d^3 x \rho(x) \frac{\partial v_{\lambda}}{\partial \lambda}, \]

since \( \rho(x) \) does not vary with \( \lambda \) by construction. Using \( E_\lambda = \langle \psi_\lambda | \hat{H}_\lambda | \psi_\lambda \rangle \), we get

\[ \frac{\partial E_\lambda}{\partial \lambda} = \frac{\partial}{\partial \lambda} \langle \psi_\lambda | \hat{H}_\lambda | \psi_\lambda \rangle = \langle \psi_\lambda | \hat{H}_\lambda | \psi_\lambda \rangle + E_\lambda \frac{\partial}{\partial \lambda} \langle \psi_\lambda | \psi_\lambda \rangle = \langle \psi_\lambda | \hat{V} | \psi_\lambda \rangle + \langle \psi_\lambda | \frac{\partial \hat{E}_\lambda}{\partial \lambda} | \psi_\lambda \rangle = \lambda^{-1} \langle \psi_\lambda | \hat{V}_\lambda | \psi_\lambda \rangle + \int d^3 x \rho(x) \frac{\partial v_{\lambda}}{\partial \lambda}, \]

so that

\[ F_{HK}[\rho] = T_s[\rho] + \int_0^1 d\lambda \lambda^{-1} \langle \psi_\lambda | \hat{V}_\lambda | \psi_\lambda \rangle. \]

From Eqs. (2.4) and (2.21), we get the expression for the exchange-correlation functional as

\[ E_{xc}[\rho] = \int_0^1 d\lambda \lambda^{-1} \langle \psi_\lambda | \hat{V}_\lambda | \psi_\lambda \rangle - E_{H}[\rho]. \]

Defining the pair correlation function as

\[ g(x, y) = \langle \tilde{\rho}(x) [\delta(x - y)] \rangle_{\lambda} - \rho(x) \rho(y), \]

we interpret the xc density \( n_{xc}(x, x'; \lambda) \) as the normalised pair correlation function [5]:

\[ n_{xc}(x, y; \lambda) = \frac{g(x, y)}{\rho(x)}. \]
Now, the form for $E_{xc}[^\rho]$ is given by
\[ E_{xc}[\rho] = \frac{1}{2} \int d^3x \int d^3y \rho(x)n_{xc}^{av}(x,y)V(x,y). \] (2.25)

The exchange-hole satisfies the sum rule given by Eq. (2.15), and also the following:
\[ n_x(x,y) \leq 0. \] (2.26)

The correlation-hole density is defined by the following
\[ n_c^{av}(x,y) = n_{xc}^{av}(x,y) - n_x(x,y), \] (2.27)
and satisfies the condition
\[ \int d^3y n_c^{av}(x,y) = 0. \] (2.28)

The success of LDA owes to the fact that it satisfies the sum-rule [14]. The immediate extension to LDA is in the form of Local Spin-density approximation (LSD) [4], which satisfies the same sum-rule and retains the good points of LDA. It is motivated by the fact that the exchange-correlation hole is very different for particles with parallel or antiparallel spins. In this scheme, separate densities of spin-up and spin-down fermions are used as a pair of functional variables: $\rho_+(x)$ and $\rho_-(x)$, and the Hamiltonian contains separate potentials for them. The general form for the LSD is as follows:
\[ E_{xc}^{LSD}[\rho] = \int d^3x \rho(x)\epsilon_{xc}(\rho_+(x), \rho_-(x)). \] (2.29)

For Coulomb systems, $\epsilon_{xc}(\rho_+(x), \rho_-(x))$ is obtained from the results for a homogeneous spin-polarized electron gas. As in LDA, LSD is exact for a uniform density system, or for one where density varies slowly over space relative to length scales such as the local Fermi wavelength. However, it can break exact spin symmetries. It is
also not exact in the one-particle limit in the sense that the requirement $E_c[\rho(\mathbf{x})] = 0$ is not satisfied. It also does not exhibit the “derivative-discontinuity” feature \cite{9, 10} that requires the exchange-correlation potential $v_{xc}(\mathbf{x})$ to tend to zero as $|\mathbf{x}| \to \infty$. The last two difficulties are handled better in the “self-interaction” correction (SIC) to LSD, but not in a satisfying manner \cite{12}. Therefore, let us take a look at what has been done to improve the situation from the standpoint of gradient expansions.

### 2.2.2 Gradient Expansion Approximation (GEA)

The idea behind the GEA is that for any sufficiently slowly varying density, an expansion of a functional in gradients should be of ever increasing accuracy. If LSD is moderately accurate for inhomogeneous systems, we expect GEA to be more accurate.

The first measure of inhomogeneity is given by the following dimensionless measure which is referred to as the reduced density gradient in literature:

$$s(\mathbf{x}) = \frac{|\nabla \rho(\mathbf{x})|}{2k_F(\mathbf{x})\rho(\mathbf{x})} \sim \frac{|\nabla \rho|}{\rho^{4/3}}. \quad (2.30)$$

Another dimensionless measure of density inhomogeneity is

$$p(\mathbf{x}) = \frac{\nabla^2 \rho(\mathbf{x})}{[2k_F(\mathbf{x})]^{2}\rho(\mathbf{x})} \sim \frac{\nabla^2 \rho}{\rho^{5/3}}. \quad (2.31)$$

The measures $s$ and $p$ are small for a slow density variation. The proper slow-varying limit is the one in which $p/s$ is also small \cite{4}. The inter-particle spacing $r_0 \sim k_F^{-1}$ is the length scale in the system. For an electronic system, it is also known as the Wigner-Seitz radius. A slowly varying density is characterized by the condition that $r_0/\ell$ is much less than 1, where $\ell$ is a typical length over which there is an appreciable change in density \cite{4}. For nuclear systems, $\ell \sim 1$fm. Note that these lengths are
normally expressed in units of the Bohr radius \( a_0 \) for electronic systems, but we are interested in the ratio.

Let us take the case of a typical radial nuclear density profile. We can invoke some basic hand waving to justify the above statements. The variation of density is appreciable only near the surface, and otherwise can be taken as a constant \( \rho \) :

\[
s(\mathbf{x}) \sim \frac{1}{k_F(\mathbf{x})} \frac{1}{\rho(\mathbf{x})} \sim \frac{1}{k_F(\mathbf{x})} \frac{1}{\ell} = \frac{k_F^{-1}}{\ell} \sim \frac{r_0}{\ell}.
\]

This justifies the statement that the measure \( s \) is a small parameter for slow density variation. Next, observe that \( \nabla^2 \rho = (2/R) \nabla \rho \sim (2/R) \nabla \rho \), where \( R \) is the measure of extent of the density profile. We have neglected the second radial derivative of \( \rho \) since the first derivative is sharply peaked only at the surface. Then,

\[
p(\mathbf{x}) \sim \frac{1}{[k_F(\mathbf{x})]^2} \frac{\nabla^2 \rho(\mathbf{x})}{\rho(\mathbf{x})} \sim \frac{r_0^2}{R} \frac{1}{\rho(\mathbf{x})} \frac{1}{\ell} = \frac{r_0}{R} \frac{r_0}{\ell} = \frac{r_0}{R} s.
\]

Thus, the condition that \( p/s \) is also small reduces to the condition that \( r_0 \ll R \).

The basic form of a GEA is conventionally assumed to be given by the following:

\[
T_s[\rho] = A_s \int d\mathbf{x} \rho^{5/3}(1 + \alpha_1 s^2 + \alpha_2 s^4 + \ldots), \tag{2.34}
\]

\[
E_x[\rho] = A_x \int d\mathbf{x} \rho^{4/3}(1 + \beta_1 s^2 + \beta_2 s^4 + \ldots). \tag{2.35}
\]

For a spin one-half system, leading coefficients are \( A_s = C_{TF} = \frac{3}{10}(3\pi^2)^{2/3} \). Eq. (2.35) is valid for Coulombic systems. One obtains \( A_x = -\frac{3}{4\pi}(3\pi^2)^{1/3} \) by evaluating the Fock integral for a Slater determinant of orbitals.
Scaling

One of the major requirements of any type of functional expansion is that each term should exhibit proper scaling. For any scale parameter $\gamma > 0$, the uniformly-scaled wavefunction is defined as

$$
\Psi_\gamma(x_1, \ldots, x_A) = \gamma^{3A/2} \Psi(\gamma x_1, \ldots, \gamma x_A),
$$

so that the normalisation is preserved. The density corresponding to the scaled wavefunction is the scaled density, which conserves the particle number and is given by

$$
\rho_\gamma(x) = \gamma^3 \rho(\gamma x), \quad \int d^3x \rho_\gamma(x) = A.
$$

Irrespective of the kind of interaction or the type of external confining potential, the kinetic energy functional always scales the same way as follows:

$$
T_s[\rho_\gamma] = \gamma^2 T_s[\rho].
$$

In general, if $F[\rho] = \int d^3x [\rho(x)]^b$, and $F[\rho_\gamma] = \gamma^a F[\rho]$, then

$$
b = 1 + a/3.
$$

For $T_s[\rho]$, $b = 5/3$ so that $a = 2$. Let us see how we get the above.

$$
F[\rho_\gamma] = \int d^3x [\rho_\gamma(x)]^b = \int d^3x \gamma^3 [\rho(\gamma x)]^b = \gamma^{3b-3} \int d^3(\gamma x) [\rho(\gamma x)]^b = \gamma^{3b-3} F[\rho].
$$

This establishes the validity of Eq. (2.39). One can easily deduce that the kinetic energy density $\tau(x)$ scales in the following way.

$$
\tau_\gamma(x) = \gamma^5 \tau(\gamma x).
$$
If one wants to get an idea about what functional form appears beyond the LDA term when one semiclassically expands the kinetic energy density, scaling analysis can be a great help. Suppose the term has the form $G[\rho] = \rho^a (\nabla \rho)^b$. This should scale in the same way as the LDA term. Note that $b$ has to be either even or zero. Then,

$$
G[\rho_\gamma] = \rho_\gamma^{a}(x) [\nabla_x \rho_\gamma(x)]^b = \gamma^{3(a+b)} \rho^{a}(\gamma x) [\nabla_x \rho(\gamma x)]^b \\
= \gamma^{3(a+b)} \rho^{a}(\gamma x) [\gamma \nabla_x \rho(\gamma x)]^b \\
= \gamma^{3a+4b} G[\rho].
$$

(2.42)

This tells us that $3a + 4b = 5$. When $b = 0$, $a = 5/3$, corresponding to the LDA term. For $b = 2$, $a = -1$. One notes that scaling merely fixes the possible combinations of the ingredients and its derivatives. It does not give us the factors preceding those terms. Dimensional analysis tells us about the dimensions of these factors. The dimension of $G[\rho]$ is $[L]^{-3a-4b} = [L]^{-5}$. Note that one can write this down by merely looking at the way $G[\rho]$ scales. Since for a non-relativistic system, the energy density has dimensions $[L]^{-5}[M]^{-1}$, it is easy to see that the factor preceding $G[\rho]$ should be of the form $\kappa/M$, where $\kappa$ is a dimensionless constant. This is indeed the case as shown in Eq. (D.42). This discussion may give the impression that a scaling analysis is completely equivalent to a dimensional one, but this is not quite true. When there is a well defined perturbative expansion, the functionals appearing at different orders will scale differently. However, at a particular order, the dimensionality of the functional completely determines its scaling. We shall come back to this point later.

The scaling of the exchange functional depends on the type of interaction. It scales the same way as the Hartree term since they both appear at the same order in
perturbation theory. For the Coulomb case, it scales as follows:

$$E_x[\rho_\gamma] = \gamma E_x[\rho]. \quad (2.43)$$

Let us prove the above by studying the scaling of the Hartree term.

$$E_H[\rho_\gamma] = \frac{1}{2} \int \int d^3x \, d^3y \, \rho_\gamma(x) \frac{1}{|x - y|} \rho_\gamma(y)$$

$$= \frac{\gamma}{2} \int \int d^3(\gamma x) \, d^3(\gamma y) \, \rho(\gamma x) \frac{1}{|\gamma x - \gamma y|} \rho(\gamma y)$$

$$= \gamma E_H[\rho]. \quad (2.44)$$

For a contact interaction, the scaling law would be different of course. Since

$$\delta^3(x - y) = \gamma^3 \delta^3(\gamma x - \gamma y), \quad (2.45)$$

the scaling law becomes $E_H[\rho_\gamma] = \gamma^3 E_H[\rho]$. The parameters $s$ and $p$ are scale invariant $(s[\rho_\gamma](x) = s[\rho](\gamma x) \ldots)$. One can easily use the scaling relations to fix the leading power of $\rho$ in Eqs. (2.34) and (2.35).

The correlation piece cannot be determined by scaling considerations in general unless there is a well defined perturbative expansion. In the high density limit ($\gamma \rightarrow \infty$), $E_c[\rho_\gamma] \rightarrow E_c[\rho]$. It has been shown by Levy and Perdew that it is impossible to partition the exact HK functional into a piece that scales as $\gamma^2$ and a piece that scales like $\gamma$, even if complete freedom with the partitioning is allowed. However, there exist scaling inequalities which are universal and are always satisfied [11]. This is something to be kept in mind in the long term, but the immediate priority is to get good functionals with appropriate scaling properties and their gradient expansions.

Expressions for the correlation energy per particle for Coulombic systems exist in the literature for the high-density limit [19, 20], and also for the low-density limit [21]. The error arising from the correlation piece is contained to a large extent by the
method of wave-vector analysis [24, 25], which involves Fourier-decomposing $E_{xc}$. An
expression encompassing both limits was proposed by Perdew and Wang [23] and is
widely used today.

The exchange-correlation piece will have gradient corrections for finite systems. A
natural way of incorporating these corrections is through density matrix expansions,
which are outlined below for the kinetic energy functional. In the KS formalism,
one exactly evaluates the kinetic energy part, and so the the following serves as an
illustration of the procedure of density matrix expansions. We shall deal with various
methods of semi-classical expansions in appendix D.

The starting point is the definition of the noninteracting Dirac density matrix as
defined in Eq. (A.11) which we write as:

$$
\gamma_s(\mathbf{x}, \mathbf{x}') = \nu \sum_k \theta(\varepsilon_F - \varepsilon_k) \psi_k(\mathbf{x}) \psi_k^*(\mathbf{x}')
$$

$$
= \nu \langle \mathbf{x} | \theta(\widehat{E}_F - \widehat{T}) | \mathbf{x}' \rangle,
$$

where $\widehat{E}_F = \varepsilon_F - \hat{v}$, and we have assumed a spin-independent Hamiltonian for a
spin one-half system. The noninteracting kinetic energy can be expressed in terms of
$\gamma_s(\mathbf{x}, \mathbf{x}')$ as

$$
T_s[\rho] = \frac{1}{2M} \int d^3 \mathbf{x} \left[ \nabla_x \cdot \nabla_x \gamma_s(\mathbf{x}, \mathbf{x}') \right]_{\mathbf{x}=\mathbf{x}'}.
$$

The next step is to write Eq. (2.46) in momentum space, and then one has to figure
out a way of evaluating $\langle \mathbf{x} | \theta(\widehat{E}_F - \widehat{T}) | \mathbf{p} \rangle$. The state $| \mathbf{p} \rangle$ is an eigenket of the
noninteracting kinetic energy operator $\widehat{T}$, and so we can look at the problem in general
as follows. The general nature of the problem is to evaluate $f(\hat{a} + \hat{c}) | a \rangle$ given that
$[\hat{a}, \hat{c}] \neq 0$. Here, $\hat{a} \rightarrow -\hat{T}$, $\hat{c} \rightarrow \widehat{E}_F$ and $f \rightarrow \theta$. To proceed, one uses the inverse
Laplace transformation to write

\[ f(\hat{\alpha} + \hat{\epsilon}) |a\rangle = \frac{1}{2\pi i} \int_{b-i\infty}^{b+i\infty} d\beta \ F(\beta) e^{\beta(\hat{\alpha} + \hat{\epsilon})} |a\rangle. \]  

(2.48)

By introducing the operator \( \hat{K}(\beta) = e^{-\beta \hat{\epsilon}} e^{\beta(\hat{\alpha} + \hat{\epsilon})} e^{-\beta \hat{\alpha}} \), Eq. (2.48) reduces to

\[ f(\hat{\alpha} + \hat{\epsilon}) |a\rangle = \frac{1}{2\pi i} \int_{b-i\infty}^{b+i\infty} d\beta \ F(\beta) e^{\beta(\hat{\alpha} + \hat{\epsilon})} \hat{K}(\beta) |a\rangle, \]

(2.49)

so that the operator \( \hat{\alpha} \) has been replaced by its eigenvalue \( a \) in the argument of the exponential. The next step is to expand \( \hat{K}(\beta) \) in a power series in \( \beta \) (in terms of \( [\hat{\alpha}, \hat{\epsilon}] \))

\[ \hat{K}(\beta) = \sum_{n=0}^{\infty} \beta^n \hat{O}_n, \]

(2.50)

so that Eq. (2.48) reduces to the following form that is central in the Kirzhnits formalism [104]:

\[ f(\hat{\alpha} + \hat{\epsilon}) |a\rangle = \sum_{n=0}^{\infty} \left[ \frac{1}{2\pi i} \int_{b-i\infty}^{b+i\infty} d\beta \ F(\beta) \beta^n e^{\beta(\hat{\alpha} + \hat{\epsilon})} \right] \hat{O}_n |a\rangle. \]

(2.51)

Then one evaluates the first few terms of this expansion and plugs it in Eq. (2.46) in momentum space to obtain the expansion of the density matrix. The density \( \rho(\mathbf{x}) \) is given by the diagonal element of the density matrix, and has the following form for our discussion:

\[ \rho(\mathbf{x}) = \gamma_s(\mathbf{x}, \mathbf{x}) = \frac{1}{3\pi^2} k_F^3 + \frac{1}{24\pi^2} \frac{\nabla^2 k_F^2}{k_F} - \frac{1}{96\pi^2} \frac{(\nabla k_F^2)^2}{k_F^4} + \cdots. \]

(2.52)

The kinetic energy density is obtained from Eq. (2.47) and has the following form to second order:

\[ \tau(\mathbf{x}) = \frac{1}{10M\pi^2} k_F^5 - \frac{1}{48M\pi^2} k_F \nabla^2 k_F^2 - \frac{1}{64M\pi^2} \frac{(\nabla k_F^2)^2}{k_F}. \]

(2.53)
\( \tau(\mathbf{x}) \) is expressed in terms of \( \rho(\mathbf{x}) \) by first obtaining the expression for \( k_F \) in terms of \( \rho(\mathbf{x}) \) from Eq. (2.52) by the method of successive approximation, and then substituting the form of \( k_F \) in Eq. (2.53). This ultimately leads to the following form of the kinetic energy density functional:

\[
\tau(\mathbf{x}) = \frac{3}{10M} (3\pi^2)^{2/3} [\rho(\mathbf{x})]^{5/3} + \frac{1}{72M} \frac{(\nabla \rho)^2}{\rho} + \cdots \tag{2.54}
\]

This approach provides a useful correction to the TF approximation for the kinetic energy functional, but seriously worsens the LSD results for \( E_c \) and \( E_{xc} \) [14]. In fact, the correlation energy turns out to be positive [13] in this formalism! This is because initial attempts at gradient corrections violated a sum rule [1, 5]. Semi-phenomenological gradient corrections [5, 23] have become steadily more sophisticated since then. The effectiveness of the KS system lies in the proper handling of \( E_{xc} \) and therefore GEA needs to be modified. The remedy is in the form of generalized gradient approximation (GGA).

### 2.2.3 Generalized Gradient Expansion Approximation (GGA)

In a GGA, spatial variations of \( \rho(\mathbf{x}) \) enter in a manner which conforms with the sum rule by construction [18], and this has reduced the errors of the LDA by a factor of 4 in Coulomb systems [5]. With the advent of various approximation schemes for the correlation part, the exchange energy is the largest remaining source of error in DFT [26]. The general form of the GGA is the following:

\[
E_{xc}^{GGA}[\rho] = \int d^3x \, f_{xc}(\rho_+, \rho_-, \nabla \rho_+, \nabla \rho_-). \tag{2.55}
\]

An empirical line of GGA development was pursued by Becke [15] who constructed a GGA for \( E_x \) by fitting two parameters to the measured energies of atoms. Lee, Yang
and Parr [16] transformed the Cole-Salvetti [17] expression for the correlation energy from a functional of KS one-particle density matrix into a functional of the density. This functional contains one empirical parameter and worked well in conjunction with Becke's work.

A powerful non-empirical way of constructing GGAs is due to Perdew and collaborators. One of the difficulties of the GEA apart from the fact that it does not respect the sum rule was that it did not satisfy Eq. (2.26). Perdew [26] showed that for GEA, the exchange hole density \( n_x(x, x + u) \) contains oscillations which are responsible for Eq. (2.26) not being satisfied. The non-empirical way of attacking the problem is to impose a real-space cutoff on this density in the sense that \( n_x \) is replaced by zero for all values of \( u \) which do not satisfy Eq. (2.26). The next step is to extend this real-space cutoff scheme from exchange to correlation with the help of a second cutoff radius that satisfies Eq. (2.28). This ultimately has culminated in the following general form for exchange-correlation [18]:

\[
E_{xc}^{GGA}[\rho_+, \rho_-] = \int d^3x \rho \epsilon_x^{\text{unif}}(\rho) F_{xc}(r_0, \zeta, s), \tag{2.56}
\]

where \( r_0 \) is the Wigner-Seitz radius, \( s \) is the reduced density gradient and \( \zeta \) is the relative spin-polarisation and is given by

\[
\zeta = \frac{(\rho_+ - \rho_-)}{(\rho_+ + \rho_-)}. \tag{2.57}
\]

\( \epsilon_x^{\text{unif}}(\rho) \) is the exchange (Fock) piece corresponding to a uniform electron gas and is \( \sim k_F. F_{xc}(r_0, \zeta, s) \), although more non-empirical than its predecessors, has numerical parameters and can be regarded as an enhanced ansatz satisfying basic rules like scaling requirements. Eq. (2.56) represents any GGA exactly when \( \zeta \) is independent of \( x \), and is always approximately valid.

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2.2.4 Meta-Generalized Gradient Expansion Approximation (Meta-GGA)

One way to go beyond the restricted GGA form of Eq. (2.55) and improve the exchange-correlation functional is to construct Meta-GGA [27], which add in another building block the semi-local kinetic energy density $\tau$ given by

$$\tau(x) = \frac{1}{2M} \sum_a |\nabla \psi_a(x)|^2 \theta(\varepsilon_F - \varepsilon_a).$$

(2.58)

However, in practice, the kinetic energy density is replaced by its local expansion in terms of the density $\rho(x)$ and its gradients [104] so that the energy is treated as a functional of the density alone. The Kohn-Sham single-particle equation still takes the form of Eq. (2.8). Early Meta-GGA’s [26, 28] preceded most GGA’s. Meta-GGA’s have the advantage of computational efficiency and higher accuracy, and are constructed as a natural extension to the GGA. The exchange and correlation functionals in this formalism are described in Ref. [27].

Other recent methods in the literature that are not described in the present work include Hyper-GGA’s [29, 30], and the optimised effective potential (OEP) formalism [31]. The latter approach leads to further development of the SIC process and may open up interesting possibilities [32].
CHAPTER 3

EFFECTIVE FIELD THEORY

In this chapter, we review the concept of an effective theory and illustrate some of its many applications in Physics. We conclude the chapter with a review of effective field theory for a dilute gas of fermions. This forms the basis of the main content of this thesis.

3.1 Effective Theory (ET)

An effective theory (ET) is a complete systematic low-energy approximation to the true theory. By systematic, we mean that there exists at least one small dimensionless parameter $s$ that can quantify the accuracy of a calculation done using an effective theory. Thus, such a calculation potentially comes with a reliable error estimate. This indicates that an ET is not a model. An ET is valid only in a specified regime determined by this small parameter, which is typically a ratio of scales present in the problem. Utilising the hierarchy of scales in the system to form this parameter is the hallmark of any ET. Any physical quantity is then expressed as an expansion in this parameter:

\[
\text{Physical Quantity} = C_0 + C_1 s + C_2 s^2 + \cdots ,
\]
although this is not always the case. The coefficients $C_k$ may be\textit{ natural} in the sense that they are dimensionful quantities multiplied by constants of order one. Under such a circumstance, the theory allows for error estimates since the coefficients can be estimated from dimensional analysis. The domain of validity of the ET is exceeded when $s \geq 1$. The radius of convergence is thus set by $s = 1$. This is the breakdown scale of the effective theory.

Let us take a simple example to illustrate this point. The gravitational potential energy of a mass $m$ distant $r$ away from the center of the earth, whose mass we denote by $M$ is given by $U = -\frac{GMm}{r}$. We have considered the case where $r > R$, the radius of the earth. The mass $m$ is at a distance $h = r - R$ above the earth’s surface. We can utilise the ratio of this length scale to the intrinsic length scale $R$ present in the problem, to form our expansion parameter. Thus, in this case, $s = \frac{h}{R}$. The gravitational potential can now be written as a simple Taylor expansion in $s$:

$$U = -\frac{GMm}{R + h} = \frac{GMm}{R}(1 - s + s^2 - \cdots).$$

Note that the above expansion is a natural one. The domain of validity of this theory is set by the condition $s < 1 \rightarrow h < R$. In a practical calculation, if one truncates the series at the $k$-th order, the truncation error would be of $O(s^{k+1})$.

There can be effective theories of effective theories. Consider the hydrogen atom problem. It can be thought of as an effective theory of QED. What we see in books is a nonrelativistic quantum treatment of the problem. Let us justify why. A nonrelativistic theory can be thought as an effective theory of the relativistic one as long as the kinetic energy is much smaller than the rest mass of the particle. The Bohr radius $r_B = (\alpha m_e)^{-1}$ is the length scale in the hydrogen atom problem, where $\alpha$ is the fine structure constant ($\alpha = 1/137$) and $m_e$ is the mass of the electron. $r_B^{-1}$ sets
the typical momenta scale for an electron. Thus, the ratio of the kinetic energy of
the electron to its rest mass energy goes like $\alpha^2/2$, a very small number justifying a
nonrelativistic treatment. But there is more. While writing down the Coulomb po-
tential due to the proton, we completely disregard the fact that the proton is a charge
distribution with a finite size $r_p$. There is a justification for this too. Imagine the
proton to be a charged lump of dimension $r_p$ carrying a charge $e$. The electrostatic
potential at a point $x$ outside the the proton dimension is given by

$$V(x) = \frac{1}{4\pi \varepsilon_0} \int d^3 y \frac{\rho(y)}{|x - y|}$$

$$= \frac{1}{4\pi \varepsilon_0} \sum_{n=0}^{\infty} \int d^3 y \rho(y) P_n(x, \hat{y}) \frac{1}{|x|} \left(\frac{y}{x}\right)^n , \quad (3.2)$$

where $P_n(x, \hat{y}) = P_n(\cos \theta)$ is the Legendre polynomial of order $n$, $\theta$ being the angle
between the vectors $x$ and $y$. $\rho(y)$ denotes the charge density of the proton. The
above is just a multipole expansion of the proton charge distribution. Since an electron
in its ground state is roughly at a distance $r_B$ from the center of the proton, a typical
magnitude for $x$ is $r_B$, and that for $y$ is set by the size scale of the proton, $r_p$. So we
can write the above expression as

$$V(x) \approx \frac{1}{4\pi \varepsilon_0} \frac{1}{|x|} \sum_{n=0}^{\infty} \int d^3 y \rho(y) P_n(\cos \theta) \left(\frac{r_p}{r_B}\right)^n$$

$$= \frac{e}{4\pi \varepsilon_0} \frac{1}{|x|} \left(1 + \mathcal{O}(s)\right) , \quad (3.3)$$

Thus, the finite size effect of the proton is suppressed by the the ratio $r_p/r_B$. So,
treating the proton as a structureless object makes some sense [33]. An electron
with typical momenta $r_B^{-1}$ will have a wavelength $\sim r_B$ associated with it. Since
this wavelength is much bigger than the length scale determining the structure of
the proton, it cannot resolve the fine details of the proton charge distribution. The
Figure 3.1: If a system is probed at low energies, fine details are not resolved.

fact that a low energy wave cannot probe short distance structure is the central idea
behind effective theories [Fig. 3.1]. Thus, the unresolved part can be replaced by
something simpler.

Let us discuss more on resolution examples. If one needs to study the structure
of a crystal with lattice spacing $d$, one needs to shine light having a wavelength $\lambda \leq d$
in order to resolve the atoms in the crystal. Next, consider a single-slit experiment
with slit width $d$. The slit casts a perfect shadow in the limit $\lambda \to 0$. This is
the geometrical optics limit, and in this limit, the slit is completely resolved due
to its sharp shadow. However, one encounters diffraction due to the finiteness of
$\lambda$. In particular, whenever $\lambda > d$, diffraction is a prominent effect. The effect of
diffraction is to decrease resolution. The angular spread of the central maxima given
by $\Delta \theta \sim \lambda/d$ is a measure of resolution, the more the spread, the worse the resolution.
A similar relation holds in the case of a circular aperture. Let us consider probing
a nucleus with electrons. Approximating this three-dimensional potential scattering
problem by diffraction from a circular aperture can be instructive. For a nucleus of
diameter 10 fm, one needs electrons of wavelength < 10 fm to resolve the details. This corresponds to a momenta > 120 Mev/c. If one plots the scattered intensity as a function of the scattering angle, one finds that the curves resemble those of the diffraction intensity patterns. From the position of the first minima, one can thus get an idea about the diameter of the nucleus [112]. These examples illustrate the idea behind Fig. 3.1.

Sometimes, a problem may be approached by constructing an effective Hamiltonian and restricting it to act only on a certain subspace. The separation of scales in the problem translate to the separation of spaces where the operators act. The following example illustrates this point. Let us consider how one can work with an effective picture taking the case of a Josephson junction. The objective of this example is not to derive Josephson’s equations, but to point out the utility of effective Hamiltonians utilising separation of scales in the problem. In this particular case, this leads to a strong coupling expansion.

Consider two superconductors denoted by $L$ and $R$ separated by a thin insulating barrier. Denote the total Hamiltonian of the system by $H$, where $H = H_R + H_L + H_T$. Here, $H_L$ denotes the full many-body Hamiltonian of the left superconductor, etc. $H_T$ is the tunneling piece that is responsible for transferring single electrons from the left to the right and vice versa. In the absence of this tunneling term, the two superconductors are of course decoupled. Since the electrons in the superconductors are in a paired state, it costs an energy at least equal to the gap energy $\Delta$ to break them up. This is the energy scale in the problem that forbids arbitrary gapless excitations. Thus, if we concentrate on low energy processes, $H_T$ acting only once on the system’s state is not physically viable, but its acting twice is all right because
then a pair of electrons is transferred and the system does not have to pay the gap cost. Hence it makes sense to cook up an effective Hamiltonian that will capture this low energy physics. This is achieved by a canonical transform of the form

\[ H_{\text{eff}} = e^{iS} H e^{-iS} \]

\[ = H + i[H, S] - \frac{1}{2}[[H, S], S] \cdots \]  \hspace{1cm} (3.4)

\( S \) is chosen so as to eliminate the effect of \( H_T \) to leading order in \( H_{\text{eff}} \). This condition translates to \( S \) satisfying

\[ H_T + i[H_L + H_R, S] = 0. \]  \hspace{1cm} (3.5)

Now, \( H_{\text{eff}} \) does not contain \( H_T \) and therefore has no terms that take an electron out of the low energy subspace. In other words, it purely acts on a low energy subspace where there are no quasiparticles. This achieves the separation of scales in the problem. Proceeding, one arrives at the following low energy Hamiltonian.

\[ H_{\text{eff}} = H_R + H_L - \sum_k \frac{H_T |k \rangle \langle k| H_T}{E_k - E}. \]  \hspace{1cm} (3.6)

It is instructive to note that the virtual intermediate state \( |k \rangle \) can be of arbitrarily high energy and therefore can have a broken pair. \( E_k \) is the usual quasiparticle excitation spectrum,

\[ E_k = E + \sqrt{(\epsilon_k - \mu)^2 + \Delta^2}, \]  \hspace{1cm} (3.7)

where \( \mu \) is the chemical potential and \( \epsilon_k \) is the dispersion with an effective mass. Since the denominator of the second order term in \( H_{\text{eff}} \) is of the order of \( \Delta \), we have an expansion in \( \frac{\Delta}{E} \). This is an example of a strong coupling expansion.
3.2 Effective Field Theory (EFT)

The basic ideas of an effective theory carries over to quantum field theory applications. It is then termed as an effective field theory (EFT). EFT approach allows for accurate model-independent calculations of low-energy processes and properties with well-defined error estimates (based on the order of truncation) [38, 39, 34, 37, 36]. An EFT can be constructed systematically using the following recipe:

- Identify the relevant degrees of freedom and the symmetries of the theory at the energy scale one is interested in.

- Write down the most general Lagrangian consistent with the symmetries.

- Choose a convenient regularization and renormalization prescription.

- Utilize the separation of scales to form the expansion parameter [34, 35].

Consider an example of a system interacting at low energies so that the mass of the particle mediating the interaction is huge relative to this energy scale. Equivalently, the typical momenta $k$ are small compared to the inverse range of the interaction $1/R$. The high-energy intermediate states are highly virtual because there is not enough energy to make a physical particle. These states last for a short time by the uncertainty principle, and hence cannot propagate over large distances. So, their effects are not distinguishable from those of local operators (operators with finite number of derivatives). The short-distance structure can therefore be replaced by something simpler without distorting the low-energy observables.

Even though this low-energy process is insensitive to the details of the short-distance dynamics, we cannot completely disregard this dynamics. It does have an
impact on low-energy observables [34]. This short-distance physics is accounted for by systematically including contributions from loop graphs into the coefficients of the local operators. This process is called renormalization. The prescription to handle loop divergences and make things finite is referred to as the regularization scheme.

The effective degrees of freedom (dof’s) in an EFT depend on a resolution momentum scale \( \Lambda \), which sets the radius of convergence of an EFT. Any momenta \( > \Lambda \) is high energy or short-distance physics. In the above example, we can take \( \Lambda \sim 1/R \) and then the low-energy observables can be described by a controlled expansion in \( kR \). Thus, one can carry out calculations of low-energy processes with well-defined error estimates [38, 39, 37, 36]. The goal of EFT is to get the long-distance physics (low energy physics relative to the momentum scale \( \Lambda \)) correct [37] while accounting for short-distance behaviour by simple local operators with renormalized coefficients. The true theory that is mimicked by the effective one may be known, but in most cases, either it is not known, or it cannot be solved in the regime of interest.

### 3.2.1 EFT in Vacuum

Let us consider two body scattering of heavy nonrelativistic fermions in vacuum. The scattering amplitude does not depend on the center of mass momentum \( \mathbf{P} \), but only on the relative momenta \( \mathbf{k} \) and \( \mathbf{k}' \) due to Galilean invariance. One might as well work in the center of mass (COM) frame where \( \mathbf{P} = 0 \). For elastic scattering, \( |\mathbf{k}| = |\mathbf{k}'| = k \). The COM energy is related to this momenta by \( E = k^2/M \), where \( M \) is the mass of the fermions in question. Choosing the fermions in the COM frame to approach each other along the \( z \) axis, then the scattered wavefunction is given by

\[
\Psi(x) = e^{ikz} + f(k, \theta) \frac{e^{ik|x|}}{|x|},
\]  

(3.8)
where $|x| = r$, $f(k, \theta)$ is the scattering amplitude whose modulus squared gives the differential scattering cross section, and $\theta$ is the angle between $k$ and $k'$. For spin-independent interactions via central potential, the scattering amplitude has a partial-wave expansion given by the following expression.

$$f(k, \theta) = \sum_{\ell=0}^{\infty} \frac{(2\ell + 1)}{k \cot \delta_{\ell} - i k} P_{\ell}(\cos \theta).$$ \hspace{1cm} (3.9)

The $T$ matrix is then defined as

$$T(k, \cos \theta) = \frac{2\pi}{\mu} f(k, \theta).$$ \hspace{1cm} (3.10)

The mass term $\mu$ appearing in the denominator is the effective mass and is given by $\mu = M/2$. Schwinger showed that for finite-ranged interactions, $k^{2\ell+1} \cot \delta_{\ell}$ has a power series expansion, called the effective range expansion (ERE). For $s$-wave scattering ($\ell = 0$), the ERE is given by

$$k \cot \delta_0 = -\frac{1}{a_s} + \frac{1}{2} r_s k^2 - P r_s^3 k^4 + \cdots$$ \hspace{1cm} (3.11)

The leading term for the $p$-wave ($\ell = 1$) ERE is given by

$$k^3 \cot \delta_1 = -\frac{3}{a_p^3} + \cdots$$ \hspace{1cm} (3.12)

In the above expressions, $a_s$ and $a_p$ are the S and P wave scattering lengths respectively, and $r_s$ is the S wave effective range. When these length scales are comparable to the range $R$ of the interaction, the theory is said to be natural.

Let us now construct a natural EFT for scattering of nonrelativistic fermions. The system is assumed to be invariant under Galilean, parity, and time-reversal transformations. The general local Lagrangian density respecting these symmetries is given
by the following:

\[
\mathcal{L} = \psi^\dagger \left[ i\partial_t + \frac{\vec{\nabla}^2}{2M} \right] \psi - \frac{C_0}{2} (\psi^\dagger \psi)^2 + \frac{C_2}{16} \left[ (\psi \psi)^\dagger (\psi^\dagger \nabla^2 \psi) + \text{h.c.} \right] + \frac{C_2'}{8} (\psi^\dagger \nabla^2 \psi)(\psi^\dagger \nabla \psi) - \frac{D_0}{6} (\psi^\dagger \psi)^3 + \ldots,
\]

(3.13)

where \( \nabla^2 = \nabla^\dagger - \nabla \) is the Galilean invariant derivative and h.c. denotes the Hermitian conjugate. The above Lagrangian density is complete, but it does not include all possible terms at a given order because that would involve redundancy. The terms proportional to \( C_2 \) and \( C_2' \) contribute to \( s \)-wave and \( p \)-wave scattering respectively, while the dots represent terms with more derivatives and/or more fields. It is important to note that there is nothing sacrosanct about the terms written down in the above Lagrangian. One can always write equivalent Lagrangians containing redundant terms that reduce to the above simple form after field redefinitions \[41\].

It is a good idea to get some feel about dimensions of the coefficients at this point. Recall that \( \Lambda \sim 1/R \) is the momentum scale in the problem. The Lagrangian density must have a dimension of \( [\Lambda^3]/[T] \equiv [\Lambda^5]/[M] \) to render the action dimensionless (in natural units). From the kinetic energy term in the Lagrangian density, it is easy to see that the dimensionality of the fermion field is \( [\Lambda^{3/2}] \). Denote \( A_{2i}^n \) as the coefficient of the operator in the Lagrangian with \( 2i \) derivatives and \( 2n \) fields. This coefficient will appear in all \( n \)-body vertices. The \( 2i \) derivatives have a dimension of \( [\Lambda^{2i}] \), and the \( 2n \) fields contribute a dimensionality of \( [\Lambda^{3n}] \). Thus, the dimension of \( A_{2i}^n \) is \( [\Lambda^{5-2i-3n}]/[M] \). As an example, consider the \( C_0 \) coefficient. It is just \( A_{2i}^n \), and has dimensions \( [\Lambda^{-1}]/[M] \). The \( C_2 \) coefficient is \( A_{2i}^n \), and hence has a dimension of \( [\Lambda^{-3}]/[M] \). The same holds true for the \( C_2' \) coefficient. Note that all these coefficients are natural.
From the EFT Lagrangian, one can easily write down the EFT potential in momentum space schematically.

\[ V_{\text{EFT}}(k, k') = C_0 + \frac{C_2}{2}(k'^2 + k^2) + C'_2 k' \cdot k + \cdots \quad (3.14) \]

The above is a momentum space version of interactions of the nature of delta functions and its derivatives. The unresolved high energy physics is encoded in these coefficients. The question is, how to determine them. If the underlying dynamics is unknown, these coefficients can be determined by fitting to at least three pieces of independent data [34]. If the true physics is known, then one can match these coefficients to observables calculated from the true theory. In the subsequent sections, we will illustrate the latter methodology for a natural theory [41, 33] with \( kR << 1 \).

The plan is to first expand the T matrix up to \( O((kR)^2) \) using the ERE:

\[ T(k, \cos \theta) = -\frac{2\pi a_s}{\mu} \left[ 1 - i a_s k + \left( \frac{a_s r_s}{2} - a_s^2 \right) k^2 \right] - \frac{2\pi a_s^3}{\mu} k^2 \cos \theta. \quad (3.15) \]

Next, we find out the effective range parameters from the known “true” physics. Finally, we evaluate the T matrix as a Born series in the COM frame with our EFT potential and match to the above expression.

Due to the singular nature of contact interactions, one encounters divergences while computing loop corrections to the T matrix. The one-loop graph gives a linear divergence, and this power divergence can be taken care of using dimensional regularization with minimal subtraction. This regularization prescription is convenient for natural theories [41], and makes the process of determining which graphs contribute at a given order (power counting) equivalent to dimensional analysis. This is because each graph contributes only one power of \( k \). The full power counting scheme is elucidated in Ref. [41].
The $T$ matrix expansion is shown in Fig. 3.2. The expansion upto $\mathcal{O}((kR)^2)$ is
\[
T(k, \cos \theta) = -C_0 \left[ 1 - i \frac{M}{4\pi} C_0 k + \left( \frac{C_2}{C_0} - \left( \frac{M}{4\pi} C_0 \right)^2 \right) k^2 + \frac{C'_2}{C_0} k^2 \cos \theta \right].
\] (3.16)

Matching this to the ERE of the $T$ matrix given by Eq. (3.15), one gets the coefficients in terms of the effective-range parameters:
\[
C_0 = \frac{4\pi a_s}{M}, \quad C_2 = C_0 \frac{a_s r_s}{2}, \quad \text{and} \quad C'_2 = \frac{4\pi a_p^3}{M}. \quad (3.17)
\]

Now we are in a position to look at some simple applications. Let us try to construct an EFT for low energy scattering (so that $kR \ll 1$) for some potentials. The scattering amplitude and hence the $T$ matrix will have a perturbative expansion in $kR$ as justified above.

**EFT for hard sphere potential**

Suppose that the true interaction between the fermions is a hard sphere potential with a range $R$. Inside the sphere, the scattering solution vanishes. Outside, the
solution has the form \((j_\ell(kr) \cos \delta \ell - \eta_\ell(kr) \sin \delta \ell)\). Matching at \(r = R\) gives us the phase shift for any partial wave \(\ell\) as

\[
\tan \delta \ell = \frac{j_\ell(kR)}{\eta_\ell(kR)}.
\] (3.18)

Since \(j_0(x) = \sin x/x\) and \(\eta_0(x) = -\cos x/x\), the \(s\)-wave phase shift is given by \(\delta_0 = -kR\). Thus the effective range expansion looks like

\[
k \cot \delta_0 = -\frac{1}{R} + \frac{1}{3} Rk^2 + \cdots
\] (3.19)

Comparing this to the form of ERE, we get \(a_s = R\) and \(r_s = 2R/3\). This allows us to fix the coefficients of the Lagrangian in terms of the range \(R\) of the hard sphere potential,

\[
C_0 = \frac{4\pi R}{M}, \quad C_2 = C_0 \frac{R^2}{3}.
\] (3.20)

We have yet to fix \(C'_2\). We need to find the \(p\)-wave phase shift for that:

\[
\tan \delta_1 = \frac{j_1(kR)}{\eta_1(kR)} = -\frac{\sin(kR)/(kR)^2 - \cos(kR)/(kR)}{\sin(kR)/(kR) + \cos(kR)/(kR)^2}
= \frac{kR - \tan(kR)}{1 + kR \tan(kR)}
\] (3.21)

So, the effective range expansion for \(p\)-waves looks like

\[
k^3 \cot \delta_1 = -\frac{3}{R^3} - \frac{9}{5R} k^2 + \cdots
\] (3.22)

Comparing with the leading term of the \(p\)-wave ERE, we get \(a_p = R\). So, the coefficient \(C'_2\) for the hard sphere case is given by

\[
C'_2 = \frac{4\pi R^3}{M}.
\] (3.23)

It is interesting to note that even though standard perturbation theory in the hard-sphere potential gives infinite results for this problem, the low energy physics is described by a perturbative expansion. This throws new lights on our understanding of
processes, indicating that a strongly coupled problem may be judiciously handled in the appropriate energy regime by doing perturbation in a suitable expansion parameter derived from the scales in the problem.

**EFT for repulsive square well potential**

Now, let us consider the case where the interaction potential between the fermions in a square well potential of strength $V_0$ and range $R$. Let $K = \sqrt{M |V_0|}$. Inside the well, the scattering solution looks like $A \ell j_\ell(\alpha r)$ where $\alpha = \sqrt{k^2 + K^2}$. Outside, the solution has the form $(j_\ell(kr) \cos \delta_\ell - \eta_\ell(kr) \sin \delta_\ell)$. Define $\gamma_\ell(k)$ as:

$$\frac{1}{R \gamma_\ell(k)} = \frac{d}{dr} (\ln R_\ell(r))_{in}. \tag{3.24}$$

Logarithmic matching at $r = R$ leads to the condition [111]

$$\cot \delta_\ell = \frac{k R \gamma_\ell(k) \eta'_\ell(kR) - \eta_\ell(kR)}{k R \gamma_\ell(k) j'_\ell(kR) - j_\ell(kR)}. \tag{3.25}$$

The above expression is completely general and can be applied to any scattering problem involving a finite range $R$ of the potential. The parameter $\gamma_\ell(k)$ can be determined only by solving the wave equation in the interior region. For the square well case,

$$\gamma_\ell(k) = \frac{1}{\alpha R \ j'_\ell(\alpha R)}. \tag{3.26}$$

Thus, the expression for phase shift reduces to

$$\cot \delta_\ell = \frac{k \ j_\ell(\alpha R) \eta'_\ell(kR) - \alpha \ j'_\ell(\alpha R) \eta_\ell(kR)}{k \ j_\ell(\alpha R) \ j'_\ell(kR) - \alpha \ j'_\ell(\alpha R) \ j_\ell(kR)}. \tag{3.27}$$

Now we can use the effective range expansion. For the $s$-wave, we get the effective range parameters as

$$a_s = R - \frac{1}{K} \tan(KR),$$

$$\tau_s = R - \frac{R^3}{3a_s^2} - \frac{1}{a_s K^2}. \tag{3.28}$$
ERE for the $p$-wave takes the form

$$k^3 \cot \delta_1 = -\frac{3}{R^3} \chi(K, R),$$

where

$$\chi(K, R) = \frac{K^2 R^2}{3 (KR \cot(KR) - 1) + K^2 R^2}.$$  

$$\Rightarrow a_p = R \left[ \frac{1}{\chi(K, R)} \right]^{1/3}. \quad (3.29)$$

Now, we can express the coefficients of the operators in our Lagrangian in terms of these effective range parameters. Our EFT is all set for calculations.

For free space low energy scattering of nucleons, the pion mass $M_{\pi}$ sets the resolution scale $\Lambda$. Thus, our effective Lagrangian picture can be useful as long as $k << M_{\pi}$.\(^1\) The above theory incorporates neither the spin-isospin dependence of the nucleon-nucleon potential, nor the non-central behaviour. However, in the $^1S_0$ channel, one can get away with our simple picture.

### 3.2.2 EFT at Finite Density: Infinite Dilute Fermi System

The application of EFT methods to many-body problems gets more complicated due to the appearance of another scale in the problem, the Fermi momentum $k_F$. Interaction of nucleons inside the nucleus is a whole different ball game, because the momenta $k$ of the nucleons can now be $\sim k_F > M_{\pi}$. So one has to explicitly include the pions in the theory. One can however integrate out the vector meson degrees of freedom as before.

It is instructive to formulate a systematic many-body EFT for a simpler system first, one that can be described by the EFT Lagrangian with reliable error estimates, and insight into the analytic structure of observables [40, 41]. The fact that we are

\(^1\)Ref. [37] discusses how the pion can be considered either a short- or long-distance degree of freedom in the two-nucleon problem, depending on the resolution scale.
Figure 3.3: Hugenholtz diagrams for a dilute Fermi gas through order $k_F^6$ in the energy density.

now at finite density itself complicates power counting scheme. However, for the case of dilute Fermi gas with natural scattering lengths, power counting is completely analogous to that of free space with the external momenta $k$ being replaced by by $k_F$ [41]. The expansion parameter is now $k_F/\Lambda$, where $\Lambda$ is the resolution scale separating the long and short distance physics.

The basic length scales in low-energy fermionic systems is the scattering length $a_s$ and the inter-particle spacing $r_0$. The scaled particle separation $r_0/a_s \sim 1/(k_F a_s)$ is a measure of density. The low density regime corresponds to $r_0 \to \infty$, so that $k_F a_s$ serves as a perturbative expansion parameter. Thus, the energy density for the uniform dilute fermion system with natural scattering length can be calculated as a perturbative expansion.
Consider $A$ fermions with spin-degeneracy $\nu$ in volume $V$. The density $\rho$ is

$$\rho = \frac{A}{V} = \nu \int \frac{d^3k}{(2\pi)^3} \theta(k_F - k) = \frac{\nu k_F^3}{6\pi^2}.$$  \hfill (3.30)

The non-interacting energy density at zero temperature is purely kinetic, and can be written as

$$\mathcal{E}_0 = \frac{\nu}{2M} \int \frac{d^3k}{(2\pi)^3} k^2 \theta(k_F - k) = \rho \frac{3}{5} \frac{k_F^2}{2M}, \hfill (3.31)$$

Note that $\mathcal{E}_0/\rho = E/A$, the non-interacting energy per particle. The order-by-order corrections to Eq. (3.31) due to interactions can be represented by the Hugenholtz diagrams given in Fig. 3.3. The interactions do not change the form of the above equations. The Feynman rules for evaluating these graphs are described in Ref. [41].

To reproduce the results in Ref. [41], we can write a conventional generating functional with the Lagrangian of Eq. (3.13) and Grassmann sources coupled to $\psi^\dagger$ and $\psi$, respectively [109]. The non-quadratic part of the Lagrangian is removed in favor of functional derivatives with respect to the Grassmann sources and the remaining quadratic part is evaluated in terms of a non-interacting Green’s function times the sources (appendix B). Perturbative expansions for Green’s functions (and subsequently $S$–matrix elements) follow by taking successive functional derivatives, and the ground state energy density follows by applying the linked cluster theorem (Ref. [109]).

In calculating the energy, finite density boundary conditions at $T = 0$ can be incorporated into the non-interacting Green’s function using the chemical potential $\mu$ or by including them by hand with a non-interacting chemical potential. The latter approach is simplest at $T = 0$ and was adopted in Ref. [41].

The diagrams of Fig. 3.3 each contribute to precisely one order in the energy density. The LO diagram of order $k_F^6$ [Fig. 3.3(a)] represents the Hartree-Fock result.
It contributes
\[ \mathcal{E}_1 = \rho (\nu - 1) \frac{k_F^2}{2M} \frac{2}{3\pi} k_F a_s , \]
where Eqs. (3.17) and (3.30) have been applied. At order \( k_F^2 \) (NLO) there are two diagrams. The three-loop diagram [Fig. 3.3(c)] is an example of an “anomalous diagram,” which vanishes identically for a uniform system in the zero-temperature formalism but is nonzero when calculated in the zero-temperature limit. The other diagram at this order [the “beach ball” diagram of Fig. 3.3(b)], makes the contribution
\[ \mathcal{E}_2 = \rho (\nu - 1) \frac{k_F^2}{2M} (k_F a_s)^2 \frac{4}{35\pi^2} (11 - 21 \ln 2) . \]
The first three of the graphs of order \( k_F^8 \) (NNLO) are anomalous diagrams. These graphs give the correction
\[
\mathcal{E}_3 = \rho \frac{k_F^2}{2M} \left[ (\nu - 1) \frac{1}{10\pi} (k_F a_s)^2 k_F r_s + (\nu + 1) \frac{1}{9\pi} (k_F a_p)^3 \right. \\
+ (\nu - 1) \{0.07550 + (\nu - 3) 0.05741\} (k_F a_s)^3 \],
\]
where the integrals for Figs. 3.3(g) and (h) have been obtained by Monte Carlo integration [41].

\[ ^2 \text{In the latter case, its contribution is precisely cancelled by the shift between the noninteracting and interacting chemical potentials, as dictated by the Kohn-Luttinger-Ward theorem [59, 109, 110}. \]
CHAPTER 4

DFT/EFT MERGER IN THE UNIFORM SYSTEM APPROXIMATION

EFT approaches have been making steady progress on two- and three-body nuclear systems and certain halo nuclei, and \textit{ab initio} shell model methods should be able to extend the calculations to a wide range of light nuclei [38, 39, 36, 37, 48]. While EFT has shown early promise in applications to basic many-body problems [40, 41], there are formidable challenges in carrying out many-body calculations, particularly for finite, non-uniform systems. DFT on the other hand is better suited to deal with such systems. EFT is a systematic approach, whereas DFT has uncontrolled approximations like the LDA that, though successful, is not systematic. Even beyond the LDA, much of DFT has developed along empirical lines and that is something which is not desired. Therefore, although the gradient expansions bring more order to the DFT formalism, it makes sense to merge the organizational advantages and insight provided by EFT with the calculational power and relative ease of DFT for finite systems to further expand the calculational framework in terms of computational ease and systematics.

In this chapter, we develop an effective action framework to accomplish the DFT/EFT merger. Our strategy is to apply an effective action formalism [99, 102,
100] to calculate the Kohn-Sham potential and energy functional order-by-order in an EFT expansion, and to use EFT power counting to organize and justify a derivative expansion of the functional.

4.1 The Model

We use a dilute, confined Fermi system with short-range interactions as a laboratory to explore how EFT can be used to carry out systematic DFT calculations. This model provides a prototype for more complex systems and also has a physical realization in recent experiments on fermionic atoms in optical traps [49]. We shall however not discuss the experimentally interesting case of large scattering length because our expansion parameter is the local Fermi momentum times the scattering length (and other effective range parameters), and this parameter no longer remains small in the aforementioned case. In this chapter, we shall work in the local density approximation. The next chapter deals with taking a small step beyond this approximation.

The use of functional Legendre transformations for DFT with the effective action formalism [44, 45] and the connection to Kohn-Sham DFT [46, 47, 54, 55, 56, 57, 58, 85] can be found in literature. We have taken one step further in terms of systematics by merging the Kohn-Sham density functional approach and effective field theory.

4.2 Effective Actions and The Inversion Method

A conventional effective action is a functional of the expectation value of elementary fields in the Lagrangian. It defines a classical field theory that contains all of the quantum effects of the interacting quantum field theory associated with the original
Lagrangian, so that one reproduces results of the full field theory from tree level calculations based on the propagators and vertices of the effective action \[99, 102, 100].

As noted before, the utility of DFT rests on finding an explicit expression, exact or approximate, for \( E_{xc} \). We adopt an approximation scheme based on effective action methods \[44, 45, 46\] extended with an effective field theory expansion at zero temperature in Minkowski space to achieve this goal.

To describe trapped fermions, we add to the Lagrangian (Eq. (3.13)) a term for an external confining potential \( v(x) \) coupled to the density operator \( v(x)\psi^\dagger \psi \). Here we take the external potential to be an isotropic harmonic confining potential

\[
v(x) = \frac{1}{2} m \omega^2 |x|^2,
\]

(4.1)
as might be appropriate for some atomic traps \[61\], but the discussion holds for a general external potential. We also introduce a c-number source, \( J(x) \), coupled to the composite density operator and write down the generating functional using the path integral formulation,

\[
Z[J] = e^{iW[J]} = \int D\psi D\psi^\dagger e^{i \int d^4x \left[ \mathcal{L} + J(x)\psi^\dagger(x)\psi(x) \right]}.
\]

(4.2)

For simplicity, normalization factors are considered to be implicit in the functional integration measure. (Refs. \[44, 45\] has a more careful treatment of the path integrals.) Using the definition in Eq. (4.2), we see that the density (in the presence of \( J \)) is

\[
\rho(x) \equiv \langle \psi^\dagger(x)\psi(x) \rangle_J = \frac{\delta W[J]}{\delta J(x)}.
\]

(4.3)

While it is possible to absorb \( v(x) \) into the definition of \( J(x) \), we find it more convenient to recover our original system in the limit \( J \to 0 \).
Let us now define the effective action through the functional Legendre transformation
\[
\Gamma[\rho] = W[J] - \int d^4 x \ J(x) \rho(x) .
\]  
(4.4)
This transformation ensures that \( \Gamma \) has no \textit{explicit} dependence on \( J \). This is easy to see since a functional derivative of Eq. (4.4) with respect to \( J \) gives us zero on the the right hand side when we use Eq. (4.3). The existence of such a functional follows from the concavity of \( W[J] \) which guarantees that Eq. (4.3) can be inverted to give \( J = J[\rho] \). The functional dependence between \( J \) and \( \rho \) can be used to write Eq. (4.4) entirely in terms of \( \rho \). The proof that \( W[J] \) is strictly concave is given in Ref. [46].

Since we are interested here in describing finite many-body ground states at \( T = 0 \), it is most convenient to work with functions of the particle number \( A \) rather than the chemical potential \( \mu \). This can be achieved via a conventional Legendre transformation on \( W \) or \( \Gamma \), but is more simply carried out implicitly, by choosing appropriate finite-density boundary conditions that enforce a given \( A \) by hand (the actual procedure is detailed below). In the following, we will assume this has been done. \textit{Thus, \( \Gamma \) and \( W \) are functions of \( A \) and variations over \( \rho(x) \) conserve \( A \).} In addition, we restrict the discussion to time independent sources and densities. In this case the effective action acquires a factor that corresponds to the time interval over which the source is acting, which we indicate schematically as
\[
\Gamma[\rho] = -E[\rho] \times \int_{-\infty}^{\infty} dt ,
\]  
(4.5)
as in Ref. [44]. To avoid overly cluttered notation, we will divide out this ubiquitous time factor everywhere it appears and write
\[
\tilde{\Gamma}[\rho] \equiv \Gamma[\rho] \times \left[ \int_{-\infty}^{\infty} dt \right]^{-1} = -E[\rho] .
\]  
(4.6)
and similarly with $W[J]$ and the expansions below. (We will continue to use $\tilde{\Gamma}$ rather than $E$ in this section.)

In conventional treatments [100, 102], an effective action is derived from a Legendre transformation with respect to a source coupled to one of the fields in the Lagrangian, rather than to a composite operator as in the present case. However, the usual advantages of working with an effective action are also present here. In particular, the effective action has extrema at the possible quantum ground states of the system, and when evaluated at the minimum is proportional (at zero temperature) to the ground state energy [44, 45, 62]. In particular, Eq. (4.5) defines an energy functional $E[\rho]$ equal to the ground-state energy when evaluated with the ground-state density.

The extremization condition is shown as follows. Combining Eq. (4.3) and Eq. (4.4) we find

$$
\frac{\delta \tilde{W}[J]}{\delta J(\mathbf{x})} = \int d^3y \left( \frac{\delta \tilde{\Gamma}[\rho]}{\delta \rho(\mathbf{y})} \right) \left( \frac{\delta \rho(\mathbf{y})}{\delta J(\mathbf{x})} \right) + \rho(\mathbf{x}) + \int d^3y \left( \frac{\delta \rho(\mathbf{y})}{\delta J(\mathbf{x})} \right) J(\mathbf{y}) \quad (4.7)
$$

or

$$
\int d^3y \left( \frac{\delta \tilde{\Gamma}[\rho]}{\rho(\mathbf{y})} + J(\mathbf{y}) \right) \left( \frac{\delta \rho(\mathbf{y})}{\delta J(\mathbf{x})} \right) = 0 . \quad (4.8)
$$

The invertibility of (4.3) implies

$$
\frac{\delta \rho(\mathbf{y})}{\delta J(\mathbf{x})} \neq 0 , \quad (4.9)
$$

so we must have

$$
\frac{\delta \tilde{\Gamma}[\rho]}{\delta \rho(\mathbf{x})} = -J(\mathbf{x}) . \quad (4.10)
$$

The above equation tells us that when $J(\mathbf{x}) = 0$ the effective action is extremized, which is a statement of the second HK theorem [2]. The strict concavity of $\tilde{W}[J]$
implies the strict convexity of \( \tilde{\Gamma}[\rho] \) and so the extremum is a minimum. Since \( J(\mathbf{x}) = 0 \) corresponds to the original system we see that the energy functional is minimized when evaluated at the exact expectation value of the density.

The inversion method is a systematic approximation procedure for constructing the energy functional. Now let us consider a system that can be characterized by an effective field theory power-counting parameter, which we label \( \lambda \). This parameter may be dimensionful and can appear to all orders. We will not exhibit it explicitly here but indicate by subscripts the order in \( \lambda \) of a given function or functional. In previous discussions of the inversion method \([44, 45]\), the parameter \( \lambda \) was always a coupling constant (e.g., \( e^2 \) for the Coulomb interaction). In contrast, we associate \( \lambda \) with an appropriate EFT expansion parameter. For example, \( \lambda \) could be \( 1/N \) in the dilute expansion (which we use here) or \( 1/N \) in a large \( N \) expansion, where "\( N \)" is the spin degeneracy \( \nu \) \([41]\). The effective action functional will depend on \( \lambda \) but we treat \( \rho \) and \( \lambda \) as independent variables:

\[
\tilde{\Gamma} = \tilde{\Gamma}[\rho, \lambda] .
\]  
(4.11)

However, the ground state expectation value \( \rho_g(\mathbf{x}) \) will naturally depend on \( \lambda \) as determined by

\[
\left. \frac{\delta \tilde{\Gamma}[\rho, \lambda]}{\delta \rho(\mathbf{x})} \right|_{\rho = \rho_g} = 0 .
\]  
(4.12)

That is, if \( \lambda \) is changed, a different \( \rho_g \) will be necessary to satisfy this equation.

The Legendre transformation defining \( \tilde{\Gamma} \) is

\[
\tilde{\Gamma}[\rho, \lambda] = \tilde{\mathcal{W}}[J, \lambda] - \int d^3 \mathbf{x} J(\mathbf{x}) \rho(\mathbf{x}) ,
\]  
(4.13)

where \( J \) is a functional of \( \rho \) and \( \lambda \) as well, as dictated by

\[
\left. \frac{\delta \tilde{\mathcal{W}}[J, \lambda]}{\delta J(\mathbf{x})} \right|_{\rho} = \rho(\mathbf{x}) .
\]  
(4.14)
As $\lambda$ is changed, $J$ must be adjusted so that the same $\rho$ is obtained when taking this derivative. This is how the dependence of $J$ on $\lambda$ arises; clearly this dependence can become quite complicated.

The inversion method now proceeds by expanding each of the quantities that depend on $\lambda$ in Eq. (4.13) in a Taylor series in $\lambda$:

\[
J[\rho, \lambda] = J_0[\rho] + J_1[\rho] + J_2[\rho] + \cdots, \quad (4.15)
\]

\[
\tilde{W}[J, \lambda] = \tilde{W}_0[J] + \tilde{W}_1[J] + \tilde{W}_2[J] + \cdots, \quad (4.16)
\]

\[
\tilde{\Gamma}[\rho, \lambda] = \tilde{\Gamma}_0[\rho] + \tilde{\Gamma}_1[\rho] + \tilde{\Gamma}_2[\rho] + \cdots, \quad (4.17)
\]

where, as advertised, the power of $\lambda$ associated with each function or functional is indicated by the subscript. We can substitute the expansion for $J$ into the expansion for $W$ and do a functional Taylor expansion of $W[J]$ about $J_0$; this makes the $\lambda$ dependence manifest. Equating equal powers of $\lambda$ gives ($l = 0, 1, 2, \ldots$)

\[
\tilde{\Gamma}_l[\rho] = \tilde{W}_l[J_0] - \int d^3x J_l(x) \rho(x) + \sum_{k=1}^{l} \int d^3x \frac{\delta \tilde{W}_{l-k}[J_0]}{\delta J_0(x)} J_k(x)
\]

\[
+ \sum_{m=2}^{l} \frac{1}{m!} \sum_{k_1, \ldots, k_m \geq 1} \int d^3x_1 \cdots \int d^3x_m \frac{\delta^m \tilde{W}_{l-(k_1+\cdots+k_m)}[J_0]}{\delta J_0(x_1) \cdots \delta J_0(x_m)}
\]

\[
\times J_{k_1}(x_1) \cdots J_{k_m}(x_m). \quad (4.18)
\]

Since $\rho$ is independent of $\lambda$ [63], each $J_k[\rho]$ follows from each $\tilde{\Gamma}_k$:

\[
J_k(x) = -\frac{\delta \tilde{\Gamma}_k[\rho]}{\delta \rho(x)}. \quad (4.19)
\]

We reiterate that all of the $J_l$'s as defined here are functionals of $\rho$.

Now we start with the zeroth order expression,

\[
\tilde{\Gamma}_0[\rho] = \tilde{W}_0[J_0] - \int d^3x J_0(x) \rho(x), \quad (4.20)
\]
and take its functional derivative with respect to $\rho$:
\[
\frac{\delta \tilde{\Gamma}_0[\rho]}{\delta \rho(x)} = -J_0(x) = \int d^3y \frac{\delta \tilde{W}_0[J_0]}{\delta J_0(y)} \frac{\delta J_0(y)}{\delta \rho(x)} - J_0(x) - \int d^3y \rho(y) \frac{\delta J_0(y)}{\delta \rho(x)} .
\]  
(4.21)

Rearranging,
\[
\int d^3y \left( \frac{\delta \tilde{W}_0[J_0]}{\delta J_0(y)} - \rho(y) \right) \frac{\delta J_0(y)}{\delta \rho(x)} = 0 ,
\]  
(4.22)

which implies
\[
\rho(x) = \frac{\delta \tilde{W}_0[J_0]}{\delta J_0(x)} ,
\]  
(4.23)

since the strict convexity of $\tilde{\Gamma}_0[\rho]$ prohibits $\delta J_0(y)/\delta \rho(x)$ from having zero eigenvalues.

Note that Eq. (4.23) says that $J_0(x)$ is the source (or potential, see below) that generates the expectation value $\rho$ from the noninteracting system (that is, the system defined by $\lambda = 0$, which includes the external potential and $J_0(x)$ but no interactions). $J_0(x)$ is not an arbitrary function, but the particular one that has this property. The existence of a $J_0(x)$ with this property is the cornerstone of the Kohn-Sham formalism.

Equation (4.23) also implies that the second term in Eq. (4.18) cancels with the $k = l$ term of the first sum for all $l > 0$, and thus $\tilde{\Gamma}_l$ simplifies to
\[
\tilde{\Gamma}_l[\rho] = \tilde{W}_l[J_0] - \delta_{l,0} \int d^3x J_l(x) \rho(x) + \sum_{k=1}^{l-1} \int d^3x \frac{\delta \tilde{W}_{l-k}[J_0]}{\delta J_0(x)} J_k(x)
\]
\[+ \sum_{m=2}^{l} \frac{1}{m!} \sum_{k_1,\ldots,k_m \geq 1} \int d^3x_1 \cdots \int d^3x_m \frac{\delta^m \tilde{W}_{l-(k_1+\cdots+k_m)}[J_0]}{\delta J_0(x_1) \cdots \delta J_0(x_m)} \times J_{k_1}(x_1) \cdots J_{k_m}(x_m) .
\]  
(4.24)

These equations allow us to build the $\tilde{\Gamma}_l$'s recursively. Note that the $\tilde{W}_k$ functionals have the same diagrammatic expansion as in Fig. 3.3, but the fermion lines are evaluated with Kohn-Sham (KS) propagators (see below). For a given $l$, we only need $\tilde{W}_k$'s with $k$ less than or equal to $l$ and $J_k$'s with $k$ smaller than $l$ (which means lower-order $\tilde{\Gamma}_k$'s). We will illustrate the procedure by constructing the first few orders.
Since the lowest-order term in $\widetilde{W}[J]$ corresponds to the system without interactions between the fermions, we can write $\widetilde{W}_0[J]$ explicitly by introducing normalized single-particle orbitals that satisfy the equation

$$\left(-\frac{\nabla^2}{2M} + v(\mathbf{x}) - J_0(\mathbf{x})\right) \psi_k(\mathbf{x}) = \varepsilon_k \psi_k(\mathbf{x}) .$$

(4.25)

The index $k$ represents all quantum numbers except for the spin (we consider only spin-independent interactions here). $\widetilde{W}_0[J_0]$ is then (minus) the sum of the single-particle eigenvalues up to the Fermi energy $\varepsilon_F$ (which is equal to the chemical potential)

$$\widetilde{W}_0[J_0] = -\nu \sum_{\varepsilon_k < \varepsilon_F} \varepsilon_k .$$

(4.26)

In practice, $\varepsilon_F$ is determined by simply counting orbitals until the $A$ lowest are filled (accounting for the spin degeneracy $\nu$). Now, $\varepsilon_k$’s are functionals of $J_0$ through Eq. (4.25); and hence we find

$$\frac{\delta \varepsilon_k}{\delta J_0(\mathbf{y})} = \frac{\delta}{\delta J_0(\mathbf{y})} \int d^3 \mathbf{x} \psi_k^*(\mathbf{x}) \left(-\frac{\nabla^2}{2M} + v(\mathbf{x}) - J_0(\mathbf{x})\right) \psi_k(\mathbf{x})$$

$$= -\psi_k^*(\mathbf{y}) \psi_k(\mathbf{y}) + \int d^3 \mathbf{x} \frac{\delta \psi_k^*(\mathbf{x})}{\delta J_0(\mathbf{y})} \left(-\frac{\nabla^2}{2M} + v(\mathbf{x}) - J_0(\mathbf{x})\right) \psi_k(\mathbf{x})$$

$$+ \int d^3 \mathbf{x} \psi_k^*(\mathbf{x}) \left(-\frac{\nabla^2}{2M} + v(\mathbf{x}) - J_0(\mathbf{x})\right) \frac{\delta \psi_k(\mathbf{x})}{\delta J_0(\mathbf{y})}$$

$$= -\psi_k^*(\mathbf{y}) \psi_k(\mathbf{y}) + \varepsilon_k \int d^3 \mathbf{x} \left[ \frac{\delta \psi_k^*(\mathbf{x})}{\delta J_0(\mathbf{y})} \psi_k(\mathbf{x}) + \psi_k^*(\mathbf{x}) \frac{\delta \psi_k(\mathbf{x})}{\delta J_0(\mathbf{y})} \right]$$

$$= -\psi_k^*(\mathbf{y}) \psi_k(\mathbf{y}) + \varepsilon_k \frac{\delta}{\delta J_0(\mathbf{y})} \int d^3 \mathbf{x} \psi_k^*(\mathbf{x}) \psi_k(\mathbf{x})$$

$$= -\psi_k^*(\mathbf{y}) \psi_k(\mathbf{y}) .$$

(4.27)

Then Eqs. (4.23) and (4.26) show that the density may be written as

$$\rho(\mathbf{x}) = -\nu \sum_{k}^{\text{occ.}} \frac{\delta \varepsilon_k}{\delta J_0(\mathbf{x})} = \nu \sum_{k}^{\text{occ.}} \psi_k^*(\mathbf{x}) \psi_k(\mathbf{x}) ,$$

(4.28)
where the sum is over occupied (“occ.”) states. Equation (4.28) corresponds to the famous result of Kohn and Sham, which gives the exact ground state density in terms of the orbitals of a non-interacting system [4].

With the above results, the lowest order effective action is

$$\tilde{\Gamma}_0[\rho] = -\nu \sum_{k}^{\text{occ.}} \varepsilon_k - \int d^3x \ J_0(\mathbf{x}) \rho(\mathbf{x}) .$$

(4.29)

We can also use Eq. (4.25) to eliminate $\varepsilon_k$ from Eq. (4.29) so that it reads

$$\tilde{\Gamma}_0[\rho] = -T_s[\rho] - \int d^3x \ v(\mathbf{x}) \rho(\mathbf{x}) ,$$

(4.30)

where

$$T_s[\rho] = \nu \sum_{k} \int d^3x \ \psi_k^*(\mathbf{x}) \left( -\frac{\nabla^2}{2M} \right) \psi_k(\mathbf{x})$$

(4.31)

is the total kinetic energy of the KS non-interacting system. If $\tilde{\Gamma}_0[\rho]$ were given as an explicit functional of $\rho$, then $J_0[\rho]$ could be determined by taking a functional derivative according to Eq. (4.21). However, taking the functional derivative of the expression in Eq. (4.29) merely reproduces the result of Eq. (4.23). Instead, we follow Ref. [46] and determine $J_0$ from the interacting effective action, which we now construct.

From Eq. (4.24) we can find $\tilde{\Gamma}_1[\rho]$ since

$$\tilde{\Gamma}_1[\rho] = \tilde{W}_1[J_0[\rho]] .$$

(4.32)

For the dilute Fermi system, this is easily calculated. We first introduce the Green’s function of the KS non-interacting system, $G_{ks}^0(x, x')$, which satisfies

$$\left( i\partial_t + \frac{\nabla^2}{2M} - v(\mathbf{x}) + J_0(\mathbf{x}) \right) G_{ks}^0(\mathbf{x}t, \mathbf{x}'t') = \delta^3(\mathbf{x} - \mathbf{x}') \delta(t - t')$$

(4.33)
with finite density boundary conditions [110]. The KS Green’s function has the usual spectral decomposition in terms of the orbitals of Eq. (4.25):

\[ iG^0_{ks}(xt, x't') = \sum_k \psi_k(x_0) \psi_k(x'_0) e^{-i\epsilon_k(t-t')} [\theta(t-t') \theta(\varepsilon - \varepsilon_F) - \theta(t'-t) \theta(\varepsilon_F - \varepsilon_k)] . \]

(4.34)

(Note that Eq. (4.26) can be derived by evaluating \( W_0[J_0] \propto \text{Tr} \ln(G^0_{ks})^{-1} \).) The Feynman rules in position space follow conventionally from Eq. (3.13) [41, 109] and we have from Fig. 3.3(a) [with fermion lines representing \( iG^0_{ks} \)]

\[ \widetilde{W}_1[J_0] = \frac{1}{2} \nu (\nu - 1) C_0 \int d^3x \ G^0_{ks}(x, x^+) G^0_{ks}(x, x^+) , \]

(4.35)

where the right side is independent of \( t_x \) by Eq. (4.34). The Green’s function with equal arguments can be directly expressed in terms of the density,

\[ \rho(x) = -i\nu G^0_{ks}(x, x^+) . \]

(4.36)

Using this result and Eq. (4.32), we have

\[ \tilde{\Gamma}_1[\rho] = \frac{1}{2} \frac{(\nu - 1)}{\nu} C_0 \int d^3x \ \rho^2(x) . \]  

(4.37)

Since the dependence on \( \rho(x) \) is explicit in Eq. (4.37), we can directly take the functional derivative with respect to \( \rho \) to obtain

\[ J_1(x) = C_0 \frac{(\nu - 1)}{\nu} \rho(x) . \]

(4.38)

Direct functional derivatives with respect to \( \rho \) will not be possible at higher order. However, we can find functional derivatives with respect to \( J_0 \). An alternative path to \( J_1[\rho] \) from \( \tilde{\Gamma}_1[\rho] \) is

\[ J_1(x) = -\frac{\delta \tilde{\Gamma}_1[\rho]}{\delta \rho(x)} = -\int \delta \frac{\delta \tilde{\Gamma}_1[\rho]}{\delta J_0(y)} \frac{\delta J_0(y)}{\delta \rho(x)} = \int d^3y \ D^{-1}(x, y) \frac{\delta \tilde{W}_1[J_0]}{\delta J_0(y)} , \]

(4.39)
where we have used Eq. (4.32) and we have defined the inverse “density-density”
correlator

\[
D^{-1}(x, y) \equiv - \frac{\delta J_0(y)}{\delta \rho(x)} = - \left( \frac{\delta \rho(x)}{\delta J_0(y)} \right)^{-1} = - \left( \frac{\delta^2 W_0[J_0]}{\delta J_0(x) \delta J_0(y)} \right)^{-1}.
\]  
(4.40)

Eq. (4.23) has been used in the last step of the above equation. We can find an
expression for \( D^{-1} \) by taking the functional derivative with respect to \( J_0 \) in Eq. (4.35).
\( G_{ks}^0 \) is a functional of \( J_0 \), and to get its derivative with respect to \( J_0 \), we start from
the following relation.

\[
\int d^4x \, G_{ks}^0(x_1, x_3) G_{ks}^0(x_3, x_2) = \delta^4(x_1 - x_2).
\]
\[ \Rightarrow \frac{\delta}{\delta J_0(x)} \int d^4x \, G_{ks}^0(x_1, x_3) G_{ks}^0(x_3, x_2) = 0. \]

or,

\[
\int d^4x \, \left[ \frac{\delta G_{ks}^0(x_1, x_3)}{\delta J_0(x)} G_{ks}^0(x_3, x_2) + G_{ks}^0(x_1, x_3) \frac{\delta G_{ks}^0(x_3, x_2)}{\delta J_0(x)} \right] = 0.
\]  
(4.41)

Left multiplying the above by \( G_{ks}^0(x_4, x_1) \), and integrating over \( x_1 \), we get

\[
\int d^4x \, G_{ks}^0(x_4, x_1) \int d^4x \, \frac{\delta G_{ks}^0(x_1, x_3)}{\delta J_0(x)} G_{ks}^0(x_3, x_2)
\]
\[ = - \int d^4x \, G_{ks}^0(x_4, x_1) \int d^4x \, G_{ks}^0(x_1, x_3) \frac{\delta G_{ks}^0(x_3, x_2)}{\delta J_0(x)}
\]
\[ = - \int d^4x \, \delta^4(x_4 - x_3) \frac{\delta G_{ks}^0(x_3, x_2)}{\delta J_0(x)}
\]
\[ = \frac{\delta G_{ks}^0(x_4, x_2)}{\delta J_0(x)}. \]  
(4.42)

Now, \( G_{ks}^{-1}(x_1, x_3) \) is given by (Ref. Eq. (B.78))

\[
G_{ks}^{-1}(x_1, x_3) = \left( i \partial_i - \hat{H}_x \right) \delta^4(x_1 - x_3).
\]  
(4.43)

where \( \hat{H}_x = - \nabla_x^2/2M + v(x) - J_0(x) \). So we get

\[
\frac{\delta G_{ks}^0(x_1, x_3)}{\delta J_0(x)} = \delta^3(x - x_1) \delta^4(x_1 - x_3). \]  
(4.44)
Using this, we finally get

\[
\frac{\delta G_{ks}^0(x_4,x_2)}{\delta J_0(x)} = - \int G_{ks}^0(x_4,x)G_{ks}^0(x,x_2) \, dt_x .
\]  

(4.45)

Using Eq. (4.45), the derivative of \( \widetilde{W}_1 \) becomes

\[
\frac{\delta \widetilde{W}_1[J]}{\delta J_0(x)} = -\nu(\nu - 1) \, C_0 \int d^3y \int d^3x \, G_{ks}^0(y,x)G_{ks}^0(x,y+)G_{ks}^0(y,y+)
\]

\[= -i(\nu - 1) \, C_0 \int d^3y \int d^3x \, G_{ks}^0(y,x)G_{ks}^0(x,y+) \rho(y) .
\]  

(4.46)

Comparing Eq. (4.46) to Eq. (4.39) we find

\[
D^{-1}(x,y) = \frac{i}{\nu} \left[ \int dt_y \, G_{ks}^0(x,y)G_{ks}^0(y,x+) \right]^{-1} .
\]  

(4.47)

This correlator will appear in all higher-order contributions. One can also derive the above expression in a more direct manner. Consider

\[
\frac{\delta \rho(x)}{\delta J_0(y)} = -i\nu \, \frac{\delta G_{ks}^0(x,x+)}{\delta J_0(y)} = -i\nu \int dt_y \, G_{ks}^0(x,y)G_{ks}^0(y,x+).
\]

(4.48)

Inverting, we get the expression for the density-density correlator. Now let us get back to our alternate derivation of \( J_1(x) \) using Eq. (4.39).

\[
J_1(x) = \int d^3y \, D^{-1}(x,y) \frac{\delta \widetilde{W}_1[J_0]}{\delta J_0(y)} = -i C_0 (\nu - 1) \int d^3y \left[ \int dt_y \, G_{ks}^0(x,y)G_{ks}^0(y,x) \right]^{-1}
\]

\[\times \int d^4u \int dt_y \, G_{ks}^0(w,y)G_{ks}^0(y,w+)G_{ks}^0(w,w+)
\]

\[= -i C_0 (\nu - 1) \, G_{ks}(x,x+)
\]

\[= C_0 \frac{(\nu - 1)}{\nu} \rho(x) .
\]  

(4.49)

This is exactly what we got previously.
\[ \Gamma_{\text{int}} = \quad + \quad + \quad + \quad \cdots \]

\[ = \quad + \quad + \cdots \]

Figure 4.1: Hugenholtz diagrams for the LO and NLO contributions to the Kohn-Sham interaction effective action \( \Gamma_{\text{int}} \). The cancellation of the last two diagrams on the first line is given by Eq. (4.52).

Having determined \( J_1[\rho] \) we can find \( \Gamma_2[\rho] \) from Eq. (4.24),

\[
\tilde{\Gamma}_2[\rho] = \widetilde{W}_2[J_0] + \int d^3x \frac{\delta \tilde{W}_1[J_0]}{\delta J_0(x)} J_1(x) + \frac{1}{2} \int d^3x \, d^3y \frac{\delta^2 \tilde{W}_0[J_0]}{\delta J_0(x) \delta J_0(y)} J_1(x) J_1(y)
\]

\[ = \widetilde{W}_2[J_0] + \frac{1}{2} \int d^3x \, d^3y \frac{\delta \tilde{W}_1[J_0]}{\delta J_0(x)} D^{-1}(x, y) \frac{\delta \tilde{W}_1[J_0]}{\delta J_0(y)} . \tag{4.50} \]

\( W_2[J_0] \) is calculated from the graphs Figs. 3.3(b) and (c):

\[
W_2[J_0] = i\nu(\nu - 1) \frac{C_0^2}{4} \int d^4x \, d^4y \, G_{ks}^0(x, y) G_{ks}^0(x, y) G_{ks}^0(y, x) G_{ks}^0(y, x) \\
- i\nu(\nu - 1)^2 \frac{C_0^2}{2} \int d^4x \, d^4y \, G_{ks}^0(x, x^+) G_{ks}^0(x, y) G_{ks}^0(y, x) G_{ks}^0(y, y^+) . \tag{4.51} \]

By using Eqs. (4.46) and (4.47), we find that the second term in the expression for \( \tilde{\Gamma}_2 \) exactly cancels the second term in \( \widetilde{W}_2 \). The second term contributing to \( \Gamma_2 \) is

\[
i\nu(\nu - 1)^2 \frac{C_0^2}{2} \int d^4x \, d^4y \, G_{ks}^0(x, x^+) G_{ks}^0(x, y) G_{ks}^0(y, x) G_{ks}^0(y, y^+) , \tag{4.52} \]

which is the negative of the second term in Eq. (4.51). This cancellation is shown in Fig. 4.1, where \( D^{-1} \) is represented by a double line. Thus, Eq. (4.50) leads to

\[
\Gamma_2[\rho] = i\nu(\nu - 1) \frac{C_0^2}{4} \int d^4x \, d^4y \, G_{ks}^0(x, y) G_{ks}^0(x, y) G_{ks}^0(y, x) G_{ks}^0(y, x) . \tag{4.53} \]

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Figure 4.2: General cancellation of the inverse correlator $D^{-1}$ for zero-range interactions with no derivatives.

The second term in $W_2$ corresponds to the “anomalous” graph (c) in Fig. 3.3. This graph vanishes identically in the uniform system at zero temperature. However, it does not vanish at finite temperature or in a finite system (at any temperature). Rather, the cancellation exhibited above is analogous to the Kohn-Luttinger-Ward theorem mentioned earlier. Similar cancellations, of the type illustrated diagrammatically in Fig. 4.2, completely eliminate contributions of $D^{-1}$ to the effective action up to $N^3\text{LO}$ in the EFT expansion for short-range forces. This complete cancellation does not occur for long-range forces, or if the zero-range delta functions at the $C_0$ vertices are regulated by a cutoff rather than by dimensional regularization.

At NNLO, $\tilde{W}_3$ is given by the sum of Hugenholtz graphs in Fig. 3.3(d) through (j). Similar cancellations [42] precisely subtract the anomalous diagrams in $\tilde{W}_3$, leaving only Fig. 3.3(g) through (j).

All higher orders in $\tilde{\Gamma}[\rho,\lambda]$ are determined in a similar manner. Direct calculation becomes cumbersome, but one can formulate Feynman rules for $\tilde{\Gamma}$, which dictate how to make appropriate insertions of $D^{-1}$; these are given in Refs. [45, 64, 63, 46]. It is important to note that the Kohn-Sham potential $J_0$ completely determines each order in the expansion of $\tilde{\Gamma}$.

The cancellations exhibited here at low orders are expected from a comparison of the DFT/EFT expansion to perturbation theory. In perturbation theory for the
confined system, the energy is calculated by evaluating the diagrams in Fig. 3.3 using the noninteracting propagator in the presence of the external potential for the fermion lines. Using the self-consistent $G_{ks}$ instead sums an infinite class of higher-order diagrams at each order. The cancellation of anomalous diagrams from $\tilde{\Gamma}$ corresponds to the removal of contributions already included through self-consistency (e.g., tadpoles). Although the nonperturbative contributions for the dilute, natural system are not required by power counting, the self-consistent calculation of the energy and density together is actually easier in practice than the purely perturbative calculation.

The appearance of the inverse density-density correlator $D^{-1}$ can be understood by comparison to the effective actions for local fields and non-local composite fields. In the former case, the Legendre transformation removes one-particle intermediate states (leaving only one-particle-irreducible diagrams), while in the latter case, the Legendre transformation removes two-particle intermediate states (leaving two-particle-irreducible diagrams). Thus we conclude that the role of $D^{-1}$ is to remove intermediate states created by $\psi^{\dagger}\psi$. The difference here is that we cannot write a closed-form expression for the effective action, which is possible in the other cases. However, we have seen that for short-range interactions, the extra diagrams at low orders cancel against anomalous diagrams, which is a great simplification.

To find an expression for $J_0$, we apply the variational principle satisfied by $\tilde{\Gamma}[\rho, \lambda]$ to its expansion:

$$
\left. \frac{\delta \tilde{\Gamma}[\rho, \lambda]}{\delta \rho(\mathbf{x})} \right|_{\rho = \rho_{gs}} = 0 = \left. \frac{\delta (\tilde{\Gamma}_0[\rho] + \tilde{\Gamma}_{\text{int}}[\rho])}{\delta \rho(\mathbf{x})} \right|_{\rho = \rho_{gs}} = -J_0(\mathbf{x})|_{\rho_{gs}} + \left. \frac{\delta \tilde{\Gamma}_{\text{int}}[\rho]}{\delta \rho(\mathbf{x})} \right|_{\rho = \rho_{gs}}, \quad (4.54)
$$
$J_0(\mathbf{x}) = \begin{array}{c} \text{interaction terms} \end{array} + (\text{perms.}) + \cdots$

$= \begin{array}{c} \text{interaction terms} \end{array} + (\text{perms.}) + \cdots$

Figure 4.3: Contributions to the Kohn-Sham potential $J_0$ through NLO [Eq. (4.56)].

where the interaction effective action is

$$\tilde{\Gamma}_{\text{int}}[\rho] \equiv \sum_{k=1} \tilde{\Gamma}_k[\rho] , \quad (4.55)$$

or

$$J_0(\mathbf{x}) \bigg|_{\rho=\rho_{\text{gs}}} = \frac{\delta \tilde{\Gamma}_{\text{int}}[\rho]}{\delta \rho(\mathbf{x})} \bigg|_{\rho=\rho_{\text{gs}}} = - \int d^3y \: D^{-1}(\mathbf{x},\mathbf{y}) \: \frac{\delta \tilde{\Gamma}_{\text{int}}[\rho]}{\delta J_0(\mathbf{y})} \bigg|_{\rho=\rho_{\text{gs}}} . \quad (4.56)$$

We stress that these relations hold only when we are solving for the Kohn-Sham potential corresponding to the ground-state density $\rho_{\text{gs}}(\mathbf{x})$.

The second equality in Eq. (4.56), which is shown diagrammatically through NLO in Fig. 4.3, is the key to the general Kohn-Sham self-consistent procedure:

1. Choose an approximation for $\tilde{\Gamma}_{\text{int}}[\rho]$ by truncating the expansion in $\lambda$ at some order.

2. Make a reasonable initial guess for the Kohn-Sham potential $J_0(\mathbf{x})$.

3. Calculate $\tilde{\Gamma}_{\text{int}}[\rho]$ starting from $J_0$.

4. Use Eq. (4.56) to determine a new Kohn-Sham potential $J_0(\mathbf{x})$.  

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5. Repeat the last two steps until self-consistency is reached (i.e., until some measure of the change in \( J_0 \) is less than a given tolerance).

In the next section, we will apply an LDA to \( \tilde{\Gamma}_{\text{int}} \), which means that it will given explicitly as a functional of \( \rho \). In this case, the second equality in Eq. (4.56) is superfluous.

To this point we have neglected to mention that expressions such as \( \tilde{\Gamma}_2 \) in Eq. (4.53) are divergent. For a uniform system, \( J_0 \) is constant. In this case, \( \tilde{W}_2 \) and subsequently \( \tilde{\Gamma}_2 \) are renormalized by dimensional regularization and minimal subtraction as in Ref. [41]. In a finite system, with \( J_0 \) a function of \( \mathbf{x} \), the ultraviolet linear divergence in Eq. (4.53) is renormalized by the same counterterm [103], but it is computationally awkward to renormalize in the finite system. By using a derivative expansion, we can perform all renormalizations in the uniform system. This will be carried out explicitly in future work. With the LDA truncation applied below, we can simply use the renormalized expressions for the energy density from Ref. [41] to calculate the renormalized Kohn-Sham potential and energy functional.

### 4.3 Results for Dilute Fermi System in a Trap

In this section, we present representative numerical results for the dilute Fermi system when confined in a harmonic oscillator trap. Our principal goal here is to illustrate the nature of the convergence of the EFT in a finite system both qualitatively and quantitatively. We consider effective range parameters corresponding to both attractive and repulsive underlying interactions (but we do not allow for pairing). To emphasize the difference between Kohn-Sham (KS) and Thomas-Fermi (TF)
approaches and since we are ultimately interested in nuclear systems, we consider relatively small numbers of trapped fermions. Typical experiments with trapped atoms use $10^5$–$10^6$ atoms [49]; as noted below, for such large systems the differences between KS and TF get washed out.

### 4.3.1 The Local Density Approximation

To carry out the Kohn-Sham self-consistent procedure, we need to evaluate the expressions in the expansion of $\tilde{\Gamma} [\rho]$, so that we can use Eq. (4.56) to find $J_0(x)$. In applications to Coulomb systems, the Kohn-Sham energy functional is conventionally written as

$$ E[\rho] = T_s[\rho] + \int d^3x v(x) \rho(x) + E_H[\rho] + E_{xc}[\rho] \, , $$

(4.57)

where $T_s$ is given in Eq. (4.31), $E_H$ is the Hartree energy and $E_{xc}[\rho]$ is known as the exchange-correlation energy. The Hartree energy is singled out because it can be explicitly written in terms of the density. When we have contact interactions only, the Fock term has the same dependence on the density as the Hartree term, and so we can also include it explicitly and replace $E_H$ by $E_{HF}$, redefining $E_{xc}$ as the pure correlation energy $E_c$.

This decomposition corresponds to writing the effective action as [46]

$$ \tilde{\Gamma} [\rho] = \tilde{\Gamma}_0[\rho] + \tilde{\Gamma}_1[\rho] + \sum_{i=2}^{\infty} \tilde{\Gamma}_i[\rho] \, , $$

(4.58)

up to an overall minus sign. The expression for $\tilde{\Gamma}_0$ given in Eq. (4.30) shows that it has the same form as the first two terms in the energy functional in Eq. (4.57). In general, the explicit functional dependence of $T_s$ on the density is unknown since it enters implicitly through the orbitals. In practice it is easiest to calculate the first
two terms by writing them as in Eq. (4.29):

\[
\tilde{\Gamma}_0[\rho] = -\nu \sum_k \varepsilon_k - \int d^3x \; J_0(x) \; \rho(x) .
\] (4.59)

The other terms in \( \tilde{\Gamma} \) may be written using the Green’s function for the KS non-interacting system as shown in Sec. 4.2. The KS Green’s functions are explicit functionals of \( J_0 \) not \( \rho \), however, and therefore almost all of \( \tilde{\Gamma} \) is not given as an explicit functional of the density; the general exception is the Hartree term and here the Fock term since we have only contact interactions. Furthermore, the actual expressions are quite difficult to evaluate in a finite system.

The results from the calculation of the energy density in the case of a uniform system [41] is the starting point of the DFT calculation of the energy density of a dilute Fermi gas confined by an external harmonic potential with short-range, spin-independent interactions. In extending these results to a finite system, the simplest approximation that can be invoked is the local density approximation (LDA). The LDA may be considered the lowest-order term in a derivative expansion of the energy functional. The idea is to expand around the uniform system where the energy functional can be written as an explicit function of \( \rho \). The LO diagram [Fig. 3.3(a)] is the Hartree-Fock contribution, which is purely local. Thus, it is an exact evaluation and Eq. (4.37) can be used directly for the energy contribution:

\[
E_{\text{HF}}[\rho(x)] = \int d^3x \; \mathcal{E}_1[\rho(x)] = \frac{1}{2} \frac{(\nu - 1)}{\nu} \; C_0 \int d^3x \; |\rho(x)|^2 .
\] (4.60)

The contributions to the energy from NLO and NNLO diagrams are computed in LDA by simply integrating the corresponding uniform energy densities evaluated at the local density. The correlation energy, to third order (NNLO) in the EFT expansion
becomes
\[
E_c^{\text{LDA}}[\rho(\mathbf{x})] = \int d^3x \{ \mathcal{E}_2(\rho_0) + \mathcal{E}_3(\rho_0) \} \big|_{\rho_0 \rightarrow \rho(\mathbf{x})} \\
= b_1 \frac{a^2_s}{2M} \int d^3x [\rho(\mathbf{x})]^{7/3} \\
+ (b_2 a^2_s r_s + b_3 a^3_p + b_4 a^3_s) \frac{1}{2M} \int d^3x [\rho(\mathbf{x})]^{8/3}, \quad (4.61)
\]
where the dimensionless \( b_k \) are
\[
b_1 &= \frac{4}{35 \pi^2} (\nu - 1) \left( \frac{6 \pi^2}{\nu} \right)^{4/3} (11 - 2 \ln 2), \\
b_2 &= \frac{1}{10 \pi} (\nu - 1) \left( \frac{6 \pi^2}{\nu} \right)^{5/3}, \\
b_3 &= \frac{1}{5 \pi} (\nu + 1) \left( \frac{6 \pi^2}{\nu} \right)^{5/3}, \\
b_4 &= \left( \frac{6 \pi^2}{\nu} \right)^{5/3} \left( 0.0755 (\nu - 1) + 0.0574 (\nu - 1)(\nu - 3) \right). \quad (4.62)
\]
\( \mathcal{E}_2 \) and \( \mathcal{E}_3 \) are the second and third order EFT energy density of the uniform system respectively.

### 4.3.2 Scaling Properties

In an EFT, the two-body short-range interaction potential is basically a Delta-function. The terms in the Eq. (4.61) satisfy the required scaling properties corresponding to this potential. One could have written down these terms without carrying out an explicit calculation. Let us see how.

The Hartree piece \( E_H[\rho] \) scales in the following way for such a potential :
\[
E_H[\rho] = \gamma^3 E_H[\rho]. \quad (4.63)
\]

Since the exchange functional scales the same way as the Hartree piece [Fig. 3.3(a)] that represents the LO diagram, we expect from Eq. (2.39) that \( (a = 3 \text{ here}) \)
\[
\mathcal{E}_1(\rho(\mathbf{x})) \sim [\rho(\mathbf{x})]^2, \quad (4.64)
\]
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which conforms with the fact that this LO term is of order \((k_F)^6\). The next term has to be of order \((k_F)^7\), since our expansion parameter is \(k_F a_s\). So we expect \(E_2(\rho(\mathbf{x})) \sim [\rho(\mathbf{x})]^{7/3}\). Now we back-calculate and find the appropriate scaling relation for this piece. Solving for \(a\) in the equation \(1 + a/3 = 7/3\), we get \(E_2[\rho] = \gamma^4 E_2[\rho]\). Clearly, we can generalise this scaling relation for the energy density functional of order \((k_F)^{5+k}\) as

\[
E_k[\rho] = \gamma^{k+2} E_k[\rho]. \tag{4.65}
\]

The kinetic energy density \((E_0)\) corresponds to \(k = 0\) term and scales as \(\gamma^2\) as expected.

With the knowledge of how the energy density scales at each order, we can, as the next step, incorporate gradient expansion corrections in the framework consistent with the scaling relation given by Eq. (4.65).

### 4.3.3 Expression for Energy

In order to solve for the orbitals in Eq. (4.25) and to calculate the energy we need the expression for \(J_0(\mathbf{x})\). In the LDA, this is simple since

\[
J_0(\mathbf{x}) = \frac{\delta}{\delta \rho(\mathbf{x})} \left( \tilde{\Gamma}_1[\rho] + \sum_{i=2}^{\infty} \tilde{\Gamma}_k[\rho] \right) = -\frac{\delta}{\delta \rho(\mathbf{x})} \left( E_{HF}[\rho] + E_{xc}[\rho] \right). \tag{4.66}
\]

To NNLO we find:

\[
J_0(\mathbf{x}) = -\left(\frac{\nu - 1}{\nu}\right) \frac{4\pi a_s}{M} \rho(\mathbf{x}) - \frac{7}{3} b_1 \frac{a_s^2}{2M} [\rho(\mathbf{x})]^{4/3} + \frac{8}{3} \left( b_2 a_s^2 r_s + b_3 a_p^3 + b_4 a_s^3 \right) \frac{1}{2M} [\rho(\mathbf{x})]^{5/3}. \tag{4.67}
\]

A convenient expression for the total binding energy (through NNLO) follows by substituting for \(J_0(\mathbf{x})\) and combining terms:

\[
E[\rho(\mathbf{x})] = \nu \sum_{k=0}^{\infty} \varepsilon_k - \frac{1}{2} \left(\frac{\nu - 1}{\nu}\right) \frac{4\pi a_s}{M} \int d^3\mathbf{x} [\rho(\mathbf{x})]^2 - \frac{4}{3} b_1 \frac{a_s^2}{2M} \int d^3\mathbf{x} [\rho(\mathbf{x})]^{7/3}
\]

\[
- \frac{5}{3} \left( b_2 a_s^2 r_s + b_3 a_p^3 + b_4 a_s^3 \right) \frac{1}{2M} \int d^3\mathbf{x} [\rho(\mathbf{x})]^{8/3}. \tag{4.68}
\]
In the numerical calculations given below, the noninteracting case \( C_0 = 0 \) uses \( J_0(x) \equiv 0 \) and the first term in Eq. (4.68), LO uses the first term in Eq. (4.67) and the first two terms in Eq. (4.68), and so on for NLO and NNLO.

### 4.3.4 Kohn-Sham Self-Consistent Procedure

Here we describe the numerical procedure used to find the Kohn-Sham orbitals. We assume closed shells, so the density and potentials are functions only of the radial coordinate \( r \equiv |x| \). The Kohn-Sham iteration procedure is as follows:

1. Start by solving the Schrödinger equation with the external potential profile \( v(r) \) for the lowest \( A \) states (including degeneracies) to find a set of orbitals and Kohn-Sham eigenvalues \( \{\psi_k, \varepsilon_k\} \).

2. Compute the density from the occupied orbitals:

\[
\rho(r) = \nu \sum_k |\psi_k(x)|^2, \quad (4.69)
\]

All other ground-state observables are functionals of \( \{\psi_k, \varepsilon_k\} \).

3. Find \( J_0(r) \) using Eqs. (4.67) at the chosen level of approximation (e.g., NLO). Evaluate the local single-particle potential

\[
v_s[\rho(r)] \equiv v_s(r) \equiv v(r) - J_0(r) \quad (4.70)
\]

4. Solve the Schrödinger equation for the lowest \( A \) states (including degeneracies), to find a set of orbitals and Kohn-Sham eigenvalues \( \{\psi_k, \varepsilon_k\} \):

\[
[-\frac{\nabla^2}{2M} + v_s(r)] \psi_k(x) = \varepsilon_k \psi_k(x). \quad (4.71)
\]
5. Repeat steps 2–4. until changes are acceptably small ("self-consistency"). In practice, the changes in the density are "damped" by using a weighted average of the densities from the \((n - 1)\)th and \(n\)th iterations:
\[
\rho(r) = \beta \rho_{n-1}(r) + (1 - \beta) \rho_n(r),
\]
with \(0 < \beta \leq 1\).

This procedure has been implemented for dilute fermions in a trap using computer codes written both in C and in Mathematica. Two methods for carrying out step 4. were tested. The Kohn-Sham single-particle equations are solved in one approach by direct integration of the differential equations via the Numerov method [65] and in the other approach by diagonalization of the single-particle Hamiltonian in a truncated basis of unperturbed harmonic oscillator wavefunctions. The same results are obtained to high accuracy. For closed shells, either method is efficient and easy to code. The matrix diagonalization approach is described in the next section.

### 4.3.5 Fermions in a Harmonic Trap

The interaction through NNLO is specified in terms of the three effective range parameters \(a_s, r_s,\) and \(a_p\). For the numerical calculations presented here, we consider two cases in the dilute limit, \(a_s \ll \{r_s, a_p\} \approx 0\) with both signs for \(a_s\), and hard sphere repulsion with radius \(R\), in which case \(a_s = a_p = R\) and \(r_s = 2R/3\).

Lengths are measured in units of the oscillator parameter \(b \equiv \sqrt{\hbar/m_\omega}\), masses in terms of the fermion mass \(M\), and \(\hbar = 1\). In these units, \(h\omega\) for the oscillator is unity and the Fermi energy of a non-interacting gas with filled shells up to \(N_F\) is \(E_F = (N_F + 3/2)\). The total number of fermions \(A\) is related to \(N_F\) by
\[
A = \frac{\nu}{6} (N_F + 1)(N_F + 2)(N_F + 3).
\]
Since we have only considered spin-independent interactions, our results are independent of whether the spin degeneracy \( \nu \) actually originates from spin, isospin, or some flavor index.

With interactions included, single-particle states are labeled by a radial quantum number \( n \), an orbital angular momentum \( \ell \) with \( z \)-component \( m_\ell \), and the spin projection. The radial functions depend only on \( n \) and \( \ell \), so the degeneracy of each level is \( \nu \times (2\ell + 1) \). Excluding spin, the solutions are of the form

\[
\psi_{n\ell m}(\mathbf{x}) = \frac{u_{n\ell}(r)}{r} Y_{\ell m}(\Omega),
\]

where the radial function \( u_{n\ell}(r) \) satisfies

\[
\left[ -\frac{1}{2} \nabla^2 + v_s(r) + \frac{\ell(\ell + 1)}{2r^2} \right] u_{n\ell}(r) = \varepsilon_{n\ell} u_{n\ell}(r).
\]

The \( u_{n\ell} \)'s are normalized according to

\[
\int_0^\infty |u_{n\ell}(r)|^2 dr = 1.
\]

Thus the density is given by:

\[
\rho(\mathbf{x}) = \nu \sum_{n\ell m} |\psi_{n\ell m}(\mathbf{x})|^2
\]

\[
= \nu \sum_{n\ell} \frac{|u_{n\ell}(r)|^2}{r^2} \sum_{m=-\ell}^{\ell} |Y_{\ell m}(\Omega)|^2
\]

\[
= \nu \sum_{n\ell} (2\ell + 1) \frac{|u_{n\ell}(r)|^2}{4\pi r^2}.
\]

We have used a special case of the “Addition Theorem” [113] in the above derivation. The interactions are sufficiently weak that the occupied states are in one-to-one correspondence with those occupied in the non-interacting harmonic oscillator potential.

One of the ways to solve the Kohn-Sham single-particle equation was by diagonalizing the single-particle Hamiltonian in a truncated basis of unperturbed harmonic
oscillator wavefunctions, denoted by $v_{nt}(r)$. The highest filled shell number ($N_F$) serves as the input along with other parameters such as effective-range values and spin-isospin multiplicity. For a given shell number $N$ and a given value of $\ell$, the number of states is easily determined by the relation

$$\begin{align*}
n &= \frac{1}{2}(N - \ell) + 1,
\end{align*}$$

where $n$ denotes the principal quantum number. The dimension of the basis ($D$) is required to be at least equal to the number of states of the outermost shell. In the outermost loop, the value of $\ell$ is varied from zero to $N_F$ in steps of unity. For each value of $\ell$, the Hamiltonian matrix $\langle v_{d\ell} | \hat{H} | v_{d'\ell'} \rangle \equiv H_{d'd'}^{\ell\ell'}$ is computed ($d, d'$ range from one to $D$). For this $\ell$ value, the different possible states are easily found. An efficient way to find the different $(N, n)$ combinations for a given $\ell$ is to loop through the shell number variable starting from one up to $N_F$, and determining the corresponding $n$ using Eq. (4.78). Diagonalizing the Hamiltonian matrix gives the eigenvalues of these states. The corresponding eigenfunctions are easily constructed as a linear combination of the basis functions weighted with the corresponding eigenvector elements. This is the basic methodology. Other quantities like the density, energy and Kohn-Sham potentials are calculated in the whole process.

In computing the matrix elements, one can reduce the computing time by noting that the Hamiltonian is symmetric, and also by getting rid of the kinetic second-derivative term and the centrifugal term using the fact that we know the eigenvalue spectrum for a simple harmonic oscillator potential.

$$\begin{align*}
\langle v_{n't} \rangle - \frac{1}{2} \frac{d^2}{dr^2} + \frac{\ell(\ell + 1)}{2r^2} |v_{nt}\rangle &= (N + \frac{3}{2}) \delta_{nn'} - \langle v_{n't} \rangle \frac{r^2}{2} |v_{nt}\rangle.
\end{align*}$$

(4.79)

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\[
\begin{array}{cccccc}
\nu & N_F & A & a_s & E/A & \langle k_F \rangle & \sqrt{\langle r^2 \rangle} & \text{approximation} \\
2 & 7 & 240 & - & 6.75 & 3.27 & 2.60 & C_0 = 0 \text{ exact} \\
2 & 7 & 240 & -0.16 & 5.98 & 3.61 & 2.35 & \text{KS LO} \\
2 & 7 & 240 & -0.16 & 6.25 & 3.44 & 2.47 & \text{KS NLO (LDA)} \\
2 & 7 & 240 & -0.16 & 6.23 & 3.46 & 2.46 & \text{KS NNLO (LDA)} \\
2 & 7 & 240 & 0.16 & 7.36 & 3.08 & 2.76 & \text{KS LO} \\
2 & 7 & 240 & 0.16 & 7.51 & 3.03 & 2.81 & \text{KS NLO (LDA)} \\
2 & 7 & 240 & 0.16 & 7.52 & 3.02 & 2.82 & \text{KS NNLO (LDA)} \\
2 & 7 & 240 & 0.16 & 7.66 & 2.97 & 2.87 & \text{KS NNLO (LDA)} \\
4 & 4 & 140 & - & 4.50 & 2.66 & 2.12 & C_0 = 0 \text{ exact} \\
4 & 4 & 140 & -0.10 & 3.62 & 3.27 & 1.72 & \text{KS LO} \\
4 & 4 & 140 & -0.10 & 3.83 & 3.01 & 1.87 & \text{KS NLO (LDA)} \\
4 & 4 & 140 & -0.10 & 3.75 & 3.12 & 1.81 & \text{KS NNLO (LDA)} \\
4 & 4 & 140 & 0.10 & 5.09 & 2.44 & 2.31 & \text{KS LO} \\
4 & 4 & 140 & 0.10 & 5.16 & 2.41 & 2.34 & \text{KS NLO (LDA)} \\
4 & 4 & 140 & 0.10 & 5.18 & 2.40 & 2.35 & \text{KS NNLO (LDA)} \\
4 & 4 & 140 & 0.10 & 5.20 & 2.39 & 2.36 & \text{KS NNLO (LDA)} \\
\end{array}
\]

Table 4.1: Energies per particle, averages of the local Fermi momentum \( k_F \), and rms radii for a variety of different parameters and particle numbers for a dilute Fermi gas in a harmonic trap. See the text for a description of units. The effective range and p-wave scattering length are set to zero, \( r_s = a_p = 0 \), except for the two lines where \( a_s \) has an asterisk, in which case they are given by \( a_s = a_p = 3r_s/2 \).

The Kohn-Sham self-consistent procedure is carried out in this code until a prescribed tolerance is reached.

To check our numerical calculations, we first compared to density distributions at zero temperature from Ref. [61], which used a contact interaction with strength corresponding to \( a_s = -0.16 \) in our units. In that work, non-interacting and mean-field (Hartree-Fock) results for the normal state (for possible comparison to superfluid solutions) were presented for systems with 240 and 330 atoms. The corresponding densities in our EFT expansion are the curves labeled “\( C_0 = 0 \) exact” and “Kohn-Sham LO” in Figs. 4.4 and 4.8. Note that spin-multiplicity \( \nu \) is denoted as \( g \) in the
**Figure 4.4:** Kohn-Sham approximations (see text) for a dilute gas of fermions in a harmonic trap with degeneracy \( \nu = 2 \) filled up to \( N_F = 7 \), which implies there are 240 particles in the trap. The scattering length is \( a_s = -0.16 \) and the other effective range parameters are set to zero.

**Figure 4.5:** Kohn-Sham approximations (see text) for a dilute gas of fermions in a harmonic trap with degeneracy \( \nu = 2 \) filled up to \( N_F = 7 \), which implies there are 240 particles in the trap. The scattering length is \( a_s = +0.16 \) and the other effective range parameters are set to zero.
Figure 4.6: Kohn-Sham approximations (see text) for a dilute gas of fermions in a harmonic trap with degeneracy $\nu = 4$ filled up to $N_F = 4$, which implies there are 140 particles in the trap. The scattering length is $a_s = -0.10$ and the other effective range parameters are set to zero.

Figure 4.7: Kohn-Sham approximations (see text) for a dilute gas of fermions in a harmonic trap with degeneracy $\nu = 4$ filled up to $N_F = 4$, which implies there are 140 particles in the trap. The scattering length is $a_s = +0.10$ and the other effective range parameters are set to zero.
Figure 4.8: Kohn-Sham approximations (see text) for a dilute gas of fermions in a harmonic trap with degeneracy $\nu = 2$ filled up to $N_F = 8$, which implies there are 330 particles in the trap. The scattering length is $a_s = -0.16$ and the other effective range parameters are set to zero.

Figure 4.9: Kohn-Sham approximations (see text) for a dilute gas of fermions in a harmonic trap with degeneracy $\nu = 2$ filled up to $N_F = 8$, which implies there are 330 particles in the trap. The scattering length is $a_s = +0.16$ and the other effective range parameters are set to zero.
Figure 4.10: Kohn-Sham approximations (see text) for a dilute gas of fermions in a harmonic trap with degeneracy $\nu = 2$ filled up to $N_F = 7$, which implies there are 240 particles in the trap. The scattering lengths are $a_s = a_p = 0.16$ and the effective range is $r_s = 2a_s/3$ (hard sphere repulsion).

Figure 4.11: Kohn-Sham approximations (see text) for a dilute gas of fermions in a harmonic trap with degeneracy $\nu = 4$ filled up to $N_F = 4$, which implies there are 140 particles in the trap. The scattering lengths are $a_s = a_p = 0.10$ and the effective range is $r_s = 2a_s/3$ (hard sphere repulsion).
NNLO Convergence with Basis Dimension

\[ A = 240, \ g = 2, \ a_s = 0.16, \ N_F = 7 \]

Area under curves:
- \( D_{10} : D_{20} \rightarrow 4.67406e-04 \)
- \( D_{20} : D_{30} \rightarrow 7.05414e-05 \)
- \( D_{30} : D_{40} \rightarrow 0.0 \)

Figure 4.12: Convergence of the second moment of the density for different basis dimensions.
plots. We also show densities for the same systems but with $a_s = +0.16$ in Figs. 4.5 and 4.9. As one might expect, the attractive interaction pulls the density in while the repulsive interaction pushes it out relative to the non-interacting density. Values for the energy per particle, the average Fermi momentum, and the rms radius for each calculation are given in Table 4.1. Averages are defined as

$$\langle f(x) \rangle \equiv \frac{1}{A} \int d^3 x \ f(x) \ \rho(x) \ .$$  \hspace{1cm} (4.80)

In each of these figures, the other effective range parameters, $r_s$ and $a_p$, are set to zero. We have also shown results for a representative system with spin degeneracy $\nu = 4$ with weaker attractive ($a_s = -0.10$) and repulsive ($a_s = +0.10$) interactions in Figs. 4.6 and 4.7. To illustrate the impact of $r_s$ and $a_p$ on the NNLO results, we have also included two calculations where the underlying interaction is hard-sphere repulsion with $R = 0.16$ ($\nu = 2$) and $R = 0.10$ ($\nu = 4$) in Figs. 4.10 and 4.11.

From Figs. 4.4 and 4.5, we see what seems to be good convergence of the density by NNLO. Note that the LO results are not well converged in either case. From Table 4.1, we find that the average Fermi momentum

$$\langle k_F \rangle \equiv \frac{1}{A} \int d^3 x \ \left[ \frac{6 \pi^2 \rho(x)}{\nu} \right]^{1/3} \ \rho(x) \ \hspace{1cm} (4.81)$$

is such that the expansion parameter in an LDA sense, $\langle k_F \rangle a_s$, is equal to or greater than one-half, which implies poor convergence. In fact, the convergence is misleading, as seen by comparison to the hard-sphere repulsive case in Fig. 4.10. We postpone the discussion of energy convergence till Sec. 4.3.7. The systems with $\nu = 4$ have $\langle k_F \rangle a_s \approx 1/4 - 1/3$, and the convergence of even the hard-sphere case is good. Fig. 4.12 gives a measure of how the density varies when we choose different dimensions of our harmonic basis.
4.3.6 Comparison to Thomas-Fermi

In this section, we compare the LDA Kohn-Sham (KS) results to those from a Thomas-Fermi (TF) approximation. By Thomas-Fermi, we mean that the entire energy, including the kinetic energy, is calculated in a local density approximation. In particular, the Thomas-Fermi kinetic energy functional is [5]

\[ T_{TF}[\rho] = \frac{3}{10M} \left( \frac{6\pi^2}{\nu} \right)^{2/3} \int d^3r \left[ \rho(\mathbf{x}) \right]^{5/3} , \]  

(4.82)
rather than being computed as the sum of the kinetic energy of Kohn-Sham orbitals. We define the Thomas-Fermi potential energy functional to have the same form as the Kohn-Sham potential energy functional in the LDA. Historically, the Thomas-Fermi approach, as applied to atoms and molecules, was the first attempt to use the (electron) density as the basic variable rather than solving for the wavefunction. In its original form, only the Hartree term and the external nuclear-electron attractive potential were included in the potential energy. We will generalize to define LO, NLO, and NNLO Thomas-Fermi approximations.

The idea behind Thomas-Fermi is that in each volume element \( dV \) we have chemical equilibrium, with chemical potential \( \mu \). Each volume element is labeled by \( r \) (we assume spherical symmetry for convenience). Local eigenvalues \( E_k(r) \) are computed at each \( r \) as if in a uniform system:

\[ E_k(r) = \frac{k^2}{2M} + v_s(r) , \]  

(4.83)
and levels are filled until

\[ E_{k_F}(r) = \mu , \]  

(4.84)
which defines the local Fermi momentum \( k_F(r) \). This is turn defines the Thomas-Fermi density \( \rho_{TF}(r, \mu) \) for a given chemical potential \( \mu \) as:

\[
\rho_{TF}(r, \mu) = \begin{cases} 
\frac{\nu}{6\pi^2} (2M[\mu - v_s(r)])^{3/2} & \text{if } \mu > v_s(r) \\
0 & \text{if } \mu \leq v_s(r)
\end{cases},
\]

where the potential \( v_s(r) \) includes the external trap potential and the LDA Kohn-Sham potential [Eq. (4.70)]. The conventional TF procedure combines this equation with an equation for the potential (e.g., a Poisson equation in the Coulomb case) by substituting for the potential. Here we solve it in a two-step process closely analogous to the Kohn-Sham solution procedure.

For a given choice of \( \mu \), the number of fermions \( A_{TF} \) is given by:

\[
A_{TF}(\mu) = 4\pi \int_0^\infty r^2 \rho_{TF}(r, \mu) \, dr,
\]

where we’ve assumed a spherically symmetric distribution. We find the correct value of \( \mu \) for an input value of \( A \) using a root finding program, which finds the zero of

\[
f(\mu) \equiv A - A_{TF}(\mu)
\]

in the interval \( \mu_{\text{min}} < \mu < \mu_{\text{max}} \). The procedure to find the self-consistent \( \rho_{TF} \) is iterative:

1. Guess an initial \( \rho_{TF}(r) \) (for example, the unperturbed density);
2. given \( \rho_{TF}(r) \), compute \( v_s(r) \) for the noninteracting, LO, NLO, or NNLO case;
3. using this \( v_s(r) \) in Eq. (4.85), find \( \mu \) so that \( f(\mu) = 0 \);
4. with the new value of \( \mu \), calculate a new \( \rho_{TF}(r, \mu) \) from Eq. (4.85);
5. return to step 2., continuing until \( \rho_{TF} \) and \( \mu \) do not change within a prescribed tolerance.

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Table 4.2: Comparisons of energies per particle, averages of the local Fermi momentum $k_F$, and rms radii between Thomas-Fermi and Kohn-Sham treatments of a dilute Fermi gas in a harmonic trap. See the text for a description of units. In all cases, $r_s = a_p = 0$.

This procedure is rather simple and scales very well with the number of particles. There are deficiencies to the Thomas-Fermi approach, however, for many problems of interest. These deficiencies are most evident for the Coulomb problem, where it is proven that molecules do not bind (the separate atoms always have lower energy) [67]. Gradients expansions can improve the approximation but have not had a quantitative impact compared to Kohn-Sham approaches.

The kinetic energy contribution is a leading source of nonlocality in the energy functional. One of the chief virtues of the Kohn-Sham approach is that it treats this component much more effectively than a derivative expansion would. The comparison with Thomas-Fermi calculations highlights this difference. The most visible consequences are the absence of shell structure in ground state densities in the
Thomas-Fermi approach and the incorrect treatment of the low-density asymptotic region (dominated by the last Kohn-Sham orbitals). In contrast, the last Kohn-Sham orbital has the correct energy (the ionization energies in the exact and Kohn-Sham systems are equal), so the exponential tail of the distribution is correct. These deficiencies of Thomas-Fermi are relevant for the calculation of nuclear charge and matter densities.

In Figs. 4.13 and 4.14, Thomas-Fermi and Kohn-Sham densities are compared for a small system of 20 atoms (the other parameters are given in the figures). Both non-interacting and NNLO curves are shown in each figure. The shell structure is evident in the non-interacting density and is only slightly damped by the interactions in the Kohn-Sham approach. In contrast, the Thomas-Fermi curves are featureless. The same comparisons but with an order of magnitude more atoms \((A = 240)\) are shown in Figs. 4.15 and 4.16. In these case the differences are much smaller. For a small number of particles, the Kohn-Sham procedure is a comparable computation to Thomas-Fermi. With thousands of atoms, the Thomas-Fermi approximation should be accurate and efficient.

In Table 4.2, the energies per particle and other properties are compared for Kohn-Sham and Thomas-Fermi solutions. With \(A = 20\) atoms, the energy is reproduced at about the 2% level and the average Fermi momentum at the 1% level. With \(A = 240\) atoms, the energy is reproduced better than 1% and the average Fermi momentum to a third of a percent. Thus the Thomas-Fermi density will be quite adequate in making error estimates, which we turn to next.
Figure 4.13: Thomas-Fermi and Kohn-Sham approximations for dilute gas of fermions in a harmonic trap with degeneracy $\nu = 2$ filled up to $N_F = 2$, which implies there are 20 particles in the trap. The scattering length is $a_s = -0.16$ and the other effective range parameters are set to zero.

Figure 4.14: Thomas-Fermi and Kohn-Sham approximations for dilute gas of fermions in a harmonic trap with degeneracy $\nu = 2$ filled up to $N_F = 2$, which implies there are 20 particles in the trap. The scattering length is $a_s = +0.16$ and the other effective range parameters are set to zero.
Figure 4.15: Thomas-Fermi and Kohn-Sham approximations for dilute gas of fermions in a harmonic trap with degeneracy $\nu = 2$ filled up to $N_F = 7$, which implies there are 240 particles in the trap. The scattering length is $a_s = -0.16$ and the other effective range parameters are set to zero.

Figure 4.16: Thomas-Fermi and Kohn-Sham approximations for dilute gas of fermions in a harmonic trap with degeneracy $\nu = 2$ filled up to $N_F = 7$, which implies there are 240 particles in the trap. The scattering length is $a_s = +0.16$ and the other effective range parameters are set to zero.
4.3.7 Power Counting and Convergence

A major motivation for the use of effective field theory for many-body problems is the promise of error estimates. We face two challenges in making such estimates for a Kohn-Sham DFT. There are usually new low-energy constants (LEC’s) at each successive order in the EFT expansion. We first need to estimate the size of the LEC’s in the omitted orders. Second, we need to estimate their numerical impact on the functional and subsequently on observables in finite systems. In the present case, where we have a perturbative low-density expansion, we can do both directly.

Naive dimensional analysis, or NDA, is frequently used to estimate unknown LEC’s in an EFT Lagrangian. The idea is to identify the relevant dimensional momentum and mass scales in the problem and to rescale each term in the Lagrangian as an appropriate combination of scales times a dimensionless coefficient. An estimate of the truncation error follows by assuming the dimensionless coefficient is order unity (e.g., from 1/3 to 3).

In Ref. [68], NDA appropriate to low-energy chiral effective field theories of QCD was applied to covariant energy functionals for nuclei. While these functionals were viewed as approximate Kohn-Sham energy functionals, their form was directly derived from a chiral Lagrangian in the Hartree approximation. That is, there was a one-to-one correspondence between terms in the Lagrangian and terms in the corresponding energy functional. As a result, estimates of coefficients in the Lagrangian were immediately translated into error estimates in the functional, which led to estimates in specific finite nuclei through local density approximations [68].

In the present case, the Hartree (actually Hartree-Fock) terms again provide an immediate connection between NDA estimates in the Lagrangian and estimates of
the energy per particle in terms of the fermion density. Using LDA estimates of the average density, we get energy estimates for specific systems of trapped atoms. EFT power counting then provides estimates for the higher-order terms using the normalization established by the Hartree terms. For a purely short-ranged interaction, the NDA is simple: the estimate of the Hartree-Fock energy contribution from a given term in the Lagrangian is found by replacing $\psi^\dagger \psi$ by the average density (and including an appropriate spin factor). Any reasonable density (e.g., the Thomas-Fermi result) can be used to find the average density, since we already allow for a much larger uncertainty in the coefficients. Local density estimates for derivatives of densities are also sufficiently accurate.
In Fig. 4.17, the contributions to the energy per particle from LO, NLO, and NNLO terms in the energy per particle are shown as round symbols for three of the systems from Table 4.1. So, for example, the NLO contribution is from \( |E_{\text{NLO}} - E_{\text{LO}}| / A \). The square symbol denote estimates based on naive dimensional analysis, with error bars indicating a 1/2 to 2 uncertainty in the coefficients. In particular, the LO contribution is an estimate of the Hartree-Fock term and the NLO and NNLO estimates were found by multiplying the LO result by \( \langle k_F \rangle a_s \) and \( (\langle k_F \rangle a_s)^2 \), respectively. With one exception, the NDA estimates are good predictors of the actual contribution. Therefore, we can use these estimates to predict the uncertainty in the energy per particle from higher orders. The exception is the NNLO estimate for the \( \nu = 2 \) system, which greatly overestimates the actual contribution at that order. The reason is evident from the \( b_4 \) coefficient in Eq. (4.62), which determines the size of this contribution. Each of the two terms in \( b_4 \) are the size expected from NDA, but for \( \nu = 2 \) they happen to largely cancel. There is always this possibility of unnaturally small coefficients (and subsequent contributions) because of accidental cancellations. If we compare instead the NNLO energy from the hard-sphere-repulsion case, which has additional contributions at NNLO, we find that it is close to the estimate.

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CHAPTER 5

THE KINETIC ENERGY DENSITY IN KS DFT

DFT has the generality to deal with any interaction but has had little explicit impact on nuclear structure phenomenology so far [72, 73, 74, 106], although the Skyrme-Hartree-Fock formalism is often considered to be a form of DFT [51]. In the previous chapter, EFT methods were applied in a DFT framework, with the ultimate goal of calculating bulk observables for medium to heavy nuclei in a systematic fashion. In this chapter, we take another step toward this goal by generalizing the EFT framework for DFT to include the kinetic energy density in the same way it appears in the Skyrme approach, leading to Kohn-Sham equations with position-dependent $M^*$'s [87]. We take a (small) step beyond the LDA by evaluating the full $\tau$ dependence in the Hartree-Fock diagrams with two-derivative vertices, which leads to an energy expression similar to the standard Skyrme energy (excepting the spin-orbit parts).

5.1 Skyrme-Hartree-Fock

The Skyrme-Hartree-Fock approach to nuclei is based on energy functionals and single-particle equations, which suggests a link between the traditional DFT and
nuclear mean-field approaches [51, 52, 53]. In calculations with the usual density-dependent Skyrme force, the energy density for spherical, even-even $N = Z$ nuclei takes the form of a local expansion in density [107, 76, 77],
\[
E_{SK}(\mathbf{x}) = \frac{1}{2M} \tau(\mathbf{x}) + \frac{3}{8} t_0 [\rho(\mathbf{x})]^2 + \frac{1}{16} t_3 [\rho(\mathbf{x})]^{2+\alpha} + \frac{1}{16} (3t_1 + 5t_2) \rho(\mathbf{x}) \tau(\mathbf{x}) + \frac{1}{64} (9t_1 - 5t_2) |\nabla \rho(\mathbf{x})|^2 - \frac{3}{4} W_0 \rho(\mathbf{x}) \nabla \cdot \mathbf{J}(\mathbf{x}) + \frac{1}{32} (t_1 - t_2) |\mathbf{J}(\mathbf{x})|^2.
\]

(5.1)

The density $\rho$, kinetic density $\tau$, and the spin-orbit density $\mathbf{J}$ are expressed as sums over single-particle orbitals $\psi_k(\mathbf{x})$ as:
\[
\rho(\mathbf{x}) = \nu \sum_k |\psi_k(\mathbf{x})|^2, \quad \tau(\mathbf{x}) = \nu \sum_k |\nabla \psi_k(\mathbf{x})|^2, \\
i\mathbf{J}(\mathbf{x}) = \nu_{iso} \sum_k \psi_k^\dagger(\mathbf{x})(\nabla \times \mathbf{\sigma}) \psi_k(\mathbf{x}),
\]

(5.2)

where the sums are over occupied states and $\nu$ denotes the spi-isospin multiplicity as usual. $\nu_{iso}$ denotes just the isospin multiplicity. The $t_i$'s, $W_0$, and $\alpha$ are generally obtained from numerical fits to experimental data. Varying the energy with respect to the wavefunctions leads to a Schrödinger-type equation with a position-dependent mass term [76, 107]:
\[
\left(-\nabla \frac{1}{2M^*(\mathbf{x})} \nabla + U(\mathbf{x}) + W(\mathbf{x})\right) \psi_k(\mathbf{x}) = \varepsilon_k \psi_k(\mathbf{x}),
\]

(5.3)

where $M^*(\mathbf{x})$ is given by
\[
\frac{1}{2M^*(\mathbf{x})} = \frac{1}{2M} + \left[ \frac{3}{16} t_1 + \frac{5}{16} t_2 \right] \rho(\mathbf{x}),
\]

(5.4)

and $W(\mathbf{x})$ is a spin-orbit potential [77]. The appearance of $M^*(\mathbf{x})$ and $W(\mathbf{x})$ are a consequence of not expanding $\tau$ and $\mathbf{J}$ in terms of $\rho$. 

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5.2 EFT/DFT with the Kinetic Energy Density

In this section, we extend the EFT/DFT construction for a dilute Fermi system to include a source coupled to the kinetic energy density operator. We carry out a double Legendre transformation via the inversion method, and get an energy functional of $\rho$ and $\tau$, and Kohn-Sham equations with a position dependent mass term $M^*(x)$.

5.2.1 Effective Action and the Inversion Method

We introduce a generating functional in the path integral formulation with $\mathcal{L}$ from Eqs. (3.13) with the external potential supplemented by c-number sources $J(x)$ and $\eta(x)$, coupled to the composite density operator and to the kinetic energy density operator, respectively,

$$Z[J, \eta] = e^{iW[J, \eta]} = \int D\psi D\psi^\dagger e^{i \int d^4x \left[ \mathcal{L} + J(x)\psi^\dagger(x)\psi(x) + \eta(x)\nabla\psi^\dagger(x)\nabla\psi(x) \right]} . \quad (5.5)$$

For simplicity, normalization factors are considered to be implicit in the functional integration measure [44, 45]. The fermion density in the presence of the sources is

$$\rho(x) \equiv \langle \psi^\dagger(x)\psi(x) \rangle_{J, \eta} = \frac{\delta W[J, \eta]}{\delta J(x)} , \quad (5.6)$$

and the kinetic energy density is given by

$$\tau(x) \equiv \langle \nabla\psi^\dagger(x) \cdot \nabla\psi(x) \rangle_{J, \eta} = \frac{\delta W[J, \eta]}{\delta \eta(x)} , \quad (5.7)$$

where functional derivatives are taken keeping the other source fixed. The effective action is defined through the functional Legendre transformation

$$\Gamma[\rho, \tau] = W[J, \eta] - \int d^4x \ J(x)\rho(x) - \int d^4x \ \eta(x)\tau(x) , \quad (5.8)$$

which implies that $\Gamma$ has no explicit dependence on $J$ and $\eta$. 
As in Ref. [42], we choose finite-density boundary conditions that enforce a given particle number \( A \) by hand, so that \( \Gamma \) and \( W \) are functions of \( A \) and variations over \( \rho(x) \) and \( \tau(x) \) conserve \( A \). This is naturally achieved by working with a fixed number of Kohn-Sham orbitals, as seen below. Just as before, we limit ourselves to time independent sources and densities, so that

\[
\tilde{\Gamma}[\rho, \tau] \equiv \Gamma[\rho, \tau] \times \left[ \int_{-\infty}^{\infty} dt \right]^{-1} = -E[\rho, \tau].
\] (5.9)

and similarly with \( W[J, \eta] \) and the expansions below. The effective action has extrema at the possible quantum ground states of the system, and when evaluated at the minimum is proportional (at zero temperature) to the ground-state energy [44, 45, 62]. In particular, Eq. (5.9) defines an energy functional \( E[\rho, \tau] \), which when evaluated with the exact ground-state density \( \rho \) and kinetic energy density \( \tau \), is equal to the ground-state energy.

If we take functional derivatives of Eq. (5.8) with respect to \( J(x) \) and \( \eta(x) \), and then apply Eqs. (5.6) and (5.7) [42], we obtain two equations that can be written in matrix form as

\[
\int d^3 y \begin{pmatrix} \frac{\delta \rho(y)}{\delta J(x)} & \frac{\delta \tau(y)}{\delta J(x)} \\ \frac{\delta \rho(y)}{\delta \eta(x)} & \frac{\delta \tau(y)}{\delta \eta(x)} \end{pmatrix} \begin{pmatrix} \frac{\delta \tilde{\Gamma}[\rho, \tau]}{\delta \rho(y)} + J(y) \\ \frac{\delta \tilde{\Gamma}[\rho, \tau]}{\delta \tau(y)} + \eta(y) \end{pmatrix} = 0. \] (5.10)

The invertibility of the transformation from \( \{J, \eta\} \) to \( \{\rho, \tau\} \) implies that the matrix in Eq. (5.10) has no zero eigenvalues, which means that the elements of the vector vanish identically for each \( x \), so that

\[
\frac{\delta \tilde{\Gamma}[\rho, \tau]}{\delta \rho(x)} = -J(x), \quad \frac{\delta \tilde{\Gamma}[\rho, \tau]}{\delta \tau(x)} = -\eta(x). \] (5.11)

Thus, the effective action when evaluated at the exact ground state density and kinetic energy density is an extremum when the sources are set to zero, which corresponds to
the original (source-free) system. The convexity of $\Gamma$ implies that the energy (equal to minus $\tilde{\Gamma}[\rho, \tau]$ at the extremum) is a minimum.\(^3\)

These properties are analogous to conventional applications of effective actions where the Legendre transformation is with respect to one of the fields rather than a composite operator [99, 102, 100]. A possible complication in the present case would be if new divergences arose in $W[J, \eta]$, which generally happens when adding a source coupled to a composite operator [88, 103]. However, that is not the case here. On the other hand, sources coupled to operators such as $\psi\psi + \psi^\dagger\psi^\dagger$, which arise when considering pairing, will introduce new divergences [75], including for the kinetic energy density.

To carry out the inversion and Legendre transformation, we apply the inversion method of Fukuda et al. [44, 45, 55, 46, 47, 54] just as described in the previous chapter. We introducing a parameter $\lambda$ associated with our dilute expansion parameter. The effective action is given a dependence on $\lambda$

$$\tilde{\Gamma} = \tilde{\Gamma}[\rho, \tau, \lambda] , \quad (5.12)$$

which is treated as an independent variable. The Legendre transformation defining $\tilde{\Gamma}$ follows from Eq. (5.8):

$$\tilde{\Gamma}[\rho, \tau, \lambda] = \tilde{W}[J, \eta, \lambda] - \int d^3x \ J(x) \ \rho(x) - \int d^3x \ \eta(x) \ \tau(x) , \quad (5.13)$$

where $J$ and $\eta$ depend on $\lambda$ as well as being functionals of $\rho$ and $\tau$.

Now we expand each of the quantities that depend on $\lambda$ in Eq. (5.13) in a series in $\lambda$ [42], treating $\rho$ and $\tau$ as order unity, and substitute the expansion for $J$ and $\eta$

\(^3\)In Ref. [46], a proof is given of the invertibility of the Legendre transformation for the Euclidean version of the functions. The proof extends directly to our Minkowski functions with any number of sources, as long as they are coupled linearly.
into the expansion for $\tilde{W}$. Equating terms with equal powers of $\lambda$ on both sides of
Eq. (5.13) after carrying out a functional Taylor expansion of $\tilde{W}[J, \eta]$ about $J_0$ and
$\eta_0$ gives a series of equations relating the $\tilde{\Gamma}_i$, $\tilde{W}_i$, $J_i$, and $\eta_i$, where the subscript $l$
indicates the power of $\lambda$. These equations allow the $\tilde{\Gamma}_i$’s to be constructed recursively
(see Ref. [42] for explicit expressions). Since $\rho$ and $\tau$ are independent of $\lambda$, the sources
for any $l$ satisfy

$$J_l(x) = -\frac{\delta \tilde{\Gamma}_l[\rho, \tau]}{\delta \rho(x)}, \quad \eta_l(x) = -\frac{\delta \tilde{\Gamma}_l[\rho, \tau]}{\delta \tau(x)}, \quad (5.14)$$

which is just the term-by-term expansion of Eq. (5.11). All of the $J_l$’s and $\eta_l$’s
as defined here are functionals of $\rho$ and $\tau$, and this functional dependence will be
understood even if not explicitly shown from now on (and functional derivatives with
respect to $\rho$ will have $\tau$ held fixed, and vice versa). We identify the $\tilde{W}_l$’s for $l \geq 1$ in
the present case with the diagrammatic expansion in Fig. 3.3 [41, 42]. That is, $\tilde{W}_1$
is given by diagram (a), $\tilde{W}_2$ by diagrams (b) and (c), and $\tilde{W}_3$ by diagrams (d) through
(j).

The zeroth-order equation from Eq. (5.13) is

$$\tilde{\Gamma}_0[\rho, \tau] = \tilde{W}_0[J_0, \eta_0] - \int d^3x \ J_0(x) \ \rho(x) - \int d^3x \ \eta_0(x) \ \tau(x) . \quad (5.15)$$

The corresponding zeroth order expansion of Eqs. (5.6) and (5.7) is

$$\rho(x) = \frac{\delta \tilde{W}_0[J_0, \eta_0]}{\delta J_0(x)} , \quad \tau(x) = \frac{\delta \tilde{W}_0[J_0, \eta_0]}{\delta \eta_0(x)} , \quad (5.16)$$

(this also follows by taking functional derivatives of Eq. (5.15) with respect to $\rho$ and
$\tau$ and using invertibility again, see [42]). Note that these are the exact ground-state
densities. Because $\rho$ and $\tau$ are treated as order unity, this is the only equation in
the expansion of Eqs. (5.6) and (5.7) in which they appear. Thus, the sources $J_0(x)$
and \( \eta_0(\mathbf{x}) \) are particular functions that generate the expectation values \( \rho \) and \( \tau \) from the noninteracting system defined by \( \lambda = 0 \). (The existence of \( J_0(\mathbf{x}) \) and \( \eta_0(\mathbf{x}) \) is the heart of the Kohn-Sham approach.) The inversion method achieves this end by construction.

The exponent in the non-interacting generating functional \( Z_0[J, \eta] \) is quadratic in the fermion fields,

\[
\int d^4 x \, \psi^\dagger \left[ i \partial_t + \frac{\nabla^2}{2M} - v(\mathbf{x}) + J_0(\mathbf{x}) \right] \psi + \int d^4 x \, \eta_0(\mathbf{x}) \nabla \psi^\dagger \cdot \nabla \psi \\
= \int d^4 x \, \psi^\dagger \left[ i \partial_t + \frac{\nabla^2}{2M} - v(\mathbf{x}) + J_0(\mathbf{x}) - \nabla \cdot \eta_0(\mathbf{x}) \nabla \right] \psi ,
\]

which leads us to define the Green’s function \( G^0_{\text{ks}} \) of the Kohn-Sham non-interacting system. This Green’s function satisfies

\[
\left( i \partial_t + \nabla \cdot \frac{1}{2M^*(\mathbf{x})} \nabla - v(\mathbf{x}) + J_0(\mathbf{x}) \right) G^0_{\text{ks}}(\mathbf{x}t, \mathbf{x}'t') = \delta^3(\mathbf{x} - \mathbf{x}')\delta(t - t')
\]

with finite density boundary conditions [110] and a position-dependent effective mass defined by

\[
\frac{1}{2M^*(\mathbf{x})} \equiv \frac{1}{2M} - \eta_0(\mathbf{x}) .
\]

Kohn-Sham orbitals arise as solutions to

\[
[- \nabla \cdot \frac{1}{2M^*(\mathbf{x})} \nabla + v(\mathbf{x}) - J_0(\mathbf{x})] \psi_k(\mathbf{x}) = \varepsilon_k \psi_k(\mathbf{x}) ,
\]

where the index \( k \) represents all quantum numbers except for the spin. Note that Eq. (5.20) is in the form of the Skyrme single-particle equation [Eq. (5.3)] (without the spin-orbit part).
As before, the spectral decomposition of \( G_{ks}^0 \) in terms of the Kohn-Sham orbitals is given by

\[
iG_{ks}^0(x, x') = \sum_k \psi_k(x) \psi_k^*(x') e^{-i \varepsilon_k (t-t')} [\theta(t - t') \theta(\varepsilon_k - \varepsilon_F) - \theta(t' - t) \theta(\varepsilon_F - \varepsilon_k)] .
\] (5.21)

It follows that \( \tilde{W}_0[J_0, \eta_0] \propto \text{Tr} \ln(G_{ks}^0)^{-1} \) (since it is quadratic it yields a simple determinant), corresponding to the system without interactions, and can be written explicitly in terms of the single-particle Kohn-Sham eigenvalues as [109]

\[
\tilde{W}_0[J_0, \eta_0] = -\nu \sum_{\varepsilon_k \leq \varepsilon_F} \varepsilon_k ,
\] (5.22)

where \( \nu \) is the spin-isospin degeneracy, as expected for a system without interactions.

Equation (5.16) applied to Eq. (5.22) [with the help of Eq. (5.20)] implies that \( \rho(x) \) and \( \tau(x) \) follow as in Eq. (5.2) from the orbitals [42]. By using Eq. (5.22) in Eq. (5.15) and then eliminating \( \varepsilon_k \) using Eq. (5.20), the lowest order effective action can be written two ways,

\[
\tilde{\Gamma}_0[\rho, \tau] = -\nu \sum_k \varepsilon_k - \int d^3x \ J_0(x) \ \rho(x) - \int d^3x \ \eta_0(x) \ \tau(x) \\
= -T_s[\tau] - \int d^3x \ \nu(x) \ \rho(x) ,
\] (5.23)

where

\[
T_s[\tau] = \nu \sum_k \int d^3x \ \psi_k^*(x) \left(-\frac{\nabla^2}{2M}\right) \psi_k(x) = \frac{\nu}{2M} \sum_k \int d^3x \ |\nabla \psi_k(x)|^2 \\
= \frac{1}{2M} \int d^3x \ \tau(x)
\] (5.24)

is the total kinetic energy of the KS non-interacting system.

The first-order equation in \( \lambda \) from Eq. (5.13) is

\[
\tilde{\Gamma}_1[\rho, \tau] = \tilde{W}_1[J_0, \eta_0] + \int d^3x \ \frac{\delta \tilde{W}_0[J_0, \eta_0]}{\delta J_0(x)} J_1(x) + \int d^3x \ \frac{\delta \tilde{W}_0[J_0, \eta_0]}{\delta \eta_0(x)} \eta_1(x)
\]
\[- \int d^3x \, J_1(x) \, \rho(x) - \int d^3x \, \eta_1(x) \, \tau(x) \]
\[= \tilde{W}_1[J_0, \eta_0]. \] (5.25)

The complete cancellation of the \(J_1\) and \(\eta_1\) terms from applying Eq. (5.16) occurs for the \(J_l\) and \(\eta_l\) terms in the equation for \(\tilde{\Gamma}_l\) for all \(l \geq 1\). Thus for a given \(l\), we only need \(\tilde{W}_{k}\)’s with \(k\) less than or equal to \(l\), and \(J_k\)’s and \(\eta_k\)’s with \(k\) smaller than \(l\). The \(\tilde{W}_k\) functionals are constructed using conventional Feynman rules in position space with factors as in Ref. [41], but with fermion lines representing \(iG_{ks}^0\).

In particular, the LO effective action is given by [42]
\[\tilde{\Gamma}_1[\rho, \tau] = \tilde{W}_1[J_0, \eta_0] = \frac{1}{2} \nu (\nu - 1) C_0 \int d^3x \, G_{ks}^0(x, x^+) \, G_{ks}^0(x, x^+). \] (5.26)

The density can be directly expressed in terms of the Kohn-Sham Green’s function with equal arguments as
\[\rho(x) = -i \nu \, G_{ks}^0(x, x^+), \] (5.27)
so that we have
\[\tilde{\Gamma}_1[\rho, \tau] = -\frac{1}{2} \frac{(\nu - 1)}{\nu} C_0 \int d^3x \, |\rho(x)|^2 \equiv \Gamma_1[\rho], \] (5.28)
which is minus the Hartree-Fock energy. Using Eq. (5.14), we obtain
\[J_1(x) = C_0 \frac{(\nu - 1)}{\nu} \rho(x), \quad \eta_1(x) = 0. \] (5.29)

After canceling the \(J_2\) and \(\eta_2\) terms as advertised above, the second-order effective action is given by
\[\tilde{\Gamma}_2[\rho, \tau] = \tilde{W}_2[J_0, \eta_0] + \int d^3x \, \left( \frac{\delta \tilde{W}_1[J_0, \eta_0]}{\delta J_0(x)} \right) J_1(x) + \int d^3x \, \frac{\delta \tilde{W}_1[J_0, \eta_0]}{\delta \eta_0(x)} \eta_1(x) \]
\[+ \frac{1}{2} \int d^3x \, d^3y \, \left( \frac{\delta^2 \tilde{W}_0[J_0, \eta_0]}{\delta J_0(x) \delta J_0(y)} \right) J_1(x) \, J_1(y) + \frac{1}{2} \int d^3x \, d^3y \, \left( \frac{\delta^2 \tilde{W}_0[J_0, \eta_0]}{\delta \eta_0(x) \delta \eta_0(y)} \right) \eta_1(x) \, \eta_1(y) \]
\[+ \int d^3x \, d^3y \, \left( \frac{\delta^2 \tilde{W}_0[J_0, \eta_0]}{\delta J_0(x) \delta \eta_0(y)} \right) J_1(x) \, \eta_1(y). \] (5.30)
$W_2[J_0, \eta_0]$ is calculated from the graphs Figs. 3.3(b) and (c):

$$W_2[J_0, \eta_0] = i\nu(\nu - 1) \frac{C_0^2}{4} \int d^4x \, d^4y \, G_{ks}^0(x, y) G_{ks}^0(y, x) G_{ks}^0(y, x)$$

$$- i\nu(\nu - 1)^2 \frac{C_0^2}{2} \int d^4x \, d^4y \, G_{ks}^0(x, y) G_{ks}^0(y, x) G_{ks}^0(y, x) G_{ks}^0(y, x)$$

The other terms in $\tilde{\Gamma}_2$ completely cancel against the “anomalous” graph of Fig. 3.3(c) so that\(^4\)

$$\Gamma_2[\rho, \tau] = i\nu(\nu - 1) \frac{C_0^2}{4} \int d^4x \, d^4y \, G_{ks}^0(x, y) G_{ks}^0(x, y) G_{ks}^0(y, x) G_{ks}^0(y, x),$$

(5.32)

which is equal to the contribution made by the “beachball” diagram [Fig. 3.3(b)] to the energy [up to the time factor of Eq. (5.9)]. This cancellation is proven exactly as in Ref. [42] after generalizing to the matrix notation of Eq. (5.10). Calculation of the third-order effective action in the inversion method similarly leads to cancellation of the “anomalous” graphs in $\tilde{W}_3$ given by Figs. 3.3(d), (e), and (f), leaving only Fig. 3.3(g) through (j) as contributors. All higher orders in $\tilde{\Gamma}[\rho, \tau, \lambda]$ are determined in a similar manner, as described in Refs. [46, 42].

In order to solve for the orbitals in Eq. (5.20) and to calculate the energy, we need expressions for $J_0(\mathbf{x})$ and $\eta_0(\mathbf{x})$. Since $J(\mathbf{x}) = \eta(\mathbf{x}) = 0$ in the ground state, Eq. (5.11) becomes a variational principle that, together with Eq. (5.14), yields self-consistent expressions for $J_0$ and $\eta_0$ [42]:

$$J_0(\mathbf{x}) \Big|_{gs} = - \sum_{l \geq 1} J_l(\mathbf{x}) \Big|_{gs} = \frac{\delta \tilde{\Gamma}_{\text{int}}[\rho, \tau]}{\delta \rho(\mathbf{x})} \Big|_{gs},$$

(5.33)

$$\eta_0(\mathbf{x}) \Big|_{gs} = - \sum_{l \geq 1} \eta_l(\mathbf{x}) \Big|_{gs} = \frac{\delta \tilde{\Gamma}_{\text{int}}[\rho, \tau]}{\delta \tau(\mathbf{x})} \Big|_{gs},$$

(5.34)

\(^4\)This complete cancellation does not occur for long-range forces, or if the zero-range delta functions at the $C_0$ vertices are regulated by a cutoff rather than by dimensional regularization, as used here.
where \( \tilde{\Gamma}_{\text{int}}[\rho, \tau] \) is the interaction effective action

\[
\tilde{\Gamma}_{\text{int}}[\rho, \tau] = \sum_{l \geq 1} \tilde{\Gamma}_l[\rho, \tau],
\]

(5.35)

and the subscript “gs” refers to the ground-state. (Note that at this stage \( \lambda = 1 \), and Eqs. (5.33) and (5.34) mix all orders of the original inversion-method expansion into the Kohn-Sham potentials \( J_0 \) and \( \eta_0 \).) A given approximation corresponds to truncating Eq. (5.35) at \( l_{\text{max}} \) and then carrying out the self-consistent calculation. We refer to \( l_{\text{max}} = 1 \) as leading order, or LO, \( l_{\text{max}} = 2 \) as next-to-leading order or NLO, and \( l_{\text{max}} = 3 \) as NNLO.

### 5.2.2 Including \( \tau \) in Hartree-Fock Diagrams

The contributions to \( E_c^{\text{LDA}}[\rho(x)] \) from the Hartree-Fock graphs containing the \( C_2 \) and \( C_2' \) vertices [Figs. 3.3(i) and (j)], which have gradients, were approximately evaluated in the LDA in Eq. (4.61) to obtain a functional of \( \rho \) alone. In the DFT formalism generalized to include the kinetic energy density \( \tau(x) \), however, we observe that they can be evaluated exactly in terms of \( \rho(x) \) and \( \tau(x) \) (for closed shells). These contributions to \( \tilde{W}_3[J_0, \eta_0] \) can be simply expressed in terms of gradients acting on the Kohn-Sham Green’s functions [cf. Eq. (5.26)]:

\[
\tilde{W}_3[J_0, \eta_0] = -\frac{1}{16} \int d^3x \left[ C_2 \nu (\nu - 1) \left\{ (\nabla_1 - \nabla_2)^2 + (\nabla_3 - \nabla_4)^2 \right\} 
+ 2C_2' \nu (\nu + 1) \left\{ (\nabla_1 - \nabla_2) \cdot (\nabla_3 - \nabla_4) \right\} \right]
+ \sum_{k} \sum_{\text{occ}} G_{ks}^0(x_4, x_2^+) G_{ks}^0(x_3, x_1^+) \bigg|_{x_1=x_2=x_3=x_4=x} + \cdots \tag{5.36}
\]

Equation (5.36) is evaluated by carrying out the gradients and then setting all of the \( x_i \) equal to \( x \). For this purpose, the replacement

\[
G_{ks}^0(x, x') \rightarrow \delta \sum_k \psi_k(x) \psi_k^*(x')
\]

(5.37)
can be made and, since in the end we integrate over \( \mathbf{x} \), we can partially integrate any term. It is not difficult to write the resulting expressions in terms of \( \rho(\mathbf{x}), \tau(\mathbf{x}) \), and a current density \( j(\mathbf{x}) \),

\[
j(\mathbf{x}) = \frac{i}{2^\nu} \sum_k \left[ \nabla \psi_k^*(\mathbf{x}) \psi_k(\mathbf{x}) - \psi_k^*(\mathbf{x}) \nabla \psi_k(\mathbf{x}) \right]. \tag{5.38}
\]

The current density vanishes when summed over closed shells, leaving simple expressions for the Hartree-Fock energy functionals:

\[
E_{C_2}[\rho(\mathbf{x}), \tau(\mathbf{x})] = \frac{B_2 a_s^2 r_s}{2M} \int d^3 \mathbf{x} [\rho(\mathbf{x})\tau(\mathbf{x}) + \frac{3}{4} (\nabla \rho)^2], \tag{5.39}
\]

\[
E_{C_2'}[\rho(\mathbf{x}), \tau(\mathbf{x})] = \frac{B_3 a_s^3}{2M} \int d^3 \mathbf{x} [\rho(\mathbf{x})\tau(\mathbf{x}) - \frac{1}{4} (\nabla \rho)^2]. \tag{5.40}
\]

The dimensionless constants \( B_2 \) and \( B_3 \) are given by

\[
B_2 = \pi \left( \frac{\nu - 1}{\nu} \right), \quad B_3 = 2 \pi \left( \frac{\nu + 1}{\nu} \right). \tag{5.41}
\]

The total contribution to the energy from NLO and NNLO diagrams is

\[
E_c[\rho(\mathbf{x}), \tau(\mathbf{x})] = \frac{b_1 a_s^2}{2M} \int d^3 \mathbf{x} [\rho(\mathbf{x})]^{7/3} + E_{C_2}[\rho(\mathbf{x}), \tau(\mathbf{x})] \\
+ E_{C_2'}[\rho(\mathbf{x}), \tau(\mathbf{x})] + \frac{b_4 a_s^3}{2M} \int d^3 \mathbf{x} [\rho(\mathbf{x})]^{8/3}. \tag{5.42}
\]

Since this functional now has the semi-local \( \tau(\mathbf{x}) \) as one of its ingredients, it represents a step beyond LDA, even though the contributions from Figs. 3.3(b), (g), and (h) are still evaluated with the LDA prescription. The next step in the DFT/EFT program will be to develop systematic expansions to these contributions in terms of \( \rho \) and \( \tau \).

For now, we carry out the DFT/EFT formalism in the effective action framework using the hybrid functional with \( \tau(\mathbf{x}) \). The full effective action is given by

\[
\tilde{\Gamma}[\rho, \tau] = \tilde{\Gamma}_0[\rho, \tau] + \tilde{\Gamma}_1[\rho, \tau] + \sum_{k=2}^\infty \tilde{\Gamma}_k[\rho, \tau]. \tag{5.43}
\]
We proceed to calculate the sources using Eqs. (5.33), (5.34), and (5.42) to NNLO; first \( J_0(\mathbf{x}) \) is

\[
J_0(\mathbf{x}) = \frac{\delta}{\delta \rho(\mathbf{x})} \left( \tilde{\Gamma}_1[\rho, \tau] + \sum_{k=2}^3 \tilde{\Gamma}_k[\rho, \tau] \right) = -\frac{\delta}{\delta \rho(\mathbf{x})} (E_{\text{HF}}[\rho] + E_c[\rho, \tau])
\]

\[
= -\frac{(\nu - 1)}{\nu} \frac{4\pi a_s}{M} \rho(\mathbf{x}) - \frac{7}{3} b_1 \frac{a_s^2}{2M} [\rho(\mathbf{x})]^{4/3} - \frac{8}{3} b_1 \frac{a_s^3}{2M} [\rho(\mathbf{x})]^{5/3}
\]

\[
- \left( B_2 a_s^2 r_s + B_3 a_p^3 \right) \frac{1}{2M} \tau(\mathbf{x}) + \left( 3B_2 a_s^2 r_s - B_3 a_p^3 \right) \frac{1}{4M} \nabla^2 \rho(\mathbf{x})
\]

and then \( \eta_0(\mathbf{x}) \) is:

\[
\eta_0(\mathbf{x}) = -\frac{\delta}{\delta \tau(\mathbf{x})} (E_{\text{HF}}[\rho] + E_c[\rho, \tau]) = - \left( B_2 a_s^2 r_s + B_3 a_p^3 \right) \frac{1}{2M} \rho(\mathbf{x}) .
\]

The spatially dependent effective mass \( M^*(\mathbf{x}) \) is therefore

\[
\frac{1}{2M^*(\mathbf{x})} = \frac{1}{2M} - \eta_0(\mathbf{x}) = \frac{1}{2M} + \left[ \frac{(\nu - 1)}{4\nu} C_2 + \frac{(\nu + 1)}{4\nu} C_2' \right] \rho(\mathbf{x}) ,
\]

where Eq. (3.17) has been used. An expression for the total binding energy (through NNLO) follows by substituting for \( J_0(\mathbf{x}) \) and \( \eta_0(\mathbf{x}) \) in Eq. (5.23) and then using Eq. (5.43) and Eq. (5.9),

\[
E[\rho(\mathbf{x}), \tau(\mathbf{x})] = \nu \sum_k^{\text{occ.}} \varepsilon_k - \int d^3 \mathbf{x} \left\{ \frac{1}{2} \frac{(\nu - 1)}{\nu} \frac{4\pi a_s}{M} [\rho(\mathbf{x})]^2 + \frac{4}{3} b_1 \frac{a_s^2}{2M} [\rho(\mathbf{x})]^{7/3}
\]

\[
+ \frac{5}{3} b_1 \frac{a_s^3}{2M} [\rho(\mathbf{x})]^{8/3} + (3B_2 a_s^2 r_s - B_3 a_p^3) \frac{1}{8M} [\nabla \rho(\mathbf{x})]^2
\]

\[
+ \left( B_2 a_s^2 r_s + B_3 a_p^3 \right) \frac{1}{2M} \rho(\mathbf{x}) \tau(\mathbf{x}) \right\} .
\]

The noninteracting case \( (C_i \equiv 0) \) uses \( J_0(\mathbf{x}) \equiv 0, \eta_0(\mathbf{x}) \equiv 0 \) and the first term in Eq. (5.47). Leading order (LO) uses the first term in Eq. (5.44) and the first two terms in Eq. (5.47), and so on for NLO and NNLO. An alternative expression for the energy is obtained by using the second part of Eq. (5.23) followed by Eqs. (5.24),
(5.43), and (5.9):

\[
E[\rho(\mathbf{x}), \tau(\mathbf{x})] = \int d^3x \left\{ \frac{1}{2M} \tau(\mathbf{x}) + v(\mathbf{x}) \rho(\mathbf{x}) + \frac{1}{2} \left( \frac{\nu - 1}{\nu} \right) \frac{4\pi a_s}{M} [\rho(\mathbf{x})]^2 \right. \\
+ \left. (B_2 a_s^2 r_s + B_3 a_p^3) \frac{1}{2M} \rho(\mathbf{x}) \tau(\mathbf{x}) + \frac{1}{8M} |\nabla \rho(\mathbf{x})|^2 \right. \\
+ \left. b_1 \frac{a_s^2}{2M} [\rho(\mathbf{x})]^{7/3} + b_4 \frac{a_s^3}{2M} [\rho(\mathbf{x})]^{8/3} \right\} .
\]

(5.48)

5.2.3 Comparison to Skyrme Hartree-Fock

A nucleus is a self-bound system, so the external potential \( v(\mathbf{x}) = 0 \). To compare the DFT/EFT functional to the conventional Skyrme energy density functional of Eq. (5.1), we set the spin multiplicity \( \nu = 4 \) and use Eq. (3.17) to rewrite Eq. (5.48) in terms of the \( C_i \)'s, obtaining the energy density:

\[
\mathcal{E}[\rho(\mathbf{x}), \tau(\mathbf{x})] = \frac{1}{2M} \tau(\mathbf{x}) + \frac{3}{8} C_0 [\rho(\mathbf{x})]^2 + \frac{1}{16} (3C_2 + 5C_2') \rho(\mathbf{x}) \tau(\mathbf{x}) \\
+ \frac{1}{64} (9C_2 - 5C_2') (\nabla \rho)^2 + b_1 \frac{a_s^2}{2M} [\rho(\mathbf{x})]^{7/3} + b_4 \frac{a_s^3}{2M} [\rho(\mathbf{x})]^{8/3}.
\]

(5.49)

We observe that we get all the terms of \( \mathcal{E}_{SK}(\mathbf{x}) \) from Eq. (5.1) except for the one with coefficient \( t_3 \) and the spin-dependent terms, if we make the correspondence \( t_0 \leftrightarrow C_0, \ t_1 \leftrightarrow C_2 \) and \( t_2 \leftrightarrow C_2' \). This correspondence is not surprising since the Skyrme interaction was originally motivated as a low-momentum expansion of the \( G \) matrix \([82]\). The two additional terms in Eq. (5.49) of the form \( \rho(\mathbf{x})^{2+\alpha} \) come from correlations (i.e., terms beyond Hartree-Fock), but there is no direct association with the \( t_3 \) term in the Skyrme energy density, which was originally motivated as a three-body contribution (so \( \alpha = 1 \)). However, it is clear that the Skyrme functional is incomplete as an expansion; a direct connection to microscopic interactions by matching to an EFT will include at least these additional terms. Thus we see that a dilute Fermi system with short-range interactions is not only an ideal test laboratory
for effective field theory at finite density, but it is also directly relevant for comparison to Skyrme functionals.

5.2.4 Spin-Isospin Dependence

The generalization of the DFT/EFT to include spin and isospin dependence is straightforward. If one writes a complete set of four-fermion terms with $\sigma$ and $\tau$ matrices in the EFT Lagrangian, there are redundant terms because of Fermi statistics. In conventional discussions of the Skyrme approach, this observation is typically cast in terms of antisymmetrization of the interaction [76, 107]. For a path integral formulation of the DFT/EFT, using Fierz rearrangement is a convenient alternative. We illustrate the procedure for the leading spin dependence.

First consider just spin-1/2 (no isospin, so $\nu = 2$). We expand the product of Grassmann fields $\psi_i \psi_j^\dagger$ ($i$ and $j$ are spin indices) in the complete basis of $\delta_{ij}$ and $\sigma_{ij}^a$ ($a = \{1, 2, 3\}$), identifying the coefficients by contracting in turn with $\delta_{ij}$ and $\sigma_{ij}^b$. Let us see how. Let us start with

$$\psi_i \psi_j^\dagger = A \delta_{ij} + B \sigma_{ij}^a . \quad (5.50)$$

Contracting with $\delta_{ij}$, we get

$$\delta_{ij} \psi_i \psi_j^\dagger = A \delta_{ij} \delta_{ij} + B \delta_{ij} \sigma_{ij}^a$$

or, $\psi_i \psi_i^\dagger = A \delta_{ii} + B \sigma_{ii}^a = A \delta_{ii} = 2A$

$$\rightarrow A = \frac{1}{2} \psi_i \psi_i^\dagger = -\frac{1}{2} \psi_i^\dagger \psi_i. \quad (5.51)$$

The minus sign comes from interchanging Grassmann fields. Next we contract with the Pauli matrix.

$$\sigma_{ji}^b \psi_i \psi_j^\dagger = A \sigma_{ji}^b \delta_{ij} + B \sigma_{ji}^b \sigma_{ij}^a$$

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or, \(- \psi_i^\dagger \sigma_{ij}^b \psi_j = A \sigma_{ii}^b + B \sigma_{ij}^a \sigma_{ij}^a = B \left( \sigma^b \sigma^a \right)_{ii} \)

or, \(- \psi^\dagger \sigma^b \psi = B \left( \delta_{ba} + i \epsilon_{bac} \sigma^c \right)_{ii} = 2B \delta_{ba} \)

\[ \rightarrow B = - \frac{1}{2} (\psi^\dagger \sigma^a \psi) . \] (5.52)

Thus, we finally get the following expression.

\[ \psi_i^\dagger \psi_j = - \frac{1}{2} (\psi^\dagger \psi) \delta_{ij} - \frac{1}{2} (\psi^\dagger \sigma^a \psi) \sigma_{ij}^a . \] (5.53)

If we substitute this result into \((\psi^\dagger \psi)^2 = \psi_i^\dagger \{ \psi_i \psi_j \} \psi_j\), we find

\[ (\psi^\dagger \psi)^2 = - \frac{1}{2} (\psi^\dagger \psi)^2 - \frac{1}{2} (\psi^\dagger \sigma \psi)^2 , \] (5.54)

or

\[ (\psi^\dagger \sigma \psi)^2 = -3 (\psi^\dagger \psi)^2 . \] (5.55)

(We could also start with \((\psi_i^\dagger \sigma_{iv}^a \psi_v)(\psi_j^\dagger \sigma_{jv}^a \psi_v)\) and obtain the same result with a bit more effort). Therefore

\[ C_0(\psi^\dagger \psi)^2 + C_0^\sigma (\psi^\dagger \sigma \psi)^2 = (C_0 - 3C_0^\sigma)(\psi^\dagger \psi)^2 \] (5.56)

and the single term \(\tilde{C}_0(\psi^\dagger \psi)^2\) with \(\tilde{C}_0 \equiv C_0 - 3C_0^\sigma\) yields the same results for all diagrams as the original two terms. This is illustrated in appendix C for HF and the beachball diagrams.

For the \(\nu = 4\) case with spin and isospin, we perform a similar procedure to find

\[ \psi_i^\dagger \psi_j^\dagger = - \frac{1}{4} (\psi^\dagger \psi) \delta_{ij} \delta_{\alpha \beta} - \frac{1}{4} (\psi^\dagger \sigma^a \psi) \sigma_{ij}^a \delta_{\alpha \beta} - \frac{1}{4} (\psi^\dagger \tau^b \psi) \delta_{ij} \tau_{\alpha \beta}^b - \frac{1}{4} (\psi^\dagger \sigma^a \tau^b \psi) \sigma_{ij}^a \tau_{\alpha \beta}^b . \] (5.57)

Substituting into any two of \((\psi^\dagger \psi)^2\), \((\psi^\dagger \sigma \psi)^2\), \((\psi^\dagger \tau \psi)^2\), and \((\psi^\dagger \sigma \tau \psi)^2\), we find two independent relations, which can be solved simultaneously to find:

\[ (\psi^\dagger \tau \psi)^2 = -2(\psi^\dagger \psi)^2 - (\psi^\dagger \sigma \psi)^2 \] (5.58)

\[ (\psi^\dagger \sigma \tau \psi)^2 = -3(\psi^\dagger \psi)^2 , \] (5.59)
which allow us to eliminate explicit dependence on $\tau$ matrices in favor of just two independent couplings:

$$
C_0(\psi^\dagger\psi)^2 + C_0^\tau(\psi^\dagger\sigma\psi)^2 + C_0^\sigma(\psi^\dagger\tau\psi)^2 + C_0^\sigma^\tau(\psi^\dagger\sigma\tau\psi)^2
$$

$$
= (C_0 - 2C_0^\tau - 3C_0^\sigma)(\psi^\dagger\psi)^2 + (C_0^\sigma - C_0^\sigma^\tau)(\psi^\dagger\sigma\psi)^2.
$$

(5.60)

This agrees with the usual discussion in terms of antisymmetrized interactions [107, 76]. The choice to eliminate the $\tau$ terms is purely conventional. The convention with Skyrme interactions is to choose the independent couplings to be $t_i$ and $x_i$, which multiply terms in the effective interaction in the combination $t_i(1 + x_i P_\sigma)$, with $P_\sigma$ the spin exchange operator. Extending to more derivatives and the spin-orbit (and tensor) terms follows systematically in the EFT approach, but introduces many more constants; complete sets of contact terms with more derivatives in the EFT Lagrangian can be found in Refs. [89] and [90]. The proliferation of constants leads to a clash of philosophies between the minimalist, phenomenological approach (use as few terms as possible), which is necessarily model dependent, and the model-independent EFT approach (use a complete set of terms).

The similarities of the successful Skyrme functional and the DFT functional for a dilute Fermi gas prompts an analysis of typical Skyrme parameters as effective range parameters. One can use the association of the $t_i$’s and the $C_i$’s along with numerical values from successful Skyrme parameterizations (e.g., Ref. [78]) to estimate “equivalent” values of $a_s$, $r_s$, and $a_p$. We find that $a_s \approx -2$–3 fm, which is about the inverse pion mass and is much smaller than the large, fine-tuned values of the free-space nucleon-nucleon interaction (however, some Skyrme parameterization have an “equivalent” $a_s$ of 5 femtometer or larger). However, $k_P a_s$ is still significantly larger than unity inside a nucleus, which precludes a perturbative dilute expansion. Interestingly, the
equivalent $r_s$ and $a_p$ values have magnitudes consistent with what one might expect from the nuclear hard-core radius (with $a_p < 0$), leading to $k_F r_s$ and $k_F a_p$ less than unity.

5.3 Results for Dilute Fermi System in a Trap

In this section, we present numerical results for the dilute Fermi system comprised of a small number of fermions confined in a harmonic oscillator trap. We compare the nature of the convergence of the EFT in a finite system both qualitatively and quantitatively to the analysis done purely in the LDA [42], which means the effect of treating the Hartree-Fock contributions at NNLO [Fig. 3.3(i) and (j)] exactly.

5.3.1 Kohn-Sham Self-Consistent Procedure

As in the previous chapter, we restrict our calculations to finding the Kohn-Sham orbitals for closed shells, so the density and potentials are functions only of the radial coordinate $r \equiv |\mathbf{x}|$. Note that the basic procedure is the same one used for closed-shell nuclei in Skyrme-Hartree-Fock [107], even though the DFT/EFT can include correlations to any order. The Kohn-Sham iteration procedure is the same in principle as before. We enumerate the steps once again for convenience.

1. Start by solving the Schrödinger equation with the external potential profile $v(r)$ for the lowest $A$ states (including degeneracies) to find a set of orbitals and Kohn-Sham eigenvalues $\{\psi_k, \varepsilon_k\}$.

2. Compute the density and kinetic energy density from the occupied orbitals:

$$
\rho(r) = \nu \sum_k |\psi_k(\mathbf{x})|^2, \tag{5.61}
$$

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\[ \tau(r) = \frac{\nu}{4\pi} \int d\Omega \, \tau(\mathbf{x}) = \frac{\nu}{4\pi} \sum_k \int d\Omega \, |\nabla \psi_k(\mathbf{x})|^2 . \] (5.62)

3. Using Eqs. (5.44)-(5.45), find \( J_0(r) \) and \( \eta_0(r) \). Evaluate the local single-particle potential

\[ v_s[\rho(r), \tau(r)] \equiv v_s(r) \equiv v(r) - J_0(r) \] (5.63)

at the chosen level of approximation (e.g., NLO) and the “effective” mass:

\[ \frac{1}{2M^*(r)} = \frac{1}{2M} - \eta_0(r) . \] (5.64)

4. Solve the Skyrme-type Schrödinger equation for the lowest \( A \) states (including degeneracies), to find \( \{\psi_k, \varepsilon_k\} \) as before:

\[ \left[-\nabla^2 \frac{1}{2M^*(r)} \nabla + v_s(r)\right] \psi_k(\mathbf{x}) = \varepsilon_k \psi_k(\mathbf{x}) . \] (5.65)

5. Repeat steps 2.-4. until changes are acceptably small (“self-consistency”). In practice, the changes in the density are “damped” by using a weighted average of the densities from the \((n-1)\)th and \(n\)th iterations:

\[ \rho(r) = \beta \rho_{n-1}(r) + (1 - \beta) \rho_n(r) , \] (5.66)

with \( 0 < \beta \leq 1 \).

This procedure has been implemented for dilute fermions in a trap using two different methods for carrying out step 4. The Kohn-Sham single-particle equations are solved in one approach by direct integration of the differential equations and in the other approach by diagonalization of the single-particle Hamiltonian in a truncated basis of unperturbed harmonic oscillator wavefunctions as described before. The same results are obtained to high accuracy.

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5.3.2 Fermions in a Harmonic Trap

The interaction through NNLO is specified in terms of the three effective range parameters $a_s$, $r_s$, and $a_p$. For the numerical calculations presented here, we consider the natural case of hard-sphere repulsion with radius $R$, in which case $a_s = a_p = R$ and $r_s = 2R/3$, and also the case with $a_p = 2a_s$, so we can emphasize the effect of $M^*(r)/M$ significantly less than unity.

As in the previous chapter, lengths are measured in units of the oscillator parameter $b \equiv \sqrt{\hbar/M\omega}$, masses in terms of the fermion mass $M$, and $\hbar = 1$. In these units, $\hbar\omega$ for the oscillator is unity and the Fermi energy of a non-interacting gas with filled shells up to $N_F$ is $E_F = (N_F + 3/2)$. The total number of fermions $A$ is related to $N_F$ by the same equation as before (Eq. (4.73)).

With spin-independent interactions included, single-particle states are labeled as before by $n, \ell, m_\ell$ and the radial functions depend only on $n$ and $\ell$, so the degeneracy of each level is $\nu \times (2\ell + 1)$. The solutions take the form (times a spinor, which is suppressed)

$$\psi_{n\ell m_\ell}(x) = R_{n\ell}(r) Y_{m_\ell}(\Omega) = \frac{u_{n\ell}(r)}{r} Y_{m_\ell}(\Omega) .$$  \hspace{1cm} (5.67)

Taking the Skyrme equation with the position dependent mass term, we carry out the normal separation of variables method. Proceeding in the usual straightforward manner, we find that the radial function $u_{n\ell}(r)$ satisfies

$$\left[ -\frac{1}{2M^*(r)} \frac{d^2}{dr^2} - \frac{d\eta_0}{dr} \left( \frac{1}{r} - \frac{d}{dr} \right) + v_s(r) + \frac{\ell(\ell + 1)}{2M^*(r)r^2} \right] u_{n\ell}(r) = \varepsilon_{n\ell} u_{n\ell}(r) ,$$  \hspace{1cm} (5.68)

where the $u_{n\ell}$’s are normalized according to

$$\int_0^{\infty} |u_{n\ell}(r)|^2 dr = 1 .$$  \hspace{1cm} (5.69)
As before, the density is given by

$$\rho(\mathbf{x}) = \nu \sum_{n\ell} \frac{\text{occ.}}{4\pi} |R_{n\ell}(r)|^2,$$

(5.70)

The kinetic energy density is given by

$$\tau(\mathbf{x}) = \nu \sum_{n\ell m_\ell} |\nabla \psi_{n\ell m_\ell}(\mathbf{x})|^2.$$

(5.71)

Now, from Ref. [113],

$$\nabla \psi_{n\ell m_\ell}(\mathbf{x}) = -A_{n\ell}(r) Y_{\ell \ell+1 m_\ell}(\Omega) + B_{n\ell}(r) Y_{\ell \ell-1 m_\ell}(\Omega),$$

(5.72)

where

$$A_{n\ell}(r) = \sqrt{\frac{\ell + 1}{2\ell + 1}} \left( \frac{d}{dr} - \frac{\ell}{r} \right) R_{n\ell}(r),$$

$$B_{n\ell}(r) = \sqrt{\frac{\ell}{2\ell + 1}} \left( \frac{d}{dr} + \frac{\ell + 1}{r} \right) R_{n\ell}(r),$$

(5.73)

and $Y_{j \ell m}(\Omega)$ is the vector spherical harmonics defined in terms of the ordinary spherical harmonics as

$$Y_{j \ell m}(\Omega) = \sum_{m_\ell} C(\ell 1 j |m_\ell m j) Y_{m \ell} \mathbf{e}_m.$$

(5.74)

$C(j_1 j_2 j |m_1 m_2 m)$ is the Clebsch-Gordon coefficient that comes while adding two angular momenta $j_1$ and $j_2$ to form $j$, and $\mathbf{e}_m$ are the spherical basis vectors given in terms of the cartesian basis vectors as

$$\mathbf{e}_1 = -\frac{1}{\sqrt{2}} (\mathbf{x} + i \mathbf{y}), \quad \mathbf{e}_0 = \mathbf{z}, \quad \mathbf{e}_{-1} = \frac{1}{\sqrt{2}} (\mathbf{x} - i \mathbf{y}).$$

(5.75)

The vector spherical harmonics obey the orthogonality relation

$$\int d\Omega \ Y_{j_1 \ell_1 m_{j_1}}(\Omega) \ Y_{j_2 \ell_2 m_{j_2}}(\Omega) = \delta_{j_1 j_2} \delta_{\ell_1 \ell_2} \delta_{m_{j_1} m_{j_2}}.$$

(5.76)
Table 5.1: Energies per particle, averages of the local Fermi momentum $k_F$, and rms radii for sample parameters and particle numbers for a dilute Fermi gas in a harmonic trap. See the text for a description of units. The scattering length is fixed at $a_s = 0.16$ and the effective range is set to $r_s = 2a_s/3$ when $a_p \neq 0$. Results with the DFT functional including $\tau$ are marked “$\tau$-NNLO.”

Now we can proceed with the derivation of the expression for the kinetic energy density [91]:

$$\tau(r) = \frac{1}{4\pi} \int d\Omega \tau(x)$$

$$= \frac{\nu}{4\pi} \sum_{\text{occ.}} \sum_{n\ell m} |\nabla \psi_{n\ell m}(x)|^2$$

$$= \frac{\nu}{4\pi} \sum_{\text{occ.}} \left( |A_{n\ell}(r)|^2 + |B_{n\ell}(r)|^2 \right)$$

$$= \frac{\nu}{4\pi} \sum_{\text{occ.}} \sum_{n\ell} (2\ell + 1) \left[ \left( \frac{dR_{n\ell}}{dr} \right)^2 + \frac{\ell(\ell + 1)}{r^2} |R_{n\ell}(r)|^2 \right]. \quad (5.77)$$

In the above derivation, we have used the orthogonality relation while doing the angular integral. The interactions are sufficiently weak that the occupied states are in one-to-one correspondence with those occupied in the non-interacting harmonic oscillator potential.
Figure 5.1: NNLO Kohn-Sham density distributions for a dilute gas of fermions in a harmonic trap with degeneracy $\nu = 2$ filled up to $N_F = 7$, which implies there are 240 particles in the trap. The scattering length is $a_s = 0.16$ and the effective range is $r_s = 2a_s/3$. Results for two values of $a_p$ are compared for the LDA $\rho$-only functional ($\rho$-DFT) and with $\tau$ ($\rho\tau$-DFT).

Figure 5.2: Deviation of $\rho\tau$-DFT from $\rho$-DFT results at NNLO for the same systems as in Fig. 5.1.
Figure 5.3: Kohn-Sham potential for the same systems as in Fig. 5.1. The original external harmonic potential is also plotted, along with the \( A = 20 \) case.

Figure 5.4: NNLO Kohn-Sham kinetic-energy-density distributions for the same systems as in Fig. 5.1. The upper three curves are for \( a_p = a_s \) and the lower three curves are for \( a_p = 2a_s \).
5.3.3 Numerical Results

Here we compare density distributions at zero temperature for the LDA analysis [42] to those from evaluating Figs. 3.3(i) and (j) exactly at NNLO (where the differences first appear in the present analysis). This comparison obviously makes sense only if at least one of $r_s$ and $a_p$ is non-zero. We choose 240 particles as a representative example (other numbers of particles give qualitatively similar results). Densities at different orders in the DFT expansion were shown in Ref. [42]. Results for the energy per particle $E/A$, average Fermi momentum $\langle k_F \rangle$ and the rms radius are given in Table 5.1.

In Fig. 5.1, we compare the densities at NNLO in the Kohn-Sham formalism with $\rho$-only functionals (the LDA calculation from Ref. [42]) to the same system with the
Figure 5.6: Comparison of selected single-particle energy spectra for the same systems as in Fig. 5.1.
\( \rho \tau \) functionals. For hard-sphere scattering (for which \( a_p = a_s \)), the density curves are almost indistinguishable. If we plot the difference on an expanded scale (see Fig. 5.2), we can see a small amplitude oscillation. The close agreement is not surprising given that the source of the difference is the NNLO Hartree-Fock terms, so the difference itself is higher order in the EFT expansion (note that the \( \rho \)-DFT and \( \rho \tau \)-DFT NNLO energies in Table 5.1 differ only by 0.01). We can magnify the difference by considering \( a_p = 2a_s \), which multiplies the corresponding Hartree-Fock term by a factor of eight (which also implies that the \( C_2 \) coefficient is unnaturally large). For this case, the difference in Fig. 5.1 is visible and significant oscillations are seen in Fig. 5.2. The increased oscillation is analogous to the difference between Thomas-Fermi and Kohn-Sham DFT densities (shown in Ref. [42]), although not as dramatic. The explanation is also analogous: the \( \rho \tau \)-DFT captures more non-locality into the DFT functional. Fig. 5.2 illustrates how a typical Kohn-Sham potential looks like once the iteration has converged.

The kinetic energy densities for these cases are shown in Fig. 5.4. When calculated from the Kohn-Sham wave functions, \( \tau(r) \) is quite similar for the \( \rho \)-only and \( \rho \tau \) calculations. Also shown in this figure is the leading contribution from the semiclassical approximation, which reproduces the “exact” kinetic energy densities except near the origin.

Since the densities, kinetic energy densities and energy per particle are not drastically different for the \( \rho \) and \( \rho \tau \) DFT, one may expect the single-particle energy spectra to be similar. But this is not the case (Fig. 5.6). The effective mass \( M^*(r) \) is different from unity in the \( \rho \tau \) case. It is shown in Fig. 5.5 for the two values of \( a_p \).
The values close to the origin are in the range of those obtained in Skyrme functionals fit to nuclear data. In those functionals, the value of $M^*$ is associated with the single-particle energy levels. This correspondence is seen in the single-particle energy spectra in Fig. 5.6, where we observe that the $\rho\tau$ levels will always lie lower except at the Fermi surface. In the next chapter, we shall estimate the difference in the levels in the uniform system limit.

This comparison demonstrates how the Kohn-Sham formalism can be misinterpreted. Even though the single-particle energies differ significantly, they are not observables. Indeed, the true bulk observables calculated in the DFT framework, those in Table 5.1, are barely distinguishable. One could ask whether the single-particle levels in some representation are \textit{“better”} than in other representations. In particular, they can be compared to the energy spectrum corresponding to the poles of the exact Green’s function, which can be constructed in terms of the Kohn-Sham Green’s function [47]. We shall investigate this matter in the next chapter.

It is not clear from the present calculation how close the full and Kohn-Sham spectra would be if the LDA were relaxed [e.g., for Fig. 3.3(b)]. It would be useful to add spin-orbit interactions and then to study Kohn-Sham spin-orbit splittings near the Fermi surface, since such splittings are sometimes fit in mean-field models.

\section*{5.3.4 Power Counting and Convergence}

The effective field theory approach allows us to estimate contributions to the energy. At each successive order in the EFT expansion, the low-energy constants (LEC’s) can be estimated using naive dimensional analysis, or NDA [42]. In the case of a short-range force with a natural scattering length, the underlying momentum
scale $\Lambda \sim 1/R$, where $R$ is the range of the potential, is the basic ingredient in
the NDA. The estimate of two-body Hartree-Fock energy contributions from a given
term in the Lagrangian can be found by replacing $\psi^\dagger \psi$ by the average density (and
including an appropriate spin factor) and the coefficient by the natural estimate
$C_{2i} \sim 4\pi/MA^{2\nu+1}$ [41]. As an example, the NDA estimate of the Hartree-Fock energy
per particle at LO was computed from Eq. (4.60) as :

$$
\left( \frac{E_{\text{HF}}}{A} \right)_{\text{NDA}} \approx \frac{1}{2} \left( \frac{\nu - 1}{\nu} \right) \frac{4\pi}{MA} \langle \rho(x) \rangle ,
$$

(5.78)

with $\Lambda = 1/R = 1/a_s$ for a hard-sphere potential. The Thomas-Fermi result can be
used to find the average density, or one might just take the actual computed average
value (the results will differ by much less than the uncertainty in the estimate). The
NLO estimate was found by multiplying the LO result by $\langle k_F a_s \rangle$, where $\langle k_F \rangle$ is the
average Fermi momentum [42]. At NNLO, we have three terms. The $\rho^{8/3}$ LDA term
was estimated by multiplying the LO result by $(\langle k_F a_s \rangle)^2$, and the other two terms
($\rho \tau$ and $\nabla \rho$) arising from Hartree-Fock at that order was estimated directly as in the
case of LO (using $\langle \rho \tau \rangle \approx \langle \rho \rangle \langle \tau \rangle$).

In Figs. 5.7 and 5.8, estimates and actual contributions are shown for $\nu = 4$, $A = 140$, $a_s = 0.10$ (for which $\langle k_F a_s \rangle \approx 0.24$) and for $\nu = 2$, $A = 240$, $a_s = 0.16$ (for
which $\langle k_F a_s \rangle \approx 0.5$). Square symbols denote estimates based on naive dimensional
analysis, with error bars indicating a 1/2 to 2 uncertainty in the estimate. Actual
contributions to the energy per particle from each of the orders are shown as round
symbols, i.e., the actual NLO contribution is $|E_{\text{NLO}} - E_{\text{LO}}|/A$. At NNLO, we plot
estimated contributions from the $\rho^{8/3}$ LDA, $\rho \tau$, and gradient terms separately. The
latter gives a very small contribution consistent with its NDA estimate, and it has

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been multiplied by ten in Figs. 5.7 and 5.8 to fit them on the graphs. The two sets of estimates and results correspond to $a_p = a_s$ (hard sphere) and $a_p = 0$.

We see from Figs. 5.7 and 5.8 that the actual results for LO, NLO and NNLO agree well with NDA estimates, including the new gradient contributions, with one exception. The exception is the $\rho^{8/3}$ LDA estimate for the $\nu = 2$ system, which greatly overestimates the actual contribution at that order due to an accidental cancellation when $\nu = 2$ between the two terms in the $b_4$ coefficient in Eq. (4.62) [42]. In general, however, we can use these estimates to reliably predict the uncertainty in the energy per particle from higher orders.
Figure 5.7: Energy estimates (squares and error bars) for $\nu = 4$, $a_s = 0.10$, $A = 140$ particles compared with actual values (circles) for a hard-sphere gas (solid) and with the p-wave scattering length equal to zero (shaded).

Figure 5.8: Energy estimates (squares and error bars) for $\nu = 2$, $a_s = 0.16$, $A = 240$ particles compared with actual values (circles) for a hard-sphere gas (solid) and with the p-wave scattering length equal to zero (shaded).
CHAPTER 6

SINGLE-PARTICLE PROPERTIES FROM KS GREEN’S FUNCTIONS

In this chapter, we use the effective action approach to Kohn-Sham density functional theory to illustrate how the exact Green’s function can be calculated in terms of the Kohn-Sham Green’s function. We find that single-particle Kohn-Sham spectra can be improved by adding sources used to construct the energy functional for an example based on Skyrme energy functionals.

The Skyrme formalism as an approximate implementation of Kohn-Sham density functional theory (DFT) [51] implies that only bulk observables can be calculated reliably. These do not include single-particle quantities. This is because only for the bulk observables can the DFT framework accommodate all correlations in principle (if not in practice because of the limited form of the energy functionals actually used) [4, 105, 104]. Nevertheless, single-particle energies and wave functions from Skyrme and other DFT-like formalisms are also regularly used.

In this chapter, we illustrate how to extend the effective action approach to Kohn-Sham DFT [55, 54, 42, 94] to calculate the full single-particle Green’s function in terms of Kohn-Sham Green’s functions at the same level of approximation. Our discussion directly adapts the extension described in the context of Coulomb systems
in Refs. [46, 47]. This connection between Green’s functions helps to clarify both some misconceptions and limitations of the Kohn-Sham approach, and suggests how to improve calculations of single-particle properties. At first, we consider functionals of the fermion density only, and then compare to generalized functionals that also depend on the kinetic energy density to illustrate the effect of additional sources.

6.1 Formalism

We introduce a generating functional in the path integral formulation with a Lagrangian $\mathcal{L}$ supplemented by a local c-number source $J(x)$ coupled to the composite density operator and a non-local c-number source $\xi(x, x')_{\alpha\beta}$ coupled to $\psi_\alpha(x)\psi_\beta^\dagger(x')$, 

$$Z[J, \xi] = e^{iW[J, \xi]} = \int D\psi D\psi^\dagger e^{i \int d^4x \left[ \mathcal{L} + J(x)\psi_\alpha^\dagger(x)\psi_\alpha(x) + \int d^4x' \xi(x, x')_{\alpha\beta}\psi_\alpha(x)\psi_\beta^\dagger(x') \right]}, \quad (6.1)$$

where $\alpha$ and $\beta$ are spin indices and summation of repeated indices is implied. As before, for simplicity, normalization factors are considered to be implicit in the functional integration measure [44, 45]. As a specific example, we will use the effective field theory (EFT) Lagrangian appropriate for a dilute Fermi system [41], but the discussion can be adapted to any system for which a hierarchy of approximations can be defined.

The fermion density in the presence of the sources $J$ and $\xi$ is 

$$\rho(x) = \langle \psi_\alpha^\dagger(x)\psi_\alpha(x) \rangle_{J, \xi} = \frac{1}{iZ} \frac{\delta Z[J, \xi]}{\delta J(x)} = \frac{\delta W[J, \xi]}{\delta J(x)}. \quad (6.2)$$

Note that the sources here are time dependent, in contrast to the more limited discussion with static sources in the previous chapters; however, the generalization of the formalism is direct. A functional Legendre transformation from $J$ to $\rho$, which takes us from $W$ to the effective action $\Gamma$, produces an energy functional of the density,
which is minimized at the exact ground-state density for time-independent sources.\(^5\)

The inversion method [44, 45] carries out this inversion order-by-order in a specified expansion. At the end, one sets \( J(x) \) and \( \xi(x, x') \) to zero. (Although we are unaware of any general problems, we have not excluded the possibility of complications in making the inversions with time-dependent sources.)

Solving the zeroth-order system leads us to define the Green’s function \( G_{ks}(x, x')_{\alpha\beta} \) of the Kohn-Sham non-interacting system in the presence of \( \xi(x, x')_{\alpha\beta} \), the Kohn-Sham potential \( J_0(x) \), and an external potential \( v(x) \). This Green’s function satisfies

\[
\int d^4z \ [G_{ks}(x, z)]^{-1}_{\alpha\gamma} G_{ks}(z, x')_{\gamma\beta} = \delta_{\alpha\beta} \delta^4(x - x') ,
\]

or

\[
\int d^4z \left[ i\partial_t + \frac{\nabla^2}{2M} - v(x) + J_0(x) \right] \delta_{\alpha\gamma} \delta^4(x - z) - \xi(z, x)_{\gamma\alpha} G_{ks}(z, x')_{\gamma\beta} = \delta_{\alpha\beta} \delta^4(x - x') ,
\]

with appropriate finite-density boundary conditions. Note that \( G_{ks} \) doesn’t take a simple form in terms of orbitals [see \( G_{ks}^0 \) in Eq. (5.21)] until we set \( \xi = 0 \) and restrict ourselves to time independent \( J_0 \).

Functional derivatives of \( W \) with respect to \( \xi(x, x') \) gives the two-point function in the presence of the sources,

\[
iG(x, x')_{\alpha\beta} \equiv \langle T[\psi_\alpha(x)\psi_\beta^*(x')] \rangle_{J, \xi} = \frac{1}{i\delta Z} \frac{\delta Z[J, \xi]}{\delta \xi(x, x')_{\alpha\beta}} = \frac{\delta W[J, \xi]}{\delta \xi(x, x')_{\alpha\beta}} .
\]

The exact ground-state Green’s function is obtained by setting \( \xi = J = 0 \) after taking derivatives. The key results we require in order to evaluate Eq. (6.5) in terms of Kohn-Sham quantities were given in Refs. [46, 47] and are rederived here. First,

\(^5\)Note that the energy functional is only obtained once \( \xi \) is set to zero.
functional derivatives with respect to $\xi$ of $W$ and $\Gamma$ are directly related, where

$$
\Gamma[\rho, \xi] = W[J, \xi] - \int d^4 y J(y) \rho(y)
$$

(6.6)
is the effective action. Namely, the functional derivative with respect to $\xi$ of this equation yields (spin indices are suppressed)

$$
\left( \frac{\delta \Gamma[\rho, \xi]}{\delta \xi(x, x')} \right)_\rho = \left( \frac{\delta W[J, \xi]}{\delta \xi(x, x')} \right)_J + \int d^4 y \left( \frac{\delta W[J, \xi]}{\delta J(y)} \right) \frac{ \delta J(y) }{ \delta \xi(x, x') } \rho(y),
$$

(6.7)
from which the last two terms cancel, leaving

$$
\left( \frac{\delta W[J, \xi]}{\delta \xi(x, x')} \right)_{\alpha \beta} = \left( \frac{\delta \Gamma[\rho, \xi]}{\delta \xi(x, x') \alpha \beta} \right)_\rho.
$$

(6.8)
(Here and below we repeatedly apply the functional relations

$$
\left( \frac{\delta F}{\delta \xi} \right)_\rho = \left( \frac{\delta F}{\delta \xi} \right)_J + \left( \frac{\delta F}{\delta J} \right)_{\xi} \frac{ \delta J }{ \delta \xi } \rho = \left( \frac{\delta F}{\delta \xi} \right)_J - \left( \frac{\delta F}{\delta \rho} \right)_{\xi} \frac{ \delta \rho }{ \delta \xi } J,
$$

(6.9)
where $F = F[J, \xi]$ and arguments and integrals are implied.) Equation (6.8) is a special case of a general result for Legendre transformations proved in Ref. [101].

Next, this relation applied to the zeroth order (Kohn-Sham) system yields the Kohn-Sham Green’s function,

$$
\left( \frac{\delta \Gamma_0[\rho, \xi]}{\delta \xi(x, x') \alpha \beta} \right)_\rho = \left( \frac{\delta W_0[J_0, \xi]}{\delta \xi(x, x') \alpha \beta} \right)_J = iG_{ks}(x, x')_{\alpha \beta}.
$$

(6.10)
We divide the full effective action into zeroth order and interacting pieces,

$$
\Gamma[\rho, \xi] = \Gamma_0[\rho, \xi] + \Gamma_{\text{int}}[\rho, \xi].
$$

(6.11)
Since $\Gamma_{\text{int}}[\rho, \xi]$ depends on $\xi$ only through $G_{ks},$

$$
\left( \frac{\delta \Gamma_{\text{int}}[\rho, \xi]}{\delta \xi(x, x') \alpha \beta} \right)_\rho = \int \int \frac{\delta \Gamma_{\text{int}}[\rho, \xi]}{\delta G_{ks}(y, y') \gamma} \left( \frac{\delta G_{ks}(y, y') \gamma}{\delta \xi(x, x') \alpha \beta} \right)_\rho d^4 y d^4 y'.
$$

(6.12)
The second half of the integrand can be rewritten
\[
\left( \frac{\delta G_{ks}(y, y')_{\delta \gamma}}{\delta \xi(x, x')_{\alpha \beta}} \right)_{\rho} = \left( \frac{\delta G_{ks}(y, y')_{\delta \gamma}}{\delta \xi(x, x')_{\alpha \beta}} \right)_{J_0} + \int \left( \frac{\delta G_{ks}(y, y')_{\delta \gamma}}{\delta J_0(z)} \right)_{\xi} \left( \frac{\delta J_0(z)}{\delta \xi(x, x')_{\alpha \beta}} \right)_{\rho} d^4 z
\]
\[
\quad = \left( \frac{\delta G_{ks}(y, y')_{\delta \gamma}}{\delta \xi(x, x')_{\alpha \beta}} \right)_{J_0} - \int \left( \frac{\delta G_{ks}(y, y')_{\delta \gamma}}{\delta \rho(z)} \right)_{\xi} \left( \frac{\delta \rho(z)}{\delta \xi(x, x')_{\alpha \beta}} \right)_{J_0} d^4 z
\]
\[
\quad = G_{ks}(x, y')_{\alpha \gamma} G_{ks}(x, z)_{\delta \beta} + i \int \left( \frac{\delta G_{ks}(y, y')_{\delta \gamma}}{\delta \rho(z)} \right)_{\xi} G_{ks}(x, z)_{\alpha \lambda} G_{ks}(z, x')_{\lambda \beta} d^4 z. \quad (6.13)
\]

The second line follows by applying [Eq. (6.9) with \( F \rightarrow J_0 \)]
\[
\left( \frac{\delta J_0(z)}{\delta \xi(x, x')_{\alpha \beta}} \right)_{\rho} = - \int \left( \frac{\delta J_0(z)}{\delta \rho(z')} \right)_{\xi} \left( \frac{\delta \rho(z')}{\delta \xi(x, x')_{\alpha \beta}} \right)_{J_0} d^4 z', \quad (6.14)
\]
and simplifying. The functional derivatives in the second line can be evaluated by using the expression for \( G_{ks} \) in terms of the noninteracting generating functionals.

Thus,
\[
\left( \frac{\delta G_{ks}(y, y')_{\delta \gamma}}{\delta \xi(x, x')_{\alpha \beta}} \right)_{J_0} = \frac{\delta}{\delta \xi(x, x')_{\alpha \beta}} \left[ - \frac{1}{Z_0} \frac{\delta Z_0[J_0, \xi]}{\delta \xi(y, y')_{\delta \gamma}} \right]
\]
\[
\quad = \left[ \frac{1}{Z_0} \frac{\delta Z_0[J_0, \xi]}{\delta \xi(x, x')_{\alpha \beta}} \right] \left[ \frac{1}{Z_0} \frac{\delta Z_0[J_0, \xi]}{\delta \xi(y, y')_{\delta \gamma}} \right] - \frac{1}{Z_0} \frac{\delta^2 Z_0[J_0, \xi]}{\delta \xi(x, x')_{\alpha \beta} \delta \xi(y, y')_{\delta \gamma}}
\]
\[
\quad = (-i)^2 \langle T \psi_{\alpha}(x) \psi_{\gamma}^\dagger(y) \rangle \langle T \psi_{\delta}(y) \psi_{\beta}^\dagger(x') \rangle
\]
\[
\quad = G_{ks}(x, y')_{\alpha \gamma} G_{ks}(y, x')_{\delta \beta} \quad (6.15)
\]

and
\[
\left( \frac{\delta \rho(z)}{\delta \xi(x, x')_{\alpha \beta}} \right)_{J_0} = -i \left( \frac{\delta G_{ks}(z, z')_{\delta \delta}}{\delta \xi(x, x')_{\alpha \beta}} \right)_{J_0} = -i G_{ks}(x, z)_{\alpha \delta} G_{ks}(z, x')_{\delta \beta}. \quad (6.16)
\]

Alternatively, we can expand \( \delta (G_{ks} G_{ks}^{-1}) / \delta \xi = 0 \) and use \( \delta G_{ks}^{-1} / \delta \xi = -1 \).

Substituting Eq. (6.13) back into Eq. (6.12), we find that
\[
\left( \frac{\delta \Gamma_{\text{int}}[\rho, \xi]}{\delta \xi(x, x')_{\alpha \beta}} \right)_{\rho} = \int \int G_{ks}(x, y')_{\alpha \gamma} \frac{\delta \Gamma_{\text{int}}[\rho, \xi]}{\delta G_{ks}(y, y')_{\delta \gamma}} G_{ks}(y, x')_{\delta \beta} d^4 y d^4 y'
\]
\[
\quad + i \int G_{ks}(x, y)_{\alpha \lambda} \frac{\delta \Gamma_{\text{int}}[\rho, \xi]}{\delta \rho(y)} G_{ks}(y, x')_{\lambda \beta} d^4 y. \quad (6.17)
\]
Equations (6.10) and (6.17), together with

$$iG(x, x')_{\alpha\beta} = \left( \frac{\delta W[J, \xi]}{\delta \xi(x, x')_{\alpha\beta}} \right)_J = \left( \frac{\delta \Gamma[\rho, \xi]}{\delta \xi(x, x')_{\alpha\beta}} \right)_\rho = \left( \frac{\delta \Gamma_0[\rho, \xi]}{\delta \xi(x, x')_{\alpha\beta}} \right)_\rho + \left( \frac{\delta \Gamma_{\text{int}}[\rho, \xi]}{\delta \xi(x, x')_{\alpha\beta}} \right)_\rho,$$

(6.18)

imply a Dyson equation for the exact Green’s function:

$$G(x, x')_{\alpha\beta} = G_{ks}(x, x')_{\alpha\beta} + \int G_{ks}(x, y')_{\alpha\gamma} \Sigma_{ks}(y', y)_{\gamma\delta} G_{ks}(y, x')_{\delta\beta} \, d^4y \, d^4y', \quad (6.19)$$

which defines a self-energy $\Sigma_{ks}$ as

$$\Sigma_{ks}(y', y)_{\gamma\delta} = \frac{1}{i} \frac{\delta \Gamma_{\text{int}}[\rho, \xi]}{\delta G_{ks}(y, y')_{\delta\gamma}} + \frac{\delta \Gamma_{\text{int}}[\rho, \xi]}{\delta \rho(y)} \delta_{\gamma\delta} \delta^4(y' - y)$$

$$= \Sigma'_{ks}(y', y)_{\gamma\delta} + J_0(y') \delta_{\gamma\delta} \delta^4(y' - y). \quad (6.20)$$

In the second line, the self-consistent Kohn-Sham potential $J_0$ is equal to $\delta \Gamma_{\text{int}}/\delta \rho$ only when we set $J = 0$ [42]. Neither $\Sigma_{ks}$ nor $\Sigma'_{ks}$ is the conventional self-energy, which is built from non-interacting (rather than Kohn-Sham) Green’s functions. We can obtain $\Sigma'_{ks}(y', y)$ at the diagrammatic level by opening each $G_{ks}$ line in turn in a given Feynman diagram for $\Gamma_{\text{int}}$. It consists of the same diagrams as the conventional one-particle-reducible self-energy, but with the fermion lines given by $G_{ks}$ rather than the non-interacting Green’s function (which includes only the external potential).

Now consider applying these equations with $\xi = J = 0$ after taking functional derivatives; we denote the Kohn-Sham Green’s function in this case as $G^0_{ks}$. For simplicity we will consider spin-independent interactions, so that the Green’s functions and self-energies are diagonal in spin ($G^0_{ks}(x, x')_{\alpha\beta} = \delta_{\alpha\beta} G^0_{ks}(x, x')$). Kohn-Sham orbitals arise as solutions to Eq. (4.25). The decomposition of $G^0_{ks}(x, x')_{\alpha\beta}$ in terms of these orbitals given by Eq. (4.34) corresponds (in frequency space) to simple poles, just like a Hartree Green’s function. It is well known that the Kohn-Sham single-particle
Figure 6.1: Equation for the full propagator in terms of the Kohn-Sham Green’s functions and self-energy.

eigenvalues $\varepsilon_k$ are not physical except at the Fermi surface [105, 104]. Nevertheless, the trace of this Green’s function gives the complete ground-state density $\rho(x)$ (that is, the exact result if we calculate to all orders).

We can easily show diagrammatically that Eq. (6.19) implies that the density obtained from the Kohn-Sham Green’s function is, as advertised, exactly equal to that obtained from the exact Green’s function. In Fig. 6.1, we have rewritten the last term in the Dyson equation (6.19) for the exact Green’s function using

$$\frac{\delta \Gamma_{\text{int}}}{\delta \rho(y)} = \int \frac{\delta \Gamma_{\text{int}}}{\delta J_0(z)} \frac{\delta J_0(z)}{\delta \rho(y)} \, d^3 z,$$

(6.21)

where $\delta J_0(z)/\delta \rho(y) = [\delta^2 W_0/\delta J_0(y) \delta J_0(z)]^{-1}$, which is minus the inverse density-density correlator [46, 42], is represented with a double line (with no arrow). The result of carrying out Eq. (5.27) on Eq. (6.19) is shown in Fig. 6.2, where the last two diagrams cancel as in Fig. 6.3. Note that while similar cancellations were shown in Ref. [42] in the special case of zero-range interactions, the result here is completely general. Thus we see that the exact density is reproduced by the Kohn-Sham Green’s function by construction.

We repeat the previous development to introduce a second energy functional with an additional local source coupled to the kinetic energy density, following Ch. 5. The
Figure 6.2: Equation for the density, showing the equivalence of the full and Kohn-Sham densities.

\[ \begin{array}{c}
\text{\includegraphics[width=\textwidth]{figure6.2}} \\
\end{array} \]

Figure 6.3: Cancellation of the density-density correlator with \( \delta J_0/\delta \rho \).

\[ \begin{array}{c}
\text{\includegraphics[width=\textwidth]{figure6.3}} \\
\end{array} \]

Comparison of results from the two functionals illustrates how the Kohn-Sham single-particle spectrum can be significantly different even though the bulk observables are essentially equal [75]. So we consider

\[ Z' [J, \eta, \xi] = e^{W' [J, \eta, \xi]} = \int D\psi D\psi^\dagger e^{i \int d^4 x [\mathcal{L} + J \psi^\dagger \psi + \eta \nabla \psi^\dagger \cdot \nabla \psi + \int d^4 x' \psi(x) \xi(x, x') \psi^\dagger(x')]}, \]

(6.22)

and the corresponding effective action

\[ \Gamma' [\rho, \tau, \xi] = W' [J, \eta, \xi] - \int d^4 y J(y) \rho(y) - \int d^4 y \eta(y) \tau(y), \]

(6.23)

with kinetic energy density

\[ \tau(x) \equiv \left< \nabla \psi^\dagger(x) \cdot \nabla \psi(x) \right>_{J, \eta, \xi} = \frac{\delta W' [J, \eta, \xi]}{\delta \eta(x)}. \]

(6.24)

(We use superscript primes on the functionals, and \( \kappa' \) on the self-energies and Green’s functions to distinguish the following quantities from those without \( \eta \) or \( \tau \) dependence.) Each step goes through with straightforward generalizations, yielding

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Eq. (6.19) again, but now with

\[
\Sigma_{k\sigma}(y', y)_{\gamma\delta} = \frac{\delta \Gamma_{\text{int}}^{\prime} [\rho, \tau, \xi]}{\delta G_{k\sigma}(y, y')_{\gamma\delta}} + [J_0(y') + \nabla_{y'} \cdot \nabla_y \eta_0(y')] \delta_{\gamma\delta} \delta^4(y' - y) \\
\equiv \Sigma_{k\sigma}^0(y', y)_{\gamma\delta} + [J_0(y') + \nabla_{y'} \cdot \nabla_y \eta_0(y')] \delta_{\gamma\delta} \delta^4(y' - y) \tag{6.25}
\]

after \(J(y')\) and \(\eta(y')\) are set to zero. [Note that the gradients act on the \(G_{k\sigma}\)'s to produce \(\tau\) after partial integrations in Eq. (6.19).]

### 6.2 Comparing Single-Particle Spectra

Functionals arising from “\(\rho\)” and “\(\rho\tau\)” formalism were compared for a dilute gas of fermions in a harmonic trap in the previous chapter. Two sets of parameters were used to illustrate the impact of a larger effective mass \(M^*(x)\), which appears only in the “\(\rho\tau\)” (primed) formalism. Even though the fermion density and energy per particle for the \(\rho\) and \(\rho\tau\) functionals were very similar, the single-particle spectra have significant and systematic differences as shown in Fig. 5.6. We can understand the systematics of the difference by comparing Kohn-Sham and exact spectra for a uniform system. We will drop the non-Hartree-Fock terms, which have been treated in LDA in both cases and which contribute equally to the energy spectra.

In the \(\rho\) case, the Kohn-Sham equation for the single-particle orbital (with external potential turned off) leads to the spectrum

\[
\varepsilon_k^\rho = \frac{k^2}{2M} - J_0^\rho , \tag{6.26}
\]

where

\[
J_0^\rho = -\frac{\nu - 1}{\nu} \frac{4\pi a_s}{M} - \left(\nu - 1\right) \frac{2a_s^2 r_s}{15\pi M} + \left(\nu + 1\right) \frac{4a_p^3}{15\pi M} \left(\frac{6\pi^2 \rho}{\nu}\right)^{5/3} . \tag{6.27}
\]

In the \(\rho\tau\) case, we find a different spectrum

\[
\varepsilon_k^{\rho\tau} = \frac{k^2}{2M^*} - J_0^{\rho\tau} , \tag{6.28}
\]

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where
\[ J_0^{\rho} = -\frac{\nu - 1}{\nu} \frac{4\pi a_s}{M} - \left( \frac{\nu - 1}{\nu} \frac{\pi a_s^2 r_s}{2M} + \frac{\nu + 1}{\nu} \frac{\pi a_p^3}{M} \right) \tau, \] (6.29)
and
\[ \frac{1}{2M^*} = \frac{1}{2M} - \eta_0 = \frac{1}{2M} + \left( \frac{\nu - 1}{\nu} \frac{\pi a_s^2 r_s}{2M} + \frac{\nu + 1}{\nu} \frac{\pi a_p^3}{M} \right) \rho. \] (6.30)
Using \( \tau = \frac{3}{5} k_F^2 \rho \), the difference in the single-particle energy spectra for momentum \( k \) simplifies to
\[ \varepsilon_k^\rho - \varepsilon_k^{\rho\tau} = \left( \frac{\nu - 1}{\nu} \frac{\pi a_s^2 r_s}{2M} + \frac{\nu + 1}{\nu} \frac{\pi a_p^3}{M} \right) (k_F^2 - k^2) \rho. \] (6.31)
Thus, for positive \( r_s \) and \( a_p \), the \( \rho \tau \) levels will always lie lower. The spectra differ for all momentum states except at the Fermi surface, where the spectra coincide as expected in Kohn-Sham DFT. In detail, the \( \rho \tau \) spectrum includes explicit momentum dependence that is converted to density dependence (i.e., \( k_F \) dependence) in the \( \rho \) spectrum. We can also compare the spectra to that of the exact Green’s function in the same Hartree-Fock approximation, where we find that the \( \varepsilon_{\rho\tau} \) spectrum is the same as the exact spectrum. Indeed, for this approximation the \( J_0 \) and \( \eta_0 \) terms in Eq. (6.25) precisely cancel against \( \Sigma_{ksr}^l \). In contrast, Eq. (6.20) yields a net contribution that shifts the Kohn-Sham spectrum to the exact spectrum.

This example illustrates how individual Hartree-Fock self-energies in a gradient expansion can be completely included by adding the corresponding source terms. The exact cancellations are only possible for local self-energies, which means Hartree-Fock. Beyond Hartree-Fock, the single-particle spectrum from the Kohn-Sham and exact Green’s functions will necessarily differ. We can anticipate that self-energies with large non-localities will lead to the most significant differences. This is consistent with the expectation that low-lying vibrational states can account for the difference.
in level density between Skyrme (or other mean-field) and experimental spectra near
the Fermi surface.

In this work, we have illustrated the relationship between Kohn-Sham and exact
Green’s functions within an effective action formalism. This approach goes beyond
the observation that single-particle properties are not reliably calculated in terms of
Kohn-Sham orbitals and eigenvalues. The formalism presents two ways to improve
single-particle spectra. The Kohn-Sham spectra became closer to the exact spectra
with the addition of appropriate sources. It is tempting to conclude that adding
additional sources can always improve the Kohn-Sham single-particle spectrum, but
this will require tests beyond the Hartree-Fock level. More generally, Eq. (6.19) shows
how to calculate single-particle quantities in terms of Kohn-Sham propagators at the
same level of approximation.
CHAPTER 7

INCORPORATING SPIN-ORBIT INTERACTION IN KS DFT

In this chapter, we take another step towards our ultimate goal of calculating bulk observables for medium to heavy nuclei by incorporating a spin-orbit term in our formalism. The result is an energy functional similar to the standard Skyrme energy functional.

7.1 EFT/DFT with Spin-Orbit Density

The spin-orbit density $\mathbf{J}$ is expressed in terms of single-particle orbitals $\psi_{k\alpha}(\mathbf{x})$ as given by Eq. (A.19),

$$i\mathbf{J}(\mathbf{x}) = \nu_{\text{iso}} \sum_{\text{occ}} \psi_{k\alpha}^{\dagger}(\mathbf{x})(\mathbf{\nabla} \times \mathbf{\sigma}_{\alpha\beta})\psi_{k\beta}(\mathbf{x}), \quad (7.1)$$

where the sums are over occupied states and $\nu_{\text{iso}}$ denotes the isospin multiplicity. In this section, we extend the EFT/DFT construction for a dilute Fermi system by including a source coupled to the spin-orbit density operator apart from sources coupled to the density and kinetic energy density operators. Carrying out a triple Legendre transformation via the inversion method, we obtain an expression for the ground-state energy as a functional of the density $\rho$, the kinetic energy density $\tau$ and the spin-orbit density $\mathbf{J}$. 

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7.1.1 Lagrangian

The presence of the spin-orbit term modifies our Lagrangian density given by Eq. (3.13) to the following [98]:

\[
\mathcal{L} = \psi ^\dagger \left[ i \partial_t + \frac{\nabla^2}{2M} \right] \psi - \frac{C_0}{2} (\psi ^\dagger \psi )^2 + \frac{C_2}{16} (\psi ^\dagger \psi )^4 (\psi ^\dagger \nabla^2 \psi ) + \text{h.c.} \\
+ \frac{C_2}{8} (\psi ^\dagger \nabla \psi )^4 \cdot (\psi ^\dagger \nabla \psi ) + \mathcal{L}_{\text{SO}},
\]

where

\[
\mathcal{L}_{\text{SO}} = -i \frac{C_2}{4} \sigma_{\alpha \lambda} \cdot (\psi^\dagger \nabla \psi_{\beta})^4 \times (\psi_{\beta} ^\dagger \nabla \psi_{\lambda}) = -i \frac{C_2}{4} \left[ (\psi^\dagger \nabla \psi_{\beta}) \cdot (\nabla \psi_{\alpha} ^\dagger \times \sigma_{\alpha \lambda} \psi_{\lambda}) + (\nabla \psi_{\beta} ^\dagger \psi_{\alpha}) \cdot (\psi_{\alpha} ^\dagger \sigma_{\alpha \lambda} \times \nabla \psi_{\lambda}) \right] \\
+ i \frac{C_2}{4} \left[ (\psi_{\beta} ^\dagger \psi_{\beta}) (\nabla \psi_{\alpha} ^\dagger \cdot \sigma_{\alpha \lambda} \times \nabla \psi_{\lambda}) - (\psi_{\beta} ^\dagger \sigma_{\alpha \lambda} \psi_{\lambda}) \cdot (\nabla \psi_{\beta} ^\dagger \times \nabla \psi_{\beta}) \right].
\]

The above spin-dependent Lagrangian is not complete up to second derivative terms.

The spin-dependent terms with two derivatives that are left out will be listed in section 7.3.

7.1.2 Effective Action and the Inversion Method

We introduce a generating functional in the path integral formulation with \( \mathcal{L} \) (along with an external potential term) from Eq. (7.2) and Eq. (7.3) supplemented by c-number sources \( J(x), \eta(x) \) and \( \xi(x) \), coupled to the composite density operator, the kinetic energy density operator, and the spin-orbit density operator respectively. In the following expression, we denote the spin-orbit operator simply as \( J(\psi^\dagger, \psi) \) for brevity. The generating functional thus looks like

\[
Z[J, \eta, \xi] = e^{iW[J, \eta, \xi]} = \int D\psi D\psi ^\dagger e^{i \int d^4x \left[ \mathcal{L} + J(x) \psi^\dagger (x) \psi(x) + \eta(x) \nabla \psi^\dagger (x) \nabla \psi(x) + \xi(x) \cdot J(\psi^\dagger, \psi) \right]}.
\]

(7.4)
As before, normalization factors are considered to be implicit in the functional integration measure. The fermion density in the presence of the sources is

$$\rho(x) \equiv \langle \psi^\dagger(x) \psi(x) \rangle_{J, \eta, \xi} = \frac{\delta W[J, \eta, \xi]}{\delta J(x)} . \quad (7.5)$$

The kinetic energy density is given by

$$\tau(x) \equiv \langle \nabla \psi^\dagger(x) \cdot \nabla \psi(x) \rangle_{J, \eta, \xi} = \frac{\delta W[J, \eta, \xi]}{\delta \eta(x)} , \quad (7.6)$$

and the spin-orbit density is given by

$$J(x) \equiv -i \langle \psi^\dagger(x) (\nabla \times \sigma) \psi(x) \rangle_{J, \eta, \xi} = \frac{\delta W[J, \eta, \xi]}{\delta \xi(x)} . \quad (7.7)$$

The functional derivatives are taken keeping the other sources fixed. Next, we define the effective action through the functional Legendre transformation

$$\Gamma[\rho, \tau, J] = W[J, \eta, \xi] - \int d^4x \, J(x) \rho(x) - \int d^4x \, \eta(x) \tau(x) - \int d^4x \, \xi(x) \cdot J(x) , \quad (7.8)$$

which implies that $\Gamma$ has no explicit dependence on $J$, $\eta$ and $\xi$.

As before, we choose finite-density boundary conditions that enforce a given particle number $N$ by hand by working with a fixed number of Kohn-Sham orbitals, and we limit ourselves to time-independent sources and densities. Factoring out a ubiquitous time factor, we write

$$\tilde{\Gamma}[\rho, \tau, J] \equiv \Gamma[\rho, \tau, J] \times \left[ \int_{-\infty}^{\infty} dt \right]^{-1} = -E[\rho, \tau, J] , \quad (7.9)$$

and similarly with $W[J, \eta, \xi]$. The energy functional $E[\rho, \tau, J]$ defined by Eq. (7.9) when evaluated with the exact ground-state density $\rho$, kinetic energy density $\tau$, and spin-orbit density $J$ gives the ground-state energy.
If we take functional derivatives of Eq. (7.8) with respect to \( J(x) \), \( \eta(x) \), and \( \xi(x) \), and then apply Eqs. (7.5), (7.6) and (7.7), and argue the invertibility of the transformation from \( \{ J, \eta, \xi \} \) to \( \{ \rho, \tau, J \} \) as we did in the previous chapters, we get

\[
\frac{\delta \tilde{\Gamma}[\rho, \tau, J]}{\delta \rho(x)} = -J(x) , \quad \frac{\delta \tilde{\Gamma}[\rho, \tau, J]}{\delta \tau(x)} = -\eta(x) , \quad \frac{\delta \tilde{\Gamma}[\rho, \tau, J]}{\delta J(x)} = -\xi(x) . \quad (7.10)
\]

Thus, the effective action when evaluated at the exact ground state densities is an extremum when the sources are set to zero, which corresponds to the original source-free system. The convexity of \( \Gamma \) implies that the energy at the extremum is a minimum.

We carry out the inversion and Legendre transformation as elaborated in the previous chapters by introducing a parameter \( \lambda \), which is ultimately set to unity. We associate powers of \( \lambda \) with the orders in the dilute EFT expansion as before. The effective action is given a dependence on \( \lambda \)

\[
\tilde{\Gamma} = \tilde{\Gamma}[\rho, \tau, J, \lambda] , \quad (7.11)
\]

which is treated as an independent variable. The Legendre transformation defining \( \tilde{\Gamma} \) follows from Eq. (7.8):

\[
\tilde{\Gamma}[\rho, \tau, J, \lambda] = \tilde{W}[J, \eta, \xi, \lambda] - \int d^3x \ J(x) \ \rho(x) - \int d^3x \ \eta(x) \ \tau(x) - \int d^3x \ \xi(x) \cdot J(x) , \quad (7.12)
\]

where the sources depend on \( \lambda \) as well as being functionals of \( \rho, \tau \) and \( J \).

Now we expand each of the quantities that depend on \( \lambda \) in Eq. (7.12) in a series in \( \lambda \), treating \( \rho, \tau \) and \( J \) as order unity. Equating terms with equal powers of \( \lambda \) on both sides of Eq. (7.12) and noting that \( \rho, \tau \) and \( J \) are independent of \( \lambda \), we get

\[
J_i(x) = -\frac{\delta \tilde{\Gamma}_i[\rho, \tau, J]}{\delta \rho(x)} , \quad \eta_i(x) = -\frac{\delta \tilde{\Gamma}_i[\rho, \tau, J]}{\delta \tau(x)} , \quad \xi_i(x) = -\frac{\delta \tilde{\Gamma}_i[\rho, \tau, J]}{\delta J(x)} , \quad (7.13)
\]
where $l$ denotes the power of $\lambda$. As before, we identify the $\tilde{W}_i$’s for $l \geq 1$ in the present case with the diagrammatic expansion in Fig. 3.3 [41, 42], so that $\tilde{W}_1$ is given by diagram (a), $\tilde{W}_2$ by diagrams (b) and (c), and $\tilde{W}_3$ by diagrams (d) through (j) and Fig. 7.1 arising due to spin-orbit interaction.

The zeroth-order equation from Eq. (7.12) is

$$\tilde{\Gamma}_0[\rho, \tau, J] = \tilde{W}_0[J_0, \eta_0, \xi_0] - \int d^3 x \ J_0(x) \ \rho(x) - \int d^3 x \ \eta_0(x) \ \tau(x) - \int d^3 x \ \xi_0(x) \cdot J(x).$$  \hspace{1cm} (7.14)

The corresponding zeroth order expansion of Eqs. (7.5), (7.6) and (7.7) is

$$\rho(x) = \frac{\delta \tilde{W}_0[J_0, \eta_0, \xi_0]}{\delta J_0(x)}, \quad \tau(x) = \frac{\delta \tilde{W}_0[J_0, \eta_0, \xi_0]}{\delta \eta_0(x)}, \quad J(x) = \frac{\delta \tilde{W}_0[J_0, \eta_0, \xi_0]}{\delta \xi_0(x)}. \hspace{1cm} (7.15)$$

The sources $J_0(x)$, $\eta_0(x)$ and $\xi_0$ are particular functions that generate the expectation values $\rho$, $\tau$ and $J$ from the noninteracting system defined by $\lambda = 0$.

As before, the exponent in the non-interacting generating functional $Z_0[J, \eta, \xi]$ is quadratic in the fermion fields, which leads us to define the Green’s function $G_{0s}^{0}$ of the Kohn-Sham non-interacting system that satisfies

$$\left(i\partial_t + \nabla \cdot \frac{1}{2M^*(x)} \nabla - v(x) + J_0(x) - i\xi_0 \cdot \nabla \times \sigma \right) G_{0s}^{0}(x't', x't) = \delta^3(x-x') \delta(t-t')$$ \hspace{1cm} (7.16)
with finite density boundary conditions \[110\] and a position-dependent effective mass defined by Eq. (5.19). Kohn-Sham orbitals arise as solutions to

\[
[-\nabla \cdot \frac{1}{2M^*(\mathbf{x})} \nabla + v(\mathbf{x}) - J_0(\mathbf{x}) + i\xi_0 \cdot \nabla \times \sigma] \psi_a(\mathbf{x}) = \varepsilon_a \psi_a(\mathbf{x}) ,
\]

(7.17)

where the index \(a\) represents all quantum numbers. Note that Eq. (7.17) is in the form of the Skyrme single-particle equation \[107\].

The spectral decomposition of \(G_{ks}^0\) in terms of the Kohn-Sham orbitals in the coupled basis is

\[
iG_{ks}^0(\mathbf{x}t, \mathbf{x}'t') = \sum_k \psi_k(\mathbf{x}) \psi_k^*(\mathbf{x}') e^{-i\varepsilon_k(t-t')}[\theta(t-t') \theta(\varepsilon_k - \varepsilon_F) - \theta(t' - t) \theta(\varepsilon_F - \varepsilon_k)] .
\]

(7.18)

Since \(\overline{W}_0[J_0, \eta_0, \xi_0] \propto \text{Tr} \ln(G_{ks}^0)^{-1}\), it can be written explicitly in terms of the single-particle Kohn-Sham eigenvalues as \[109\]

\[
\overline{W}_0[J_0, \eta_0, \xi_0] = - \sum_{\varepsilon_k \leq \varepsilon_F} \varepsilon_k .
\]

(7.19)

By using Eq. (7.19) in Eq. (7.14) and then eliminating \(\varepsilon_k\) using Eq. (7.17), the lowest-order effective action can be written as,

\[
\hat{\Gamma}_0[\rho, \tau, \mathbf{J}] = - \sum_a \varepsilon_a - \int d^3 \mathbf{x} \ J_0(\mathbf{x}) \ \rho(\mathbf{x}) - \int d^3 \mathbf{x} \ \eta_0(\mathbf{x}) \ \tau(\mathbf{x}) - \int d^3 \mathbf{x} \ \xi_0(\mathbf{x}) \cdot \mathbf{J}(\mathbf{x})
\]

\[
= - T_s[\tau] - \int d^3 \mathbf{x} \ v(\mathbf{x}) \ \rho(\mathbf{x}) ,
\]

(7.20)

where

\[
T_s[\tau] = \frac{1}{2M} \int d^3 \mathbf{x} \ \tau(\mathbf{x})
\]

(7.21)

is the total kinetic energy of the KS non-interacting system.

Proceeding in exactly the same manner as elaborated in the previous chapters (Ch. 4.5), we get to first-order in \(\lambda\)

\[
\tilde{\Gamma}_1[\rho, \tau, \mathbf{J}] = \tilde{W}_1[J_0, \eta_0, \xi_0] = - \frac{1}{2} \frac{\nu - 1}{\nu} \ C_0 \int d^3 \mathbf{x} \ \rho^2(\mathbf{x}) \equiv \tilde{\Gamma}_1[\rho] .
\]

(7.22)
Using Eq. (7.13), we obtain

\[ J_1(x) = C_0 \frac{(\nu - 1)}{\nu} \rho(x), \quad \eta_1(x) = 0, \quad \xi_1(x) = 0. \] (7.23)

The second-order effective action amounts to calculating the contribution made by the “beachball” diagram [Fig. 3.3(b)] to the energy (up a time factor) due to the usual cancellation of the “anomalous” graph of Fig. 3.3(c). Calculation of the third-order effective action in the inversion method similarly leads to cancellation of the “anomalous” graphs in \( \tilde{W}_3 \) given by Figs. 3.3(d), (e), and (f), leaving only Fig. 3.3(g) through (j) and Fig. 7.1 as contributors. All higher orders in \( \tilde{\Gamma}[\rho, \tau, J, \lambda] \) are determined in a similar manner.

In order to solve for the orbitals in Eq. (7.17) and to calculate the energy, we need expressions for \( J_0(x), \eta_0(x) \) and \( \xi_0(x) \). Since \( J(x) = \eta(x) = \xi(x) = 0 \) in the ground state, Eq. (7.10) becomes a variational principle that, together with Eq. (7.13), yields self-consistent expressions for \( J_0, \eta_0 \) and \( \xi_0 \):

\[ J_0(x)_{\text{gs}} = -\sum_{l \geq 1} J_l(x)_{\text{gs}} = \frac{\delta \tilde{\Gamma}_{\text{int}}[\rho, \tau, J]}{\delta \rho(x)}_{\text{gs}}, \] (7.24)

\[ \eta_0(x)_{\text{gs}} = -\sum_{l \geq 1} \eta_l(x)_{\text{gs}} = \frac{\delta \tilde{\Gamma}_{\text{int}}[\rho, \tau, J]}{\delta \tau(x)}_{\text{gs}}, \] (7.25)

\[ \xi_0(x)_{\text{gs}} = -\sum_{l \geq 1} \xi_l(x)_{\text{gs}} = \frac{\delta \tilde{\Gamma}_{\text{int}}[\rho, \tau, J]}{\delta J(x)}_{\text{gs}}, \] (7.26)

where \( \tilde{\Gamma}_{\text{int}}[\rho, \tau] \) is the interaction effective action

\[ \tilde{\Gamma}_{\text{int}}[\rho, \tau, J] = \sum_{l \geq 1} \tilde{\Gamma}_l[\rho, \tau, J], \] (7.27)

and the subscript “gs” refers to the ground-state. At this stage \( \lambda = 1 \), a given approximation corresponds to truncating Eq. (7.27) at \( l_{\text{max}} \) and then carrying out the
self-consistent calculation. As before, we refer to \( l_{\text{max}} = 1 \) as leading order, or LO, \( l_{\text{max}} = 2 \) as next-to-leading order or NLO, and \( l_{\text{max}} = 3 \) as NNLO.

### 7.1.3 The Ground State Energy

The contributions to \( E_c[\rho, \tau, J] \) from the Hartree-Fock graphs with spin-orbit interaction comes at the NNLO order [Fig. 7.1] because it is a term with two derivatives. Therefore, power counting dictates its contribution to be at NNLO. Its contribution is given by (appendix B)

\[
E_{C_2^2}[\rho, J] = - \left( \frac{\nu_{\text{iso}} + 1}{2\nu_{\text{iso}}} \right) C_2^2 \int d^3 \mathbf{x} \rho(\mathbf{x}) \mathbf{\nabla} \cdot J(\mathbf{x}) .
\]

(7.28)

As before, we deal with closed shell configurations. The contributions from the Hartree-Fock diagrams with derivatives \( (E_{C_2} \text{ and } E_{C_2'}) \) are given by Eq. (5.39) and Eq. (5.40) as before so that the total contribution to the energy from NLO and NNLO diagrams is

\[
E_c[\rho(\mathbf{x}), \tau(\mathbf{x}), J] = E_c[\rho(\mathbf{x}), \tau(\mathbf{x})] + E_{C_2^2}[\rho(\mathbf{x}), J(\mathbf{x})] ,
\]

(7.29)

where \( E_c[\rho(\mathbf{x}), \tau(\mathbf{x})] \) is given by Eq. (5.42). We quote the expression here for convenience:

\[
E_c[\rho(\mathbf{x}), \tau(\mathbf{x})] = \frac{b_1 a_0^2}{2M} \int d^3 \mathbf{x} [\rho(\mathbf{x})]^{7/3} + E_{C_2}[\rho(\mathbf{x}), \tau(\mathbf{x})]
\]

\[
+ E_{C_2'}[\rho(\mathbf{x}), \tau(\mathbf{x})] + \frac{b_1 a_0^3}{2M} \int d^3 \mathbf{x} [\rho(\mathbf{x})]^{8/3} .
\]

(7.30)

The full effective action is given by

\[
\tilde{\Gamma}[\rho, \tau, J] = \tilde{\Gamma}_0[\rho, \tau] + \tilde{\Gamma}_1[\rho] + \sum_{k=2}^{\infty} \tilde{\Gamma}_k[\rho, \tau, J]
\]

\[
= \tilde{\Gamma}_0[\rho, \tau] - E_{\text{HF}}[\rho] - E_c[\rho, \tau, J] .
\]

(7.31)
Now we proceed to calculate the sources using Eqs. (7.24), (7.25), (7.26), and (7.30) to NNLO. \( J_0(\mathbf{x}) \) is computed as

\[
J_0(\mathbf{x}) = \frac{\delta}{\delta \rho(\mathbf{x})} \left( \hat{\Gamma}_1[\rho] + \sum_{k=2}^3 \hat{\Gamma}_k[\rho, \tau, \mathbf{J}] \right) = -\frac{\delta}{\delta \rho(\mathbf{x})} \left( E_{\text{HF}}[\rho] + E_c[\rho, \tau, \mathbf{J}] \right)
\]

\[
= -\left( \frac{\nu - 1}{\nu} \right) \frac{4\pi a_s}{M} \rho(\mathbf{x}) - \frac{7}{3} b_1 \frac{a_s^2}{2M} |\rho(\mathbf{x})|^4/3 - \frac{8}{3} b_4 \frac{a_s^3}{2M} |\rho(\mathbf{x})|^{5/3}
- (B_2 a_s^2 r_s + B_3 a_p^3) \frac{1}{2M} \tau(\mathbf{x}) + (3B_2 a_s^2 r_s - B_3 a_p^3) \frac{1}{4M} \nabla^2 \rho(\mathbf{x})
+ \left( \frac{\nu_{\text{iso}} + 1}{2\nu_{\text{iso}}} \right) C_2^\sigma \nabla \cdot \mathbf{J}(\mathbf{x}) .
\]

(7.32)

\( \eta_0(\mathbf{x}) \) has the same form as Eq. (5.45),

\[
\eta_0(\mathbf{x}) = -\frac{\delta}{\delta \tau(\mathbf{x})} \left( E_{\text{HF}}[\rho] + E_c[\rho, \tau, \mathbf{J}] \right) = - \left( B_2 a_s^2 r_s + B_3 a_p^3 \right) \frac{1}{2M} \rho(\mathbf{x}) ,
\]

(7.33)

so that the spatially dependent effective mass \( M^*(\mathbf{x}) \) is given by Eq. (5.46). Finally, \( \xi_0(\mathbf{x}) \) is given by

\[
\xi_0(\mathbf{x}) = -\frac{\delta}{\delta \mathbf{J}(\mathbf{x})} \left( E_{\text{HF}}[\rho] + E_c[\rho, \tau, \mathbf{J}] \right) = - \left( \frac{\nu_{\text{iso}} + 1}{2\nu_{\text{iso}}} \right) C_2^\sigma \nabla \rho(\mathbf{x}) .
\]

(7.34)

An expression for the total binding energy (through NNLO) follows by substituting for \( J_0(\mathbf{x}) \), \( \eta_0(\mathbf{x}) \) and \( \xi_0(\mathbf{x}) \) in Eq. (7.20) and then using Eq. (7.31) and Eq. (7.9). The resulting expression is given by:

\[
E[\rho(\mathbf{x}), \tau(\mathbf{x}), \mathbf{J}(\mathbf{x})] = \sum_{k=1}^{\text{occ}} \varepsilon_k - \int d^3 \mathbf{x} \left\{ \frac{1}{2} \left( \frac{\nu - 1}{\nu} \right) \frac{4\pi a_s}{M} |\rho(\mathbf{x})|^2 + \frac{4}{3} b_1 \frac{a_s^2}{2M} |\rho(\mathbf{x})|^{4/3}
+ \frac{5}{3} b_4 \frac{a_s^3}{2M} |\rho(\mathbf{x})|^{8/3} + (3B_2 a_s^2 r_s - B_3 a_p^3) \frac{1}{8M} |\nabla \rho(\mathbf{x})|^2
+ \left( B_2 a_s^2 r_s + B_3 a_p^3 \right) \frac{1}{2M} \rho(\mathbf{x}) \tau(\mathbf{x})
+ \left( \frac{\nu_{\text{iso}} + 1}{2\nu_{\text{iso}}} \right) C_2^\sigma \rho(\mathbf{x}) \nabla \cdot \mathbf{J}(\mathbf{x}) \right\} .
\]

(7.35)

This is the same as Eq. (5.47) that we obtained in chapter (5) with an extra term. An alternative expression for the energy is obtained by using the second part of Eq. (7.20)
followed by Eqs. (7.31), and (7.9):

\[
E[\rho(\mathbf{x}), \tau(\mathbf{x}), \mathbf{J}(\mathbf{x})] = \int d^3 \mathbf{x} \left\{ \frac{1}{2M} \tau(\mathbf{x}) + \nu(\mathbf{x}) \rho(\mathbf{x}) + \frac{1}{2} (\nu - 1) \frac{4\pi a_s}{M} |\rho(\mathbf{x})|^2 \right. \\
+ \left. (B_2 a_s^2 r_s + B_3 a_p^3) \frac{1}{2M} \rho(\mathbf{x}) \tau(\mathbf{x}) \right. \\
+ \left. (3B_2 a_s^2 r_s - B_3 a_p^3) \frac{1}{8M} |\nabla \rho(\mathbf{x})|^2 \right. \\
+ b_1 \frac{a_s}{2M} [\rho(\mathbf{x})]^{7/3} + b_4 \frac{a_s^3}{2M} [\rho(\mathbf{x})]^{8/3} \\
- \left. \left( \frac{\nu_{\text{iso}} + 1}{2
}\nu_{\text{iso}} \right) C_2^\sigma \rho(\mathbf{x}) \nabla \cdot \mathbf{J}(\mathbf{x}) \right\} .
\] (7.36)

If we set the isospin multiplicity \( \nu_{\text{iso}} = 2 \) and rewrite Eq. (7.36) in terms of the \( C_i \)'s, the resulting expression takes the same form as that of the Skyrme functional.

### 7.2 Fermions in a Harmonic Trap

We intend to solve the Kohn-Sham single-particle equations in a coupled basis. The Kohn-Sham self-consistent procedure follows in exactly the same fashion as described in the previous chapters (see for example section 5.3.1). The only addition is computing and incorporating the spin-orbit source \( \xi_0 \) in the procedure, which is straightforward.

We will restrict ourselves to closed shells. Let \( k \equiv \{n, \ell, j, m_j\} \) be our short-hand index labelling the single-particle states given by

\[
\psi_k(\mathbf{x}) \equiv \psi_{ntljm_j}(\mathbf{x}) = R_{ntlj}(r) \mathcal{Y}_{ljm_j}(\Omega),
\] (7.37)

where

\[
\mathcal{Y}_{ljm_j}(\Omega) = c_1 Y_{lmdj-1/2}(\Omega) \eta_\uparrow + c_2 Y_{lmdj+1/2}(\Omega) \eta_\downarrow.
\] (7.38)

\( c_1 \) and \( c_2 \) are the Clebsch-Gordan coefficients (\(|c_1|^2 + |c_2|^2 = 1\)) and \( \eta_\uparrow, \eta_\downarrow \) denotes the spin up and down spinors respectively. In our notation, \( c_1 \) is given by \( C(\ell 1/2 j)(m_j - \frac{1}{2}) \) and
$1/2 \cdot 1/2 m_j), and c_2$ is given by $C(\ell 1/2 \, j | m_j + 1/2 ) - 1/2 m_j)$. In this basis, the expressions for $\rho$ is given by
\[ \rho(x) = \nu_{iso} \sum_k \psi_k^* (x) \psi_k (x) \theta(\varepsilon_F - \varepsilon_k), \]
so that
\[ \rho(r) = \frac{1}{4\pi} \int d\Omega \rho(x) \]
\[ = \frac{\nu_{iso}}{4\pi} \int d\Omega \sum_{n\ell jm_j} |R_{n\ell j}(r)|^2 |Y_{\ell jm_j}(\Omega)|^2 \]
\[ = \frac{\nu_{iso}}{4\pi} \int d\Omega \sum_{n\ell jm_j} |R_{n\ell j}(r)|^2 \left[ |c_1|^2 |Y_{\ell m_j-1/2}(\Omega)|^2 + |c_2|^2 |Y_{\ell m_j+1/2}(\Omega)|^2 \right] \]
\[ = \frac{\nu_{iso}}{4\pi} \sum_{n\ell j} |R_{n\ell j}(r)|^2 \left[ \sum_{m_j} 1 \right] = \frac{\nu_{iso}}{4\pi} \sum_{n\ell j} (2j + 1) |R_{n\ell j}(r)|^2, \quad (7.39) \]
where we have used the normalisation of the Clebsch-Gordan coefficients and the orthogonality of spherical harmonics.

Next, we evaluate the form of the kinetic energy density in the coupled basis. Using Eq. (7.37), Eq. (7.38), and Eq. (5.72), we get
\[ \nabla \psi_k = \nabla \left[ R_{n\ell j}(r) \left( c_1 Y_{\ell m_j-1/2}(\Omega) \eta_\uparrow + c_2 Y_{\ell m_j+1/2}(\Omega) \eta_\downarrow \right) \right] \]
\[ = (c_1 \varphi_1 \eta_\uparrow + c_2 \varphi_2 \eta_\downarrow), \quad (7.40) \]
where
\[ \varphi_1 = -A_{n\ell j}(r) Y_{\ell \ell+1 m_j-1/2}(\Omega) + B_{n\ell j}(r) Y_{\ell \ell-1 m_j-1/2}(\Omega), \]
\[ \varphi_2 = -A_{n\ell j}(r) Y_{\ell \ell+1 m_j+1/2}(\Omega) + B_{n\ell j}(r) Y_{\ell \ell-1 m_j+1/2}(\Omega). \quad (7.41) \]
The functions $A_{n\ell j}(r)$ and $B_{n\ell j}(r)$ has the form given by Eq. (5.73). Using Eq. (7.40) and the orthogonality of the spinors, we get
\[ |\nabla \psi_k|^2 = |c_1|^2 |\varphi_1|^2 + |c_2|^2 |\varphi_2|^2, \quad (7.42) \]
so that using the orthogonality of vector spherical harmonics, we get
\[ \tau(r) = \frac{1}{4\pi} \int d\Omega \tau(x) \]
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\[
= \frac{\nu_{\text{iso}}}{4\pi} \sum_{k}^{\text{occ.}} d\Omega |\nabla \psi_{k}(x)|^{2}
\]
\[
= \frac{\nu_{\text{iso}}}{4\pi} \sum_{n_{\ell}j}^{\text{occ.}} \left( |A_{n_{\ell}j}(r)|^{2} + |B_{n_{\ell}j}(r)|^{2} \right)
\]
\[
= \frac{\nu_{\text{iso}}}{4\pi} \sum_{n_{\ell}j}^{\text{occ.}} (2j + 1) \left[ \left( \frac{dR_{n_{\ell}j}}{dr} \right)^{2} + \frac{\ell(\ell + 1)}{r^{2}} |R_{n_{\ell}j}(r)|^{2} \right]. \quad (7.43)
\]

Since we are dealing with a closed shell scenario, the spin-orbit density is purely radial. Before proceeding, let us denote the spin and angular momenta operators as \( S \) and \( L \) respectively, so that the operator \( 2S \cdot L \) is diagonal in the coupled basis, and for a spin one-half system, has the following value:
\[
\phi(j, \ell) = j(j + 1) - \ell(\ell + 1) - \frac{3}{4}. \quad (7.44)
\]

Now, since the spin-orbit density is radial, we can write \( J(x) = \hat{\mathbf{r}} \cdot J(x) \), where \( \hat{\mathbf{r}} \) is the unit vector in the radial direction. Alternatively, one can write \( J(x) = J \cdot \hat{\mathbf{r}} \).

Using this in the previous expression, we get \( J = \hat{\mathbf{r}} (J \cdot \hat{\mathbf{r}}) \). Using Eq. (7.1), we get
\[
J \cdot \hat{\mathbf{r}} = -i \nu_{\text{iso}} \psi^{\dagger}_{k} \nabla \times \sigma_{k} \psi_{k}
\]
\[
= \nu_{\text{iso}} \psi^{\dagger}_{k} \sigma_{k} \cdot \nabla \times \psi_{k}
\]
\[
= \frac{2\nu_{\text{iso}}}{r} \psi^{\dagger}_{k} S \cdot L \psi_{k} = \frac{\nu_{\text{iso}}}{r} \sum_{k}^{\text{occ.}} \phi(j, \ell) \psi^{\dagger}_{k} \psi_{k}, \quad (7.45)
\]

where we have used Eq. (7.44). Using the above, we get
\[
J = \hat{\mathbf{r}} (J \cdot \hat{\mathbf{r}})
\]
\[
= \hat{\mathbf{r}} \left[ \frac{\nu_{\text{iso}}}{r} \sum_{n_{\ell}j}^{\text{occ.}} \phi(j, \ell) \psi^{\dagger}_{n_{\ell}j} \psi_{n_{\ell}j} \right], \quad (7.46)
\]

so that the radial spin-orbit density (using \( J(x) = J \cdot \hat{\mathbf{r}} \)) is given by
\[
J(r) = \frac{1}{4\pi} \int d\Omega J(x)
\]

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\[
= \frac{\nu_{\text{iso}}}{4\pi r} \sum_{m,j}^{\text{occ.}} \phi(j, \ell) |R_{nlj}|^2
\]

\[
= \frac{\nu_{\text{iso}}}{4\pi r} \sum_{n,l,j}^{\text{occ.}} (2j + 1) \phi(j, \ell) |R_{nlj}|^2.
\] (7.47)

Computing \( \nabla \cdot \mathbf{J} \) is now a matter of taking a simple derivative. Using similar algebra as illustrated in Eq. (7.45), we note that

\[
-i \sum_{k}^{\text{occ.}} \psi_k^* \nabla \rho \cdot (\nabla \times \mathbf{\sigma}) \psi_k = \frac{1}{r} \frac{d}{dr} \sum_{k}^{\text{occ.}} \phi(j, \ell) \psi_k^* \psi_k.
\] (7.48)

Carrying out the normal separation of variables method on Eq. (7.17) and using Eq. (7.34) and Eq. (7.48), we find that the radial function \( u_{nlj}(r) \) satisfies

\[
\left[-\frac{1}{2M^*(r)} \frac{d^2}{dr^2} - \frac{d\eta_0}{dr} \left( \frac{1}{r} - \frac{d}{dr} \right) + v_s(r) + \frac{\ell(\ell + 1)}{2M^*(r)r^2} \right] u_{nlj}(r)
+ \left( \frac{\nu_{\text{iso}} + 1}{2\nu_{\text{iso}}} \right) \frac{C_{lj}^2}{r} \frac{d\rho}{dr} \phi(j, \ell) u_{nlj}(r) = \varepsilon_{nlj} u_{nlj}(r).
\] (7.49)

The actual numerical calculation and studying the impact of the spin-orbit term on the density profile and single-particle spectra remains to be done.

### 7.3 Comments

Our Lagrangian (Eq. (7.3)) did not include a complete set of spin-dependent terms at second-derivative order. Here, we write down the form of the potential containing all the spin-dependent terms up to second derivatives [98]. Denote the transferred and average momenta by \( \mathbf{q} \) and \( \mathbf{p} \) respectively. They are given in terms of the COM of the particles as :

\[
\mathbf{q} = \mathbf{k}' - \mathbf{k}, \quad \mathbf{p} = \frac{1}{2}(\mathbf{k} + \mathbf{k}').
\] (7.50)

The complete potential up to terms involving two derivatives is then of the following form :

\[
V(q, p) = A_1 q^2 + A_2 p^2 + (A_3 q^2 + A_4 p^2)(\mathbf{\sigma}_1 \cdot \mathbf{\sigma}_2) + \frac{iA_5}{2} (\mathbf{\sigma}_1 + \mathbf{\sigma}_2) \cdot (\mathbf{p} \times \mathbf{q})
\]
\[ +A_6(q \cdot \sigma_1)(q \cdot \sigma_2) + A_7(p \cdot \sigma_1)(p \cdot \sigma_2). \] (7.51)

In this thesis, we have dealt with the first, second, and the fourth term. The third piece can be handled with Fierz rearrangement. Future work will encompass the rest of the terms.
CHAPTER 8

SUMMARY

In this thesis, we construct a Kohn-Sham density functional for a confined, dilute Fermi gas order-by-order as an effective field theory (EFT) expansion. The starting point is a generating functional with a source $J(x)$ coupled to the composite density operator $\psi^\dagger \psi$. A functional Legendre transformation with respect to the source leads to an effective action of the density, which is used to calculate the ground state energy, including all correlations, with what looks like a Hartree calculation (which is the many-body equivalent of tree level). This is density functional theory, but with a systematic expansion.

In a finite system, the density-weighted average of a local Fermi momentum times the effective range parameters controls one expansion, with another expansion involving gradients of the density. In the present work, we used both the local density approximation (LDA) and gradient expansion (for Hartree-Fock terms with derivative interactions only) which means that both the expansions were tested. The observed convergence of the density and energy in sample systems confirms this expansion for a finite system. An error plot of contributions to the energy per particle versus the order of the calculation shows that we can reliably estimate the truncation error in a finite system.
As a next step, we go beyond LDA by incorporating the kinetic-energy-density \( \tau(\mathbf{x}) \) into the formalism. The generating functional is constructed by including, in addition to a source \( J(\mathbf{x}) \) coupled to the composite density operator \( \psi^\dagger \psi \), another source \( \eta(\mathbf{x}) \) coupled to the (semi-local) kinetic energy density operator \( \nabla \psi^\dagger \cdot \nabla \psi \). A functional Legendre transformation with respect to the sources yields an effective action of the kinetic energy density \( \tau \) as well as the fermion density \( \rho \). This extension sets the stage for the construction of energy functionals and Kohn-Sham equations that go systematically beyond the local density approximation (LDA).

As a first step, we included the exact Hartree-Fock (HF) contribution at NNLO for a natural dilute Fermi system but treated non-HF contributions in LDA. This exact HF contribution provides explicit dependence on \( \tau \) and on the gradient of the density, unlike the LDA. The ground-state energy functional and Kohn-Sham single-particle equations constructed here take the same form as those in Skyrme Hartree-Fock calculations (excluding the spin-orbit contribution), with one basic difference. The Skyrme parametrization has only one term with a fractional power of the density, but our result has more such terms. These additional terms motivated by power counting may become important for extrapolating far from stability. An error plot of contributions to the energy per particle versus the order of the calculation showed that we can reliably estimate the truncation error in a finite system, including the gradient terms.

We note that nuclei are *not* perturbative dilute Fermi systems with natural free-space scattering lengths. But there is phenomenological evidence that power counting can apply to energy functionals that are fit to bulk nuclear properties. Phenomenologically successful functionals, both of the Skyrme type and covariant, have Hartree
terms that are consistent with NDA for a chiral low-energy theory [48, 68, 92]. This involves power counting with two scales: the pion decay constant $f_\pi$ and an underlying scale for short-range physics $\Lambda$, which empirically (for these functionals) is around 600 MeV, so that the functionals do take the form of a density expansion (with parameter $\rho/f^2_\pi\Lambda$) as well as a gradient expansion.

Next, we investigated the value of including the kinetic energy density as a functional variable and arrived at the conclusion that it leads to a single-particle spectrum closer to that of the exact Green’s function. In future work, the formalism will be applied to the calculation of spectral functions and the effect of low-lying vibrational states on the spectra tested by including self-energy diagrams that sum particle-hole bubbles.

Finally, we extended our formalism to include spin-orbit interaction by coupling a source $\xi$ to the spin-orbit density operator in addition to a source $J(\mathbf{x})$ coupled to the composite density operator, another source $\eta(\mathbf{x})$ coupled to the kinetic energy density operator. The resulting energy functional was of the same form as the Skyrme functional. Work is in progress to numerically solve for fermions in a harmonic trap and investigate whether one can estimate the spin-orbit piece of the energy functional.

### 8.1 Future Research Directions

In the immediate future, the following issues need to be addressed.

- Developing a derivative expansion of the non-relativistic Feynman propagator to compute contributions to the energy functional beyond LDA and testing for convergence is an important next step. Another possibility is to use the functional expansion of $k_F$ in terms of $\rho$, its derivatives, and $\tau$. This would allow
us to evaluate diagrams such as the NLO “beachball” diagram, or diagrams with long-range forces. A systematic derivative expansion will be of importance to nuclei for controlled extrapolations far from the valley of stability.

- Including all the terms up to two derivatives in the spin-dependent potential (Eq. (7.51)) is the next step. We also need to incorporate isospin dependence in the form of $\mathbf{\tau}_1 \cdot \mathbf{\tau}_2$. Such an isospin dependent term can be removed by Fierz rearrangement, but then we will have to include the $\mathbf{\sigma}_1 \cdot \mathbf{\sigma}_2$ term with an appropriate coefficient. Including isospin dependent terms up to two derivatives analogous to the spin terms can also be done. It is interesting to note that the Skyrme functional has no terms coming from the tensor piece. Including tensor components to study their effect on the energy functional is an interesting possibility. Investigating the effects of incorporating sources coupled to different composite operators with the same global properties but different local structure on the single particle spectra also needs to be studied.

- Any attractive interaction leads to a pairing instability. Investigating pairing for finite systems as well as carrying out finite temperature calculations remains to be done. The inversion method has been applied to conventional BCS superconductivity in Ref. [71] using a source coupled to the pair creation and destruction operator. Work to adapt this procedure to the EFT is in progress.

- A major goal of future investigations will be to elucidate the nature of the density expansion for finite nuclei and to connect it to the underlying chiral EFT. Long-range forces have to be included to make a connection between the density functional procedure and chiral effective field theories with pions.
Systematic derivative expansions are relevant in this context. Modifying the formalism for self-bound systems will require further research.

- Effective low-momentum potentials ($V_{\text{lowk}}$) combined with Pauli-blocking leads to corrections in nuclear matter in the particle-particle channel that are well converged at second order in potential [97]. Connecting this approach to DFT needs to be done.

- The current framework needs to be extended in order to incorporate time dependent DFT so that collective motion can be studied in a systematic fashion. This would serve as a generalization of the RPA formalism.

- A systematic solution to the large scattering length problem at finite density remains a challenge.
APPENDIX A

BASIC DEFINITIONS

In this appendix, we review some basic definitions [107, 108].

A.1 Density of States

The single particle density of states is defined as

\[ g(\varepsilon) = \nu \sum_k \delta(\varepsilon - \varepsilon_k), \] (A.1)

where \( \nu \) is the spin-isospin multiplicity. The canonical partition function is given by the Laplace transform of \( g(\varepsilon) \).

\[ Z(\beta) = \mathcal{L}_\beta[g(\varepsilon)] = \int_0^\infty d\varepsilon \ e^{-\beta \varepsilon} g(\varepsilon). \] (A.2)

Observe that the above expression in the discrete limit reduces to

\[ Z(\beta) = \nu \sum_k e^{-\beta \varepsilon_k} \equiv Tr[e^{-\beta \hat{H}}]. \]

Conversely, one can obtain the density of states given the partition function by taking its inverse Laplace transform.

\[ g(\varepsilon) = \mathcal{L}_\varepsilon^{-1}[Z(\beta)] = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\beta \ Z(\beta) e^{\beta \varepsilon}. \]
A.2 Bloch Density Matrix

The Bloch density matrix, also known as the canonical density matrix, or heat kernel, for a system with a spin-independent Hamiltonian is given by:

\[
C(x, y, \beta)_{\lambda\mu} = \langle x, \lambda | e^{-\beta \hat{H}} | y, \mu \rangle = \sum_k \langle x, \lambda | e^{-\beta \hat{H}} | \psi_k \rangle \langle \psi_k | y, \mu \rangle = \sum_k \psi_k(x) \psi_k^*(y) e^{-\beta \epsilon_k} = \delta_{\lambda\mu} \sum_k \psi_k(x) \psi_k^*(y) e^{-\beta \epsilon_k},
\]  

(A.3)

where \( \beta = \frac{\hbar}{k_B} \), and we have used \( \hat{H} | \psi_k \rangle = \epsilon_k | \psi_k \rangle \). From now onwards, we will be setting \( \hbar \) to unity. The partition function can then be expressed in terms of the Bloch density matrix in the following way.

\[
Z(\beta) = Tr(C) = \int d^3x C(x, x, \beta)_{\lambda\lambda} = \nu \int d^3x C(x, x, \beta).
\]  

(A.4)

The time dependent Schrödinger equation is \( [i \partial_t - \hat{H}(x)] \Psi(x, t) = 0 \). The general solution to the equation can be written as a linear superposition of the eigenstates of the Hamiltonian.

\[
\Psi(x, t) = \sum_k a_k(t) \psi_k(x), \quad a_k(t) = a_k(0) e^{-\epsilon_k t}
\]  

where \( a_k(0) = \int d^3x \Psi(x, 0) \psi_k^*(x) \).

(A.5)

Using the expression for \( a_k(0) \), we get the solution to be in the form

\[
\Psi(x, t) = \int d^3y C(x, y, \beta = it) \Psi(y, 0).
\]  

(A.6)

The above equation tells us that \( C(x, y, \beta = it) \) is the amplitude for propagation of the particle from \( y \) to \( x \) in time \( t \). In this sense, \( C(x, y, \beta) \) is like a single particle
propagator at zero density. Note that \( C(x, y, 0) = \delta^3(x - y) \).

This function satisfies the equation \( \left[ i \partial_t - \hat{H}(x) \right] C(x, y, \beta = it) = 0 \). Equivalently, the following equation is also satisfied:

\[
\left[ \partial_\beta + \hat{H}(x) \right] C(x, y, \beta) = 0.
\] (A.7)

This equation is known as Bloch’s equation. To study the state evolution for positive \( \beta \) only, one defines the retarded single particle propagator as

\[
C_R(x, y, \beta) = C(x, y, \beta) \theta(\beta).
\] (A.8)

This function serves as the Green’s function, and the following is a way to see that.

\[
\left[ \partial_\beta + \hat{H}(x) \right] C_R(x, y, \beta) = \theta(\beta) \left[ \partial_\beta + \hat{H}(x) \right] C + C \left[ \partial_\beta + \hat{H}(x) \right] \theta(\beta) = C \partial_\beta \theta(\beta) = C(x, y, 0) \delta(\beta).
\]

or,

\[
\left[ \partial_\beta + \hat{H}(x) \right] C_R(x, y, \beta) = \delta^3(x - y) \delta(\beta).
\] (A.9)

One can also define the advanced propagator as \( C_A(x, y, \beta) = C(x, y, \beta) \theta(-\beta) \). Using the fact that \( \theta(\beta) + \theta(-\beta) = 1 \) so that \( C_A = C - C_R \), it is easy to show that the advanced propagator satisfies the following equation:

\[
\left[ \partial_\beta + \hat{H}(x) \right] C_A(x, y, \beta) = -\delta^3(x - y) \delta(\beta).
\] (A.10)

Writing the above set of equations in terms of \( t \) is trivially achieved by \( \beta \to it \).

**A.3 Dirac Density Matrix**

The noninteracting Dirac density matrix for a system with a spin-independent Hamiltonian is given as a spin trace as

\[
\gamma_s(x, y) = \nu \sum_k \psi_k(x) \psi^*_k(y) \theta(\varepsilon_F - \varepsilon_k) = \nu \langle x | \theta(\varepsilon_F - \hat{H}) | y \rangle.
\] (A.11)
Since unit step function has the following representation:
\[ \theta(z) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\beta \frac{e^{\beta z}}{\beta} = \mathcal{L}_{\varepsilon_F}^{-1} \left[ \frac{1}{\beta} \right], \] (A.12)
the Dirac density matrix reduces to the following form.
\[ \gamma_s(x, y) = \frac{\nu}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\beta \, C(x, y, \beta) \frac{e^{\beta \varepsilon_F}}{\beta} = \nu \mathcal{L}_{\varepsilon_F}^{-1} \left[ \frac{C(x, y, \beta)}{\beta} \right]. \] (A.13)
The density is simply the diagonal of the Dirac density matrix.
\[ \rho(x) = \gamma_s(x, x) = \frac{\nu}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\beta \, C(x, x, \beta) \frac{e^{\beta \varepsilon_F}}{\beta}. \] (A.14)

A.4 Kinetic Energy Density

We have adopted a convention where the kinetic energy density is defined without the mass factor in the following manner.
\[ \tau(x) = \nu \sum_k (\nabla \psi_k) \cdot (\nabla \psi_k^*) \theta(\varepsilon_F - \varepsilon_k). \] (A.15)
The following is a useful relation
\[ \sum_k (\psi_k^* \nabla^2 \psi_k + \psi_k \nabla^2 \psi_k^*) \theta(\varepsilon_F - \varepsilon_k) = \frac{1}{\nu} (\nabla^2 \rho - 2\tau). \] (A.16)

A.5 Current and Spin-Orbit Density

The current density is defined as.
\[ j(x) = \frac{i \nu}{2} \sum_k [(\nabla \psi_k^*) \psi_k - \psi_k^* (\nabla \psi_k)] \theta(\varepsilon_F - \varepsilon_k). \] (A.17)
Now, we are in a position to write down the following relations.
\[ \sum_k (\nabla \psi_k^*) \psi_k \theta(\varepsilon_F - \varepsilon_k) = \frac{1}{2\nu} (\nabla \rho - 2i j), \]
\[ \sum_k \psi_k^* (\nabla \psi_k) \theta(\varepsilon_F - \varepsilon_k) = \frac{1}{2\nu} (\nabla \rho + 2i j). \] (A.18)
The spin-orbit density is given by

\[ i \mathbf{J}(x) = \nu_{\text{iso}} \sum_k \sum_{\alpha, \beta} \psi_{k\alpha}^\dagger(x) \left[ (\nabla \psi_{k\beta}) \times \sigma_{\alpha\beta} \right] \theta(\varepsilon_F - \varepsilon_k), \tag{A.19} \]

where \( \nu_{\text{iso}} \) is the isospin multiplicity.

### A.6 Application to Uniform System in 3D

For a uniform system, the energy is purely kinetic. The wavefunctions for a uniform system are just plane waves, so that \( |k\rangle \) is an eigenket of \( \hat{H} \), where \( \hat{H} = \hat{T} \). Hence, we can use the completeness relation:

\[ \int \frac{d^3k}{(2\pi)^3} |k\rangle \langle k| = 1. \]

Noting \( \hat{H}|k\rangle = \frac{k^2}{2M}|k\rangle \) for the uniform system, let us try to apply some of the above equations and see what we get. If we work in three spatial dimensions, the expression for the density reduces to

\[ \rho(x) = \frac{\nu}{2\pi i} \int_{-i\infty}^{c+i\infty} d\beta \frac{\langle x|e^{-\beta\hat{T}}|x\rangle e^{\beta \varepsilon_F}}{\beta}, \]

\[ = \frac{\nu}{2\pi i} \int_{-i\infty}^{c+i\infty} d\beta \left[ \int \frac{d^3k}{(2\pi)^3} \langle x|e^{-\beta\hat{T}}|k\rangle \langle k|x\rangle \right] \]

\[ = \frac{\nu}{2\pi i} \int_{-i\infty}^{c+i\infty} d\beta \left[ \int \frac{d^3k}{(2\pi)^3} e^{-\beta \frac{k^2}{2M}} \right] \frac{e^{\beta \varepsilon_F}}{\beta}. \]

Changing the order of integration and using the representation for the unit step function, we get

\[ \rho(x) = \nu \int \frac{d^3k}{(2\pi)^3} \theta(\varepsilon_F - \frac{k^2}{2M}) = \frac{\nu k_F^3}{6\pi^2}. \tag{A.20} \]

As expected, the density is a constant. Note that \( \varepsilon_F = \frac{k_F^2}{2M} \) where \( k_F \) is the Fermi momentum.
The Dirac density matrix is computed as follows.

\[
\gamma_s(x, y) = \nu \langle x|\theta(\varepsilon_F - \hat{H})|y\rangle \\
= \nu \int \frac{d^3k}{(2\pi)^3} \langle x|\theta(\varepsilon_F - \hat{T})|k\rangle \langle k|y\rangle \\
= \nu \int \frac{d^3k}{(2\pi)^3} e^{ikr} \theta(k_F - k) \\
= \frac{\nu}{2\pi^2} k_F^3 \frac{j_1(k_F r)}{k_F r} = 3\rho \frac{j_1(k_F r)}{k_F r}, 
\]

(A.21)

where \( r \) is the relative coordinate \((x - y)\) and \( j_1 \) is the spherical Bessel function,

\[
j_1(z) = \frac{\sin(z)}{z^2} - \frac{\cos(z)}{z}. 
\]

(A.22)

If we take the limit \( r \to 0 \) in the expression for \( \gamma_s(x, y) \), we obtain \( \rho \) as expected.

Finally, let us see how the Bloch density matrix looks like for a uniform system.

\[
C(x, y, \beta) = \langle x|e^{-\beta \hat{H}}|y\rangle = \int \frac{d^3k}{(2\pi)^3} \langle x|e^{-\beta \hat{T}}|k\rangle \langle k|y\rangle \\
= \int \frac{d^3k}{(2\pi)^3} e^{ikr} e^{-\beta \frac{k^2}{2M}} \\
= \left( \frac{M}{2\pi\beta} \right)^{\frac{3}{2}} e^{-\frac{M^* r^2}{2\beta}}. 
\]

(A.23)

It is easy to verify that the Dirac density matrix can be obtained from the Bloch density matrix by taking an inverse Laplace transform as given in Eq. (A.13).
APPENDIX B

HARTREE-FOCK (HF) CALCULATIONS

In this appendix, we review the basic technique of evaluating diagrams at the Hartree-Fock (HF) order. We will start off by deriving expressions for HF diagrams with different interactions using second quantised formalism, and then show how one gets the same results using Feynman rules. Although we are interested in closed shell configurations (for which $j = 0$), the expressions derived in this appendix will be more general.

B.1 HF in Second Quantised Formalism

The interaction Hamiltonian with two-body forces only in three spatial dimensions is given by

$$\hat{H}_{\text{int}} = \frac{1}{2} \sum_{\alpha, \beta, \lambda, \mu} \int d^3 x d^3 y \psi^\dagger_\lambda(x) \psi^\dagger_\mu(y) V(x, y) \psi_\alpha(x) \psi_\beta(y). \quad (B.1)$$

For a spin-independent interaction,

$$V(x, y)_{\alpha \lambda; \beta \mu} = \delta_{\alpha \lambda} \delta_{\beta \mu} V(x, y). \quad (B.2)$$

In order to get HF energies, we have to compute $\langle \hat{H}_{\text{int}} \rangle$, the full expectation value of the interaction Hamiltonian. Denote $N(\hat{A} \hat{B})$ as the normal-ordered product of
two operators, and \( T(\hat{A}\,\hat{B}) \) as the time-ordered one. Since \( \langle N(\hat{A}\,\hat{B}) \rangle = 0 \), Wick's theorem \cite{Wick} tells us

\[
\langle T(\hat{A}\,\hat{B}) \rangle = \langle N(\hat{A}\,\hat{B}) \rangle + \widehat{\hat{A}\,\hat{B}} = \hat{A}\,\hat{B},
\]

(B.3)

where \( \widehat{\hat{A}\,\hat{B}} \) is a c-number called contraction. Note that in general,

\[
N(\hat{A}\,\hat{B}\,\hat{C}\,\hat{D}) = -\hat{A}\hat{C} \left[ N(\hat{B}\,\hat{D}) \right],
\]

(B.4)

so that its expectation value is zero. This is because the expectation value of all uncontracted normal-ordered products vanish. The negative sign comes only if we are dealing with fermions.

The HF energy is obtained by finding the expectation value of \( \hat{H}_{\text{int}} \) in the non-interacting ground state instead of the fully interacting ground state, with the field operators written in terms of the non-interacting wavefunctions. These wavefunctions are obtained self-consistently. This is the HF approximation, and amounts to first-order perturbation theory at the first iteration.

\[
E_{\text{HF}} = \frac{1}{2} \sum_{\alpha, \beta} \int \int d^3x\,d^3y\, V(x, y) \langle \hat{\psi}_\alpha^\dagger(x) \hat{\psi}_\beta^\dagger(y) \hat{\psi}_\beta(y) \hat{\psi}_\alpha(x) \rangle.
\]

(B.5)

In a non-relativistic theory, one chooses the interaction to be instantaneous. This means that we can replace the expectation value in the above equation by a time-ordered expectation value. This allows us to use Wick's theorem, and we get a string of expectation values of normal-ordered products of the fields with all possible contractions. Only those normal-ordered products with all the fields contracted survive when the expectation value is taken. These terms are c-numbers, and there is no need to mention normal ordering for these terms any more. The order of contracting the field operators in the interaction Hamiltonian dictates whether we are computing a
direct (Hartree) or exchange (Fock) process. The corresponding expressions are

\[ E_H = \frac{1}{2} \sum_{\alpha, \beta} \int d^3x \int d^3y \, V(x, y) \, \hat{\psi}_\alpha(x) \hat{\psi}_\beta(y) \hat{\psi}_\beta(y) \hat{\psi}_\alpha(x), \]

\[ E_F = \frac{1}{2} \sum_{\alpha, \beta} \int d^3x \int d^3y \, V(x, y) \, \hat{\psi}_\alpha(x) \hat{\psi}_\beta(y) \hat{\psi}_\beta(y) \hat{\psi}_\alpha(x). \] (B.6)

Now, we can go back and replace the two-operator contractions by the corresponding
time-ordered product expectation. This of course is the same as the ordinary expecta-
tion value due to instantaneousness of the interaction. Noting that interchanging
the order of any two fermionic field operators give rise to a negative sign, we get the
following expressions for HF energies.

\[ E_H = \frac{1}{2} \sum_{\alpha, \beta} \int d^3x \int d^3y \, V(x, y) \, \langle \hat{\psi}_\alpha(x) \hat{\psi}_\beta(y) \rangle \langle \hat{\psi}_\beta(y) \hat{\psi}_\alpha(x) \rangle, \]

\[ E_F = -\frac{1}{2} \sum_{\alpha, \beta} \int d^3x \int d^3y \, V(x, y) \, \langle \hat{\psi}_\alpha(x) \hat{\psi}_\beta(y) \rangle \langle \hat{\psi}_\beta(y) \hat{\psi}_\alpha(x) \rangle. \] (B.7)

Observe that the Hartree term is like a product of two spin traces, whereas the Fock
term has a single spin trace.

B.2 Evaluation of HF Diagrams

The field operator \( \hat{\psi}_\alpha(x) \) can be written in terms of particle and hole operators
by a canonical transformation:

\[ \hat{\psi}_\alpha(x) = \sum_k \psi_{k\alpha}(x) \tilde{a}_{k\alpha} \theta(\varepsilon_k - \varepsilon_F) + \sum_k \psi_{k\alpha}(x) \tilde{b}_{k\alpha}^\dagger \theta(\varepsilon_F - \varepsilon_k). \] (B.8)

\( \psi_{k\alpha}(x) \) is the non-interacting wavefunction, and is given by

\[ \psi_{k\alpha}(x) = \psi_k(x) \eta_\alpha, \] (B.9)

where \( \eta_\alpha \) denotes the usual spinor vector satisfying \( \eta_\alpha \eta_\beta = \delta_{\alpha\beta} \). If isospin is present
too, we will merely have one more label (an isospin spinor) and things will proceed
exactly as with the pure spin case. So, we will save ourselves the trouble and denote \( \nu \) to be the spin multiplicity or the spin-isospin multiplicity depending on the context.

The operator \( \hat{a}_{ka} \) destroys a particle in the state \((ka)\) above the filled Fermi sea, whereas \( \hat{b}_{ka} \) destroys a hole in the same state inside the Fermi sea [110]. Thus the particle and hole destruction operators both annihilate the non-interacting ground state. This is because there are no particles above the filled Fermi sea, and no holes below it (since it is filled). So, the expectation values \( \langle \hat{a}_{ka} \hat{a}_{k'a}, \hat{b}_{ka} \hat{b}_{k'a} \rangle \), and \( \langle \hat{a}_{ka} \hat{b}_{k'a} \rangle \) are the only combinations that survive in any calculation. This is no surprise since the rest of the combinations are either normal ordered products, or does not have the same number of creation and annihilation operators.

Now let us consider the expectation value of \( \hat{\psi}_{\alpha}^\dagger(x) \hat{\psi}_{\beta}(y) \).

\[
\langle \hat{\psi}_{\alpha}^\dagger(x) \hat{\psi}_{\beta}(y) \rangle = \sum_k \sum_n \psi_k^* \psi_n \theta(\varepsilon_F - \varepsilon_k) \theta(\varepsilon_F - \varepsilon_n) \langle \hat{b}_{ka} \hat{b}_{k'n} \rangle \\
= \left[ \sum_k \psi_k^* \psi_k \theta(\varepsilon_F - \varepsilon_k) \right] \eta_{\alpha} \eta_{\beta} \delta_{\alpha\beta} \\
= \frac{1}{\nu} \gamma_s(x, y) \eta_{\alpha} \eta_{\beta} \delta_{\alpha\beta}, \quad (B.10)
\]

where \( \gamma_s(x, y) \) is the non-interacting Dirac density matrix as defined in Eq. (A.11).

As a special case,\n
\[
\langle \hat{\psi}_{\alpha}^\dagger(x) \hat{\psi}_{\alpha}(x) \rangle = \frac{1}{\nu} \rho(x). \quad (B.11)
\]

Let us now evaluate the Hartree term.

\[
E_H = \frac{1}{2} \sum_{\alpha, \beta} \int \int d^3 x d^3 y V(x, y) \langle \hat{\psi}_{\alpha}^\dagger(x) \hat{\psi}_{\alpha}(x) \rangle \langle \hat{\psi}_{\beta}^\dagger(y) \hat{\psi}_{\beta}(y) \rangle \\
= \frac{1}{2} \sum_{\alpha, \beta} \int \int d^3 x d^3 y \frac{\rho(x)}{\nu} V(x, y) \frac{\rho(y)}{\nu} \\
= \frac{1}{2} \int \int d^3 x d^3 y \rho(x) V(x, y) \rho(y). \quad (B.12)
\]
Note that the above expression has the same form as that of the potential energy of a charge distribution if one considers a Coulomb interaction. Next, let us handle the Fock term.

\[
E_F = -\frac{1}{2} \sum_{\alpha, \beta} \int \int d^3x \, d^3y \, V(x, y) \langle \hat{\psi}_\alpha^\dagger(x) \hat{\psi}_\beta(y) \rangle \langle \hat{\psi}_\beta^\dagger(y) \hat{\psi}_\alpha(x) \rangle \\
= -\frac{1}{2} \int \int d^3x \, d^3y \, \frac{\gamma_s(y, x)}{\nu} V(x, y) \frac{\gamma_s(x, y)}{\nu} \sum_{\alpha, \beta} (\eta_\alpha^\dagger \eta_\beta \delta_{\alpha\beta}) (\eta_\beta^\dagger \eta_\alpha \delta_{\alpha\beta}) \\
= -\frac{1}{2} \int \int d^3x \, d^3y \, \frac{\gamma_s(y, x)}{\nu} V(x, y) \frac{\gamma_s(x, y)}{\nu} \sum_{\alpha} \delta_{\alpha\alpha} \\
= -\frac{1}{2\nu} \int \int d^3x \, d^3y \, \gamma_s(y, x) V(x, y) \gamma_s(x, y). \tag{B.13}
\]

Observe that at the HF order, only the occupied states contribute. If we go to the second-order in perturbation theory, the intermediate states will be above the Fermi sea (due to Pauli blocking) and we will get contributions from the unoccupied (particle) states too.

### B.2.1 Pure Contact Interaction

For a contact interaction, \( V(x, y) = C_0 \delta(x - y) \). This is precisely the same interaction corresponding to the term in our EFT Lagrangian (Eq. (3.13)) with the coefficient \( C_0 \). The Hartree and Fock diagrams both reduce to the same “bowtie” diagram (Fig. 3.3–a). It is easy to see from Eq. (B.12) and Eq. (B.13) that the HF energy is simply given by

\[
E_{C_0} = \frac{C_0}{2} (1 - \frac{1}{\nu}) \int d^3x \, \rho^2(x). \tag{B.14}
\]
B.2.2 Contact Interaction with Derivatives

p-wave term

We start off by evaluating the contribution from the $C'_2$ term in the Lagrangian because it is less cumbersome to deal with, and so its easier to demonstrate the methodology. The corresponding potential is [76]

$$V(x, y) = C'_2 k' \cdot \delta(x - y) k,$$

where

$$k = \frac{1}{2i} \left( \nabla_x - \nabla_y \right), \quad k' = -\frac{1}{2i} \left( \nabla_x - \nabla_y \right).$$

The interaction Hamiltonian is then

$$\hat{H}_{\text{int}} = \frac{C'_2}{8} \sum_{\alpha, \beta} \int \int d^3x \, d^3y \, \hat{\psi}^\dagger_\alpha(x) \hat{\psi}^\dagger_\beta(y) \times \left[ -\left( \nabla_x - \nabla_y \right) \cdot \delta(x - y) \left( \nabla_x - \nabla_y \right) \hat{\psi}_\beta(y) \hat{\psi}_\alpha(x) \right]$$

$$= \frac{C'_2}{8} \sum_{\alpha, \beta} \int d^3x \left[ \left( \nabla_\alpha \hat{\psi}^\dagger_\beta \right) \hat{\psi}_\beta \left( \nabla_\beta \hat{\psi}^\dagger_\alpha \right) - \left( \nabla_\beta \hat{\psi}^\dagger_\alpha \right) \left( \nabla_\alpha \hat{\psi}_\beta \right) \right] \left( \hat{\psi}_\beta (\nabla_\beta \hat{\psi}_\alpha) - (\nabla_\beta \hat{\psi}_\beta) \hat{\psi}_\alpha \right)$$

where all the field operators and its derivatives are evaluated at $x$. The Hartree contribution is

$$E_H = \frac{C'_2}{8} \sum_{\alpha, \beta} \int d^3x \left[ E_{H1} - E_{H2} - E_{H3} + E_{H4} \right], \quad \text{where}$$

$$E_{H1} = \left( \nabla_\alpha \hat{\psi}^\dagger_\beta \right) \hat{\psi}_\beta \cdot (\nabla_\alpha \hat{\psi}_\alpha), \quad E_{H2} = \left( \nabla_\beta \hat{\psi}^\dagger_\alpha \right) \hat{\psi}_\beta \cdot (\nabla_\beta \hat{\psi}_\beta) \hat{\psi}_\alpha,$$

$$E_{H3} = \hat{\psi}^\dagger_\alpha (\nabla_\beta \hat{\psi}^\dagger_\beta) \hat{\psi}_\beta \cdot (\nabla_\beta \hat{\psi}_\alpha), \quad E_{H4} = \hat{\psi}^\dagger_\alpha (\nabla_\beta \hat{\psi}^\dagger_\beta) \cdot (\nabla_\beta \hat{\psi}_\beta) \hat{\psi}_\alpha.$$

As before, we can replace the contractions by the expectation values. Consider the expectation value of $\nabla_\alpha \hat{\psi}^\dagger_\alpha \cdot \nabla_\beta \hat{\psi}_\beta$.

$$\langle \nabla_\alpha \hat{\psi}^\dagger_\alpha \cdot \nabla_\beta \hat{\psi}_\beta \rangle = \sum_k \sum_n \nabla_\alpha \hat{\psi}^\dagger_{k\alpha}(x) \cdot \nabla_\alpha \hat{\psi}_n(x) \theta(\varepsilon_F - \varepsilon_k) \theta(\varepsilon_F - \varepsilon_n) \langle \delta_{k\alpha} \delta_{n\beta} \rangle.$$
\[
\begin{align*}
&= \left[ \sum_k \nabla \psi_k(x) \cdot \nabla \psi_k(x) \theta(\varepsilon_F - \varepsilon_k) \right] \eta_\alpha^\dagger \eta_\beta \delta_{\alpha\beta} \\
&= \frac{1}{\nu} \tau(x) \eta_\alpha^\dagger \eta_\beta \delta_{\alpha\beta},
\end{align*}
\]
where \(\tau(x)\) is the kinetic energy density as defined in Eq. (A.15). As a special case,
\[
\langle \nabla \hat{\psi}_\alpha^\dagger \cdot \nabla \hat{\psi}_\alpha \rangle = \frac{1}{\nu} \tau(x).
\]  
(B.20)

Finally, consider the expectation value of \(\hat{\psi}_\alpha^\dagger \nabla \hat{\psi}_\beta\).
\[
\langle \hat{\psi}_\alpha^\dagger \nabla \hat{\psi}_\beta \rangle = \sum_k \sum_n \psi_{k\alpha}^\dagger(x) \nabla \psi_{n\beta}(x) \theta(\varepsilon_F - \varepsilon_k) \theta(\varepsilon_F - \varepsilon_n) \langle \hat{b}_{kn} \hat{b}_{n\beta}^\dagger \rangle
\]
\[
= \left[ \sum_k \psi_k^\dagger(x) \nabla \psi_k(x) \theta(\varepsilon_F - \varepsilon_k) \right] \eta_\alpha^\dagger \eta_\beta \delta_{\alpha\beta}
\]
\[
= \frac{1}{2\nu} \left( \nabla \rho(x) + 2i \mathbf{j}(x) \right) \eta_\alpha^\dagger \eta_\beta \delta_{\alpha\beta},
\]  
(B.21)

where \(\mathbf{j}(x)\) is the current density defined by Eq. (A.17). In a similar manner, we get
\[
\langle (\nabla \hat{\psi}_\alpha^\dagger) \hat{\psi}_\beta \rangle = \frac{1}{2\nu} \left( \nabla \rho(x) - 2i \mathbf{j}(x) \right) \eta_\alpha^\dagger \eta_\beta \delta_{\alpha\beta}.
\]  
(B.22)

Now, we proceed with our calculation.
\[
\sum_{\alpha,\beta} \mathcal{E}_{H1} = \sum_{\alpha,\beta} \mathcal{E}_{H4} = \sum_{\alpha,\beta} \rho(x) \frac{\tau(x)}{\nu}
= \rho(x) \tau(x).
\]
\[
\sum_{\alpha,\beta} \mathcal{E}_{H2} = \sum_{\alpha,\beta} \mathcal{E}_{H3}
= \frac{1}{4} \left( \nabla \rho(x) + 2i \mathbf{j}(x) \right) \cdot \left( \nabla \rho(x) - 2i \mathbf{j}(x) \right)
= \frac{1}{4} (\nabla \rho)^2 + j^2(x).
\]  
(B.23)

So, the Hartree energy takes the form
\[
E_H = \frac{C_2'}{4} \int d^3x \left[ \rho(x) \tau(x) - \frac{1}{4} (\nabla \rho)^2 - j^2(x) \right].
\]  
(B.24)
Now, let us consider the Fock term. The expression looks like

\[
E_F = \frac{C_2'}{8} \sum_{\alpha, \beta} \int d^3 x \left[ \mathcal{E}_{F1} - \mathcal{E}_{F2} - \mathcal{E}_{F3} + \mathcal{E}_{F4} \right],
\]

where

\[
\begin{align*}
\mathcal{E}_{F1} &= \left( \nabla \hat{\psi}_\alpha^\dagger \right) \hat{\psi}_\beta \cdot \left( \nabla \hat{\psi}_\alpha \right), \\
\mathcal{E}_{F2} &= \left( \nabla \hat{\psi}_\alpha^\dagger \right) \hat{\psi}_\beta \cdot \left( \nabla \hat{\psi}_\beta \right) \hat{\psi}_\alpha, \\
\mathcal{E}_{F3} &= \hat{\psi}_\alpha^\dagger \left( \nabla \hat{\psi}_\beta \right) \hat{\psi}_\beta \cdot \left( \nabla \hat{\psi}_\alpha \right), \\
\mathcal{E}_{F4} &= \hat{\psi}_\alpha^\dagger \left( \nabla \hat{\psi}_\beta \right) \cdot \left( \nabla \hat{\psi}_\beta \right) \hat{\psi}_\alpha.
\end{align*}
\]

Clearly, \( \mathcal{E}_{F2} \) and \( \mathcal{E}_{F3} \) give the same contribution.

\[
\sum_{\alpha, \beta} \mathcal{E}_{F2} = -\sum_{\alpha, \beta} \frac{\rho(x)}{\nu} \frac{\tau(x)}{\nu} \eta_\alpha^\dagger \eta_\beta \delta_\alpha^\dagger \eta_\beta \eta_\alpha \delta_\beta \alpha \\
= -\frac{\rho(x)}{\nu} \frac{\tau(x)}{\nu} \sum_\alpha \delta_\alpha \alpha \\
= -\frac{1}{\nu} \rho(x) \tau(x).
\]

Similarly, \( \mathcal{E}_{F1} \) and \( \mathcal{E}_{F4} \) contribute equally. Carrying out the spin sum, we get

\[
\sum_{\alpha, \beta} \mathcal{E}_{F1} = -\frac{1}{\nu} \left[ \frac{1}{4} (\nabla \rho)^2 + j^2(x) \right].
\]

Proceeding, the Fock energy turns out to be \( E_H/\nu \), so that

\[
E_{HF} = \frac{C_2'}{4} \left( 1 + \frac{1}{\nu} \right) \int d^3 x \left[ \rho(x) \tau(x) - \frac{1}{4} (\nabla \rho)^2 - j^2(x) \right].
\]

s–wave term

Now, we evaluate the contribution from the \( C_2 \) term in the EFT Lagrangian. The corresponding potential is \([76]\)

\[
V(x, y) = \frac{1}{2} C_2 \left[ \delta(x - y) k^2 + k^2 \delta(x - y) \right] \equiv V_1(x, y) + V_2(x, y).
\]

Let us work with the \( V_1 \) piece first. Using the fact that \( k = (\nabla_x - \nabla_y)/2i \), the interacting Hamiltonian corresponding to the \( V_1 \) piece (after carrying out the integration
\[ \hat{H}_{\text{int}} = -\frac{C_2}{16} \sum_{\alpha,\beta} \int d^3x \hat{\psi}_\alpha^\dagger(x) \hat{\psi}_\beta^\dagger(x) \]

\[ \times \left[ \hat{\psi}_\beta(x) \nabla^2 \hat{\psi}_\alpha(x) + \nabla^2 \hat{\psi}_\beta(x) \hat{\psi}_\alpha(x) - 2 \nabla \hat{\psi}_\beta(x) \cdot \nabla \hat{\psi}_\alpha(x) \right] \] (B.30)

Before proceeding, there is one small calculation that we need to do. Consider

\[ \langle \int d^3x \rho(x) \hat{\psi}_\alpha^\dagger(x) \nabla^2 \hat{\psi}_\beta(x) \rangle = -\langle \int d^3x \nabla \left[ \rho(x) \hat{\psi}_\alpha^\dagger(x) \right] \cdot \nabla \hat{\psi}_\beta(x) \rangle \]

\[ = -\langle \int d^3x \left[ \rho(x) \nabla \hat{\psi}_\alpha^\dagger(x) \cdot \nabla \hat{\psi}_\beta(x) + \nabla \rho(x) \cdot \hat{\psi}_\alpha^\dagger(x) \nabla \hat{\psi}_\beta(x) \right] \rangle \]

\[ = -\int d^3x \left[ f(x) + g(x) \right] \eta_\alpha \eta_\beta \delta_{\alpha \beta}, \] (B.31)

where

\[ f(x) = \frac{1}{\nu} \rho(x) \tau(x), \quad g(x) = \nabla \rho(x) \cdot \frac{1}{2\nu} (\nabla \rho(x) + 2i \mathbf{j}(x)). \] (B.32)

Now we are in a position to almost read off the Hartree and Fock contributions. Contracting operators in the usual way, and using the above result, the Hartree contribution from the \( V_1 \) piece looks like

\[ E_H^1 = -\frac{C_2}{16} \left( -2\nu \left[ f(x) + g(x) \right] - \frac{1}{2} (\nabla \rho(x) + 2i \mathbf{j}(x))^2 \right). \] (B.33)

The Fock piece as usual has a relative negative sign. The spin sum as before gives a factor of \( \nu \) in the denominator. Thus, the HF contribution from the \( V_1 \) piece looks like

\[ E_{\text{HF}}^1 = -\frac{C_2}{16} \left( \frac{1}{\nu} - 1 \right) \left( 2\nu \left[ f(x) + g(x) \right] + \frac{1}{2} (\nabla \rho(x) + 2i \mathbf{j}(x))^2 \right). \] (B.34)

Now we focus on the \( V_2 \) piece. Using the fact that \( \mathbf{k}' = -(\hat{\nabla}_x - \hat{\nabla}_y)/2i \), the interacting Hamiltonian corresponding to the \( V_2 \) piece (after carrying out the integration
\[ \hat{H}_{\text{int}}^2 = \frac{C_2}{16} \sum_{\alpha,\beta} \int \! d^3x \left[ \nabla^2 \hat{\psi}_\alpha^\dagger(x) \hat{\psi}_\beta(x) + \hat{\psi}_\alpha^\dagger(x) \nabla^2 \hat{\psi}_\beta^\dagger(x) - 2 \nabla \hat{\psi}_\alpha^\dagger(x) \cdot \nabla \hat{\psi}_\beta^\dagger(x) \right] \times \hat{\psi}_\beta(x) \hat{\psi}_\alpha(x). \]  

(B.35)

Proceeding just as before, we find that

\[ \langle \int \! d^3x \rho(x) \nabla^2 \hat{\psi}_\alpha^\dagger(x) \hat{\psi}_\beta(x) \rangle = - \int \! d^3x \left[ f(x) + h(x) \right] \eta_\alpha^\dagger \eta_\beta \delta_{\alpha\beta}, \quad (B.36) \]

where

\[ f(x) = \frac{1}{\nu} \rho(x) \tau(x), \quad h(x) = \nabla \rho(x) \cdot \frac{1}{2\nu} \left( \nabla \rho(x) - 2i \, j(x) \right). \]

(B.37)

Proceeding just as before, we get the HF contribution from the \( V_2 \) piece as

\[ E_{\text{HF}}^2 = - \frac{C_2}{16} \left( \frac{1}{\nu} - 1 \right) \left( 2\nu [ f(x) + h(x) ] + \frac{1}{2} \left( \nabla \rho(x) - 2i \, j(x) \right)^2 \right). \]  

(B.38)

Thus, the total HF contribution from the \( C_2 \) term in the Lagrangian is

\[ E_{\text{HF}} = E_{\text{HF}}^1 + E_{\text{HF}}^2 = - \frac{C_2}{4} \left( \frac{1}{\nu} - 1 \right) \left[ \rho(x) \tau(x) + \frac{3}{4} \left( \nabla \rho \right)^2 - j^2(x) \right]. \]

(B.39)

**B.2.3 Spin-Orbit Interaction**

In order to deal with the spin-orbit interaction, we have to evaluate the contribution from the \( C_2^\sigma \) term in the Lagrangian. The corresponding potential is [76]

\[ V(x, y) = iC_2^\sigma (\sigma_1 + \sigma_2) \cdot k' \times \delta(x - y) k, \]  

(B.40)

where

\[ k = \frac{1}{2i} \left( \nabla_x - \nabla_y \right), \quad k' = - \frac{1}{2i} \left( \nabla_x + \nabla_y \right) \]

(B.41)
as before. In this section, we will reserve $\alpha, \beta$ etc. to denote matrix indices of spinors and spin matrices, so that the isospin is taken care of separately. Carrying out the sum over isospin index, the Hartree contribution is given by

$$E_H = \frac{iC_5^2}{4} \nu_{\text{iso}} \sum_{\alpha, \beta, \lambda} \int d^3x \left[ e_{\text{H1}} - e_{\text{H2}} - e_{\text{H3}} + e_{\text{H4}} \right],$$

where

$$e_{\text{H1}} = \sigma_{\alpha \lambda} \cdot \left( \nabla \hat{\psi}_\alpha^\dagger \right) \hat{\psi}_\beta \times \left( \nabla \hat{\psi}_\lambda \right), \quad e_{\text{H2}} = \sigma_{\alpha \lambda} \cdot \left( \nabla \hat{\psi}_\alpha^\dagger \right) \hat{\psi}_\beta \times \left( \nabla \hat{\psi}_\lambda \right),$$

$$e_{\text{H3}} = \sigma_{\alpha \lambda} \cdot \left( \nabla \hat{\psi}_\alpha^\dagger \right) \hat{\psi}_\beta \times \left( \nabla \hat{\psi}_\lambda \right), \quad e_{\text{H4}} = \sigma_{\alpha \lambda} \cdot \left( \nabla \hat{\psi}_\alpha^\dagger \right) \hat{\psi}_\beta \times \left( \nabla \hat{\psi}_\lambda \right).$$

As before, we can replace the contractions by the expectation values. We shall work in the coupled basis in this section. The field operator $\hat{\psi}_\alpha(x)$ are now written in terms of particle and hole operators as:

$$\hat{\psi}_\alpha(x) = \sum_k \psi_{ka}(x) \hat{a}_k \theta(\varepsilon_k - \varepsilon_F) + \sum_k \psi_{ka}(x) \hat{b}_k^\dagger \theta(\varepsilon_F - \varepsilon_k).
$$

Note that the spin label information is contained in the coupled basis label $k = \{l, s, j, m_j\}$. $\psi_k(x)$ is the two component spinor.

Consider the first term. It is easy to see that

$$\nu_{\text{iso}} \sum_\beta \langle \hat{\psi}_\beta^\dagger \hat{\psi}_\beta \rangle = \rho(x). \quad (B.44)$$

From Eq. (A.19), we note that

$$i \nabla \cdot J(x) = \nu_{\text{iso}} \sum_{k\alpha\beta} \nabla \psi_{ka}^\dagger(x) \cdot (\nabla \times \sigma_{\alpha\beta}) \psi_{k\beta}(x) \theta(\varepsilon_F - \varepsilon_k)$$

$$= \nu_{\text{iso}} \sum_{k\alpha\beta} \sigma_{\alpha\beta} \cdot (\nabla \psi_{ka}^\dagger(x) \times \nabla \psi_{k\beta}(x)) \theta(\varepsilon_F - \varepsilon_k), \quad (B.45)$$

where the index $k$ refers to quantum numbers in the uncoupled basis. Using the above, we find that the contribution from the first term to the Hartree energy is
given by
\[
E_{H1} = \frac{\imath C_\sigma}{4} \int d^3x \rho(x) \{ \imath \nabla \cdot J(x) \} = -\frac{C_\sigma^2}{4} \int d^3x \rho(x) \nabla \cdot J(x).
\] (B.46)

Time reversal invariance of occupied states result in the following expression [76]:
\[
\sum_{\alpha \beta} \langle \hat{\psi}_\alpha^\dagger \sigma_{\alpha \beta} \hat{\psi}_\beta \rangle = 0.
\] (B.47)

Using this, we see that the last term does not contribute \((E_{H4} = 0)\). Writing the above in terms of the spinors and taking a gradient, we get
\[
\sum_{k \alpha \beta} \sigma_{\alpha \beta} \cdot \nabla \psi_{k \alpha}^\dagger \psi_{k \beta} = -\sum_{k \alpha \beta} \sigma_{\alpha \beta} \cdot \psi_{k \alpha}^\dagger \nabla \psi_{k \beta}.
\] (B.48)

Now consider the contribution from the second term. Noting that
\[
\sum_{\alpha} \langle \hat{\psi}_\alpha^\dagger \nabla \hat{\psi}_\alpha \rangle = \sum_{k \alpha} \psi_{k \alpha}^\dagger \nabla \psi_{k \alpha} = \frac{1}{2\nu_{\text{iso}}} (\nabla \rho + 2\imath j),
\] (B.49)

we get
\[
E_{H2} = -\nu_{\text{iso}}^2 \frac{\imath C_\sigma}{4} \int d^3x \sum_{\alpha, \lambda} \left[ \sum_{k} \sigma_{\alpha \lambda} \cdot \nabla \psi_{k \alpha}^\dagger \psi_{k \lambda} \right] \times \frac{1}{2\nu_{\text{iso}}} (\nabla \rho + 2\imath j). \] (B.50)

Similarly, the third term contributes
\[
E_{H3} = \nu_{\text{iso}}^2 \frac{\imath C_\sigma}{4} \int d^3x \sum_{\alpha, \lambda} \left[ \sum_{k} \sigma_{\alpha \lambda} \cdot \psi_{k \alpha}^\dagger \nabla \psi_{k \lambda} \right] \times \frac{1}{2\nu_{\text{iso}}} (\nabla \rho - 2\imath j). \] (B.51)

Using the above two equations along with Eq. (B.48), we get
\[
E_{H2} + E_{H3} = \nu_{\text{iso}}^2 \frac{\imath C_\sigma}{4} \int d^3x \sum_{\alpha, \lambda} \left[ \sum_{k} \sigma_{\alpha \lambda} \cdot \psi_{k \alpha}^\dagger \nabla \psi_{k \lambda} \right] \times \frac{1}{\nu_{\text{iso}}} \nabla \rho
\]
\[
= \frac{C_\sigma^2}{4} \int d^3x \nabla \rho \cdot J.
\] (B.52)

So, the Hartree energy takes the form
\[
E_{H} = -\frac{C_\sigma^2}{2} \int d^3x \rho(x) \nabla \cdot J(x),
\] (B.53)
where we have used the fact that partial integration gives,

\[ \int d^3 x \nabla \rho \cdot J = - \int d^3 x \rho \cdot \nabla \cdot J. \quad (B.54) \]

Now, let us consider the Fock term. Carrying out the sum over isospin index, the Fock contribution is given by

\[
E_F = \frac{iC_2}{4} \nu_{iso} \sum_{\alpha, \beta, \lambda} \int d^3 x \left[ \mathcal{E}_{F1} - \mathcal{E}_{F2} - \mathcal{E}_{F3} + \mathcal{E}_{F4} \right], \text{ where}
\]

\[
\mathcal{E}_{F1} = \sigma_{\alpha \lambda} \cdot \left( \nabla \psi^\dagger_{\alpha} \right) \psi_{\beta} \times (\nabla \psi_{\lambda}), \quad \mathcal{E}_{F2} = \sigma_{\alpha \lambda} \cdot \left( \nabla \psi^\dagger_{\alpha} \right) \psi_{\beta} \times (\nabla \psi_{\beta}) \psi_{\lambda},
\]

\[
\mathcal{E}_{F3} = \sigma_{\alpha \lambda} \cdot \psi_{\alpha} \left( \nabla \psi^\dagger_{\beta} \right) \psi_{\beta} \times (\nabla \psi_{\lambda}), \quad \mathcal{E}_{F4} = \sigma_{\alpha \lambda} \cdot \psi_{\alpha} \left( \nabla \psi^\dagger_{\beta} \right) \times (\nabla \psi_{\beta}) \psi_{\lambda}. \quad (B.55)
\]

Using time reversal invariance trick, it can be shown that \[76]\]

\[
\nu_{iso} \sum_k \psi^\dagger_{k\alpha} \psi_{k\beta} = \rho \delta_{\alpha \beta}. \quad (B.56)
\]

In general, the \( \delta_{\alpha \beta} \) factor appears whenever we have a sum over occupied states with spinors with different spin indices. We will use this extensively in the calculations below. The contribution from the first term is given by

\[
E_{F1} = -\nu_{iso} \frac{iC_2}{4} \int d^3 x \sum_{\alpha, \beta, \lambda} \left[ \sum_k \sigma_{\alpha \lambda} \cdot \nabla \psi^\dagger_{k\alpha} \psi_{k\beta} \right] \times \frac{1}{2\nu_{iso}} (\nabla \rho + 2i j \delta \beta \lambda). \quad (B.57)
\]

Similarly, the fourth term contributes

\[
E_{F4} = \nu_{iso} \frac{iC_2}{4} \int d^3 x \sum_{\alpha, \beta, \lambda} \left[ \sum_k \sigma_{\alpha \lambda} \cdot \psi^\dagger_{k\alpha} \nabla \psi_{k\beta} \right] \times \frac{1}{2\nu_{iso}} (\nabla \rho - 2i j \delta \beta \lambda). \quad (B.58)
\]

Thus we get

\[
E_{F1} + E_{F4} = \frac{C_2}{4\nu_{iso}} \int d^3 x \nabla \rho \cdot J. \quad (B.59)
\]

Next, we note that \( E_{F3} \) will not contribute due to time reversal invariance. Finally, proceeding in the same way, the contribution from the second term to the Fock energy
is given by

\[ E_{F2} = -\frac{C^g}{4\nu_{iso}} \int d^3 x \rho(x) \nabla \cdot J(x). \]  \hspace{1cm} (B.60)

So, the Fock energy takes the form

\[ E_F = -\frac{C^g}{2\nu_{iso}} \int d^3 x \rho(x) \nabla \cdot J(x), \] \hspace{1cm} (B.61)

Thus, the Hartree-Fock energy has the following form:

\[ E_{HF} = -\frac{C^g}{2} \left( 1 + \frac{1}{\nu_{iso}} \right) \int d^3 x \rho \nabla \cdot J(x). \] \hspace{1cm} (B.62)

### B.3 Finite Density Propagator

The fully interacting finite density propagator is defined as the following vacuum expectation value.

\[ i G_{\alpha \beta}(x_t, y_t) \equiv i G_{\alpha \beta}(x, y) = \langle T \left[ \hat{\phi}_\alpha(x) \hat{\phi}_\beta^\dagger(y) \right] \rangle. \] \hspace{1cm} (B.63)

\(T\) refers to the time ordering operator and \(\hat{\phi}\) is the field operator in the Heisenberg picture. Note that “vacuum” means the fully interacting ground state by terminology. In the above definition, we have assumed that the interacting ground state is normalised.

A Heisenberg field operator is related to the corresponding Schrödinger operator (setting \(\hbar\) to unity) in the following manner:

\[ \hat{\phi}_\alpha(x_t) \equiv \hat{\phi}_\alpha(x) = e^{i\hat{H}_t} \hat{\psi}_\alpha(x) e^{-i\hat{H}_t}. \] \hspace{1cm} (B.64)

Thus, we get \(\hat{\phi}_\alpha^\dagger(x_t) \equiv \hat{\phi}_\alpha^\dagger(x) = e^{i\hat{H}_t} \hat{\psi}_\alpha^\dagger(x) e^{-i\hat{H}_t}\). Let us define \(t \equiv t_x - t_y\). The expression for the propagator in terms of the Schrödinger operators looks like

\[ i \, G_{\alpha \beta}(x, y) = \theta(t) \langle \hat{\phi}_\alpha(x) \hat{\phi}_\beta^\dagger(y) \rangle - \theta(-t) \langle \hat{\phi}_\beta^\dagger(y) \hat{\phi}_\alpha(x) \rangle \]

\[ \equiv \ i \, G_{\alpha \beta}^< (x, y) - i \, G_{\alpha \beta}^> (x, y). \] \hspace{1cm} (B.65)
Consider the case \( t > 0 \).

\[
i G_{\alpha\beta}^>(x, y) = \langle e^{i\hat{H}_\text{t}_{x}} \hat{\psi}_\alpha(x) e^{-i\hat{H}_\text{t}_{y}} \hat{\psi}^*_\beta(y) e^{-i\hat{H}_\text{t}_{y}} \rangle
\]

\[
= e^{i\epsilon_0 t} \langle \hat{\psi}_\alpha(x) e^{-i\hat{H}_\text{t}_{y}} \hat{\psi}_\beta(y) \rangle
\]

\[
= \sum_k \sum_n \psi_{k\alpha}(x) \psi_{n\beta}^*(y) \theta(\epsilon_k - \epsilon_F) \theta(\epsilon_n - \epsilon_F) \langle \hat{a}_{k\alpha} e^{-i\hat{H}_\text{t}_{y}} \hat{a}^*_n \rangle
\]

\[
= \delta_{\alpha\beta} \sum_k e^{-i\epsilon_k t} \psi_k(x) \psi_k^*(y) \theta(\epsilon_k - \epsilon_F), \quad \text{(B.66)}
\]

where \( \epsilon_0 \) is the energy eigenvalue of the interacting ground state (that we have set to zero) and we have assumed a spin-independent Hamiltonian. For the case \( t < 0 \), the other half contributes.

\[
i G_{\alpha\beta}^<(x, y) = \langle e^{i\hat{H}_\text{t}_{y}} \hat{\psi}_\beta(y) e^{i\hat{H}_\text{t}_{x}} \hat{\psi}_\alpha(x) e^{-i\hat{H}_\text{t}_{x}} \rangle
\]

\[
= e^{-i\epsilon_0 t} \langle \hat{\psi}_\beta(y) e^{i\hat{H}_\text{t}_{x}} \hat{\psi}_\alpha(x) \rangle
\]

\[
= \sum_k \sum_n \psi_{k\alpha}(x) \psi_{n\beta}^*(y) \theta(\epsilon_F - \epsilon_k) \theta(\epsilon_F - \epsilon_n) \langle \hat{b}_{n\beta} e^{i\hat{H}_\text{t}_{x}} \hat{b}^*_k \rangle
\]

\[
= \delta_{\alpha\beta} \sum_k e^{-i\epsilon_k t} \psi_k(x) \psi_k^*(y) \theta(\epsilon_F - \epsilon_k). \quad \text{(B.67)}
\]

Thus, the finite density propagator takes the form

\[
i G_{\alpha\beta}(x, y) = \delta_{\alpha\beta} \sum_k e^{-i\epsilon_k t} \psi_k(x) \psi_k^*(y) [ \theta(t) \theta(\epsilon_k - \epsilon_F) - \theta(-t) \theta(\epsilon_F - \epsilon_k) ]. \quad \text{(B.68)}
\]

It is instructive to take the zero density limit. One simulates this limit by tending the Fermi level \( \epsilon_F \) to zero. Then the propagator reduces to

\[
\delta_{\alpha\beta} \sum_k e^{-i\epsilon_k t} \psi_k(x) \psi_k^*(y) \theta(t) = \delta_{\alpha\beta} C(x, y, it) \theta(t), \quad \text{(B.69)}
\]

the same as the expression for the retarded propagator in free space derived earlier. Thus we see that at zero density (free space), it does not make sense to talk about an advanced propagator. At finite density, one defines the advanced and the retarded
propagator in the following way [109].

\[
  i G_{\alpha\beta}^R(x, y) = i \left( G_{\alpha\beta}^>(x, y) - G_{\alpha\beta}^<(x, y) \right) \theta(t),
\]

\[
  i G_{\alpha\beta}^A(x, y) = i \left( G_{\alpha\beta}^<(x, y) - G_{\alpha\beta}^>(x, y) \right) \theta(-t). \tag{B.70}
\]

Thus we get the following relation.

\[
  i G_{\alpha\beta}^R(x, y) - i G_{\alpha\beta}^A(x, y) = i G_{\alpha\beta}^>(x, y) - i G_{\alpha\beta}^<(x, y). \tag{B.71}
\]

The equation satisfied by the finite density propagator given by Eq. (B.68) is

\[
  \left( i \partial_t - \hat{H}_x \right) G_{\alpha\beta}(x, y) = \delta_{\alpha\beta} \delta^3(x - y) \delta(t) \equiv \delta_{\alpha\beta} \delta^4(x - y), \tag{B.72}
\]

where \( x = (x, t_x) \). The above can be very easily verified in the following manner.

\[
  i \partial_t G(x, y) = \partial_t \sum_k e^{-i\varepsilon_k t} \psi_k(x) \psi_k^*(y) [ \theta(t) \theta(\varepsilon_k - \varepsilon_F) - \theta(-t) \theta(\varepsilon_F - \varepsilon_k) ]
\]

\[
  = -i \sum_k \varepsilon_k e^{-i\varepsilon_k t} \psi_k(x) \psi_k^*(y) [ \theta(t) \theta(\varepsilon_k - \varepsilon_F) - \theta(-t) \theta(\varepsilon_F - \varepsilon_k) ]
\]

\[
  + \sum_k e^{-i\varepsilon_k t} \psi_k(x) \psi_k^*(y) \delta(t), \tag{B.73}
\]

where we have used \( \partial_t \theta(t) = \delta(t) \). We can use the fact that \( f(t)\delta(t) \equiv f(0)\delta(t) \) and remove the exponential factor in the second term of the above equation. Noting that

\[
  \hat{H}_x \psi_k = \varepsilon_k \psi_k,
\]

we get

\[
  \hat{H}_x G(x, y) = \hat{H}_x (-i) \sum_k e^{-i\varepsilon_k t} \psi_k(x) \psi_k^*(y) [ \theta(t) \theta(\varepsilon_k - \varepsilon_F) - \theta(-t) \theta(\varepsilon_F - \varepsilon_k) ]
\]

\[
  = -i \sum_k \varepsilon_k e^{-i\varepsilon_k t} \psi_k(x) \psi_k^*(y) [ \theta(t) \theta(\varepsilon_k - \varepsilon_F) - \theta(-t) \theta(\varepsilon_F - \varepsilon_k) ]
\]

\[
  = i \partial_t G(x, y) - \sum_k \psi_k(x) \psi_k^*(y) \delta(t)
\]

\[
  = i \partial_t G(x, y) - \delta^3(x - y) \delta(t). \tag{B.74}
\]

This proves Eq. (B.72). In the final step, we have used the completeness relation of the eigenstate \( \psi_k(x) \) of the Hamiltonian.
Now, let us derive a formal expression for the inverse of the finite density propagator. We will suppress spin indices in the following discussion to avoid clutter. The starting point is the following expression:

\[ G(x, z) = \int d^4 y \, \delta^4(x - y) G(y, z). \] (B.75)

Now, we use the above in Eq. (B.68).

\[ \left( i \partial_t - \hat{H}_x \right) G(x, z) = \delta^4(x - z). \]

or,

\[ \int d^4 y \left[ \left( i \partial_t - \hat{H}_x \right) \delta^4(x - y) \right] G(y, z) = \delta^4(x - z). \] (B.76)

Comparing the above expression with

\[ \int d^4 y G^{-1}(x, y) G(y, z) = \delta^4(x - z), \] (B.77)

we infer that

\[ G^{-1}(x, y) = \left( i \partial_t - \hat{H}_x \right) \delta^4(x - y). \] (B.78)

### B.4 HF Evaluation using Feynman Rules

Using the form of the finite density Green’s function, one can directly obtain expressions for Hartree and Fock diagrams. In this section, we illustrate the methodology for ordinary HF diagrams, and in the next section, we shall formulate the basic steps to carry out HF diagrams with derivative interactions using a path integral formalism.

The basic rules for evaluating any Feynman diagram in position space in the zero-temperature formalism are as follows.

1. Assign a space-time point and a spin index to each vertex. For every fermion line directed from \( y \) to \( x \), write down the propagator \( iG^0(x, y) \) with the relevant spin indices.
2. For each fermion line beginning and ending at the same spatial point \( x \), the corresponding propagator expression should be \( iG^0(x, x^+) \), where \( x^+ \equiv (x, t^+_x) \).

This is a special case and it picks out the contribution from the occupied state. Note that \( \rho(x) = -i\nu G^0(x, x^+) \) is the density of the non-interacting system. A good way to keep track of these things is to replace the \( t \) variable in the theta functions (in the expression for the propagator) by \( t - \eta \), \( \eta \) being a positive infinitesimal. In general, a propagator connecting points \( y \) to \( x \) but at equal times \( (t = 0) \) must be interpreted as \( iG^0(x_{t_x}, y_{t_y}) \equiv iG^0(x, y^+) \), so that the occupied part contributes. Note that \( \gamma_s(x, y) = -i\nu G^0(x, y^+) \) is the density matrix.

3. For every interaction between points \( x \) and \( y \), include a factor of \(-iV(x, y) = -iV(x, y) \delta(t_x - t_y) \) with the appropriate spin labels.

4. For spin-independent interactions, the two-body vertices for contact interactions have the structure \( (\delta_{\lambda_0 \mu_0} + \delta_{\lambda_0 \mu_0}) \) where \( (\lambda, \mu) \) are the incoming spins and \( (\alpha, \beta) \) are the outgoing ones. Do the spin summations and write down a factor of \(-\nu \) for each \( \delta_{\lambda \lambda} \) (for every closed fermion loop).

5. Multiply by a symmetry factor \( i/\xi \) where \( \xi = S \prod_{\ell=2}^{m} (\ell!)^{m} \). \( S \) is the number of vertex permutations that transform a diagram into itself, and \( m \) is the number of equivalent \( \ell \)-tuples of lines. Equivalent lines are defined as similarly directed lines that begin and end at the same vertices.

6. Integrate over all vertex co-ordinates (spatial and temporal) and divide by a time factor \( T \).
Now let us consider the Hartree diagram with spin-independent interactions. The two fermion loops gives a factor of $(−ν)^2$. The symmetry factor $ξ = 2$ since $S = 1$, $m = 1$, and $ℓ = 2$. So the Hartree energy is

$$
E_H = \frac{μ^2}{T} \left( \frac{i}{ξ} \right) \int d^4x \int d^4y \ iG^0(x, x^+) \ [-iV(x, y) \ δ(t_x - t_y)] \ iG^0(y, y^+)
$$

$$
= \frac{1}{2T} \int d^4x \int d^4y \ ρ(x) \ V(x, y) \ ρ(y)
$$

$$
= \frac{1}{2} \int \int d^3x \ d^3y \ ρ(x) \ V(x, y) \ ρ(y), \quad \text{(B.79)}
$$

where we have used the fact that $\int dt_x \int dt_y \ δ(t_x - t_y) = T$.

As the next example, let us evaluate the Fock term. There is a single fermion loop contributing a factor of $(−ν)$. The symmetry factor $ξ = 2$ since $S = 1$, $m = 1$, and $ℓ = 2$ as before. So the Fock energy is

$$
E_F = -\frac{μ}{T} \left( \frac{i}{ξ} \right) \int d^4x \int d^4y \ iG^0(x, y) \ [-iV(x, y) \ δ(t_x - t_y)] \ iG^0(y, x)
$$

$$
= -\frac{μ}{2} \int \int d^3x d^3y \ iG^0(x, y^+) \ V(x, y) \ iG^0(y, x^+)
$$

$$
= -\frac{μ}{2} \int \int d^3x d^3y \ \left[ -\frac{γ_s(x, y)}{ν} \right] \ V(x, y) \ \left[ -\frac{γ_s(y, x)}{ν} \right]
$$

$$
= -\frac{1}{2ν} \int \int d^3x d^3y \ γ_s(x, y) \ V(x, y) \ γ_s(y, x). \quad \text{(B.80)}
$$

Note that only after carrying out the HF self-consistent procedure can we get an approximation to the true density of the system. For Kohn-Sham DFT case, the true density is however equal to the density of the Kohn-Sham system by construction (assuming the correlations are accounted for exactly). Next, we illustrate the path integral way of evaluating these diagrams.
B.5 Path Integral Formulation

The path integral formulation is the most elegant way of dealing with these calculations. We will be working at zero temperatures. Let $\mathcal{L}$ denote the Lagrangian of the system. The partition function in Minkowski space in the presence of Grassman sources coupled to the fields looks like

$$Z[\eta_\alpha, \eta_\beta] = \int D\psi D\bar{\psi} e^{i \int d^4x \left[ \mathcal{L} - \psi_\alpha(x)\psi_\alpha(x) - \psi_\beta(x)\eta_\alpha(x) \right]}$$

(B.81)

These sources will be ultimately set to zero. They are introduced for reasons to be made clear shortly. The Lagrangian has a pure kinetic part and an interacting part, so that we can write

$$\mathcal{L} = \bar{\psi}_\alpha \left( i\partial + \frac{\nabla^2}{2M} \right) \psi_\alpha + \mathcal{L}_I.$$  

(B.82)

One can also include an external potential term $-v(x)\psi_\alpha^\dagger \psi_\alpha$ in the definition of the non-interacting part in general. The action is defined as $\mathcal{S} = \int d^4x \mathcal{L}$. Let us shift to Euclidean picture by replacing $it$ by $\tau$, so that $i\partial_t \rightarrow -\partial_\tau$. This means

$$i\mathcal{S} = i \int d^4x \mathcal{L} = -\int dx \left[ \psi_\alpha^\dagger \left( \partial_\tau - \frac{\nabla^2}{2M} + v(x) \right) \psi_\alpha - \mathcal{L}_I \right]$$

$$= -\int dx dy \psi_\alpha^\dagger(x) (G^0)^{-1}_{\alpha\beta}(x, y) \psi_\beta(y) + \int dx \mathcal{L}_I = -\mathcal{S}_E,$$  

(B.83)

where $dx \equiv \int d\tau_x \int d^3x$ is the space-time volume element in Euclidean space, and the inverse of the non-interacting Green’s function is defined as

$$(G^0)^{-1}_{\alpha\beta}(x, y) = \delta_{\alpha\beta} \left( \partial_\tau - \frac{\nabla^2}{2M} + v(x) \right) \delta(x - y) \delta(\tau_x - \tau_y).$$

(B.84)

The Green’s function in Euclidean picture is given by

$$G^0_{\alpha\beta}(x, y) = \delta_{\alpha\beta} \sum_k e^{-\varepsilon_k \tau} \psi_k(x) \psi_k^*(y) \left[ \theta(\tau) \theta(\varepsilon_k - \varepsilon_F) - \theta(-\tau) \theta(\varepsilon_F - \varepsilon_k) \right],$$

(B.85)
where $\tau \equiv \tau_x - \tau_y$. Note that it does not have the factor of $i$, so that the density is $\rho(\mathbf{x}) = -\nu G^0(\mathbf{x}, \mathbf{x}^+)$. The partition function now looks like

$$Z[\eta, \eta^\dagger] = \int D\psi D\psi^\dagger e^{-S_E - \int dx \left[ \eta^\dagger(\mathbf{x})\psi_{\alpha}(\mathbf{x}) + \psi^\dagger(\mathbf{x})\eta_{\alpha}(\mathbf{x}) \right]}.$$  \hspace{1cm} \text{(B.86)}

### B.5.1 Non-interacting System

In this special case, $\mathcal{L}_I = 0$ so that the partition function in a schematic notation is given by the following expression.

$$Z[\eta, \eta^\dagger] = \int D\psi D\psi^\dagger e^{-\int dx dy \psi^\dagger \mathcal{G}^{-1} \psi_{\alpha} - \int dx \left[ \eta^\dagger \psi_{\alpha} + \psi^\dagger \eta_{\alpha} \right]}.$$  \hspace{1cm} \text{(B.87)}

We can complete the square in the exponent in the following manner:

$$\psi^\dagger \mathcal{G}^{-1} \psi_{\alpha} + \eta^\dagger \psi_{\alpha} + \psi^\dagger \eta_{\alpha} = \left( \psi^\dagger + \eta^\dagger \mathcal{G}^{-1} \right) \left( \psi_{\alpha} + \mathcal{G} \eta_{\alpha} \right) - \eta^\dagger \mathcal{G} \eta_{\alpha}$$

$$= \left( \psi' \right)^\dagger \mathcal{G}^{-1} \left( \psi' \right) - \eta^\dagger \mathcal{G} \eta_{\alpha},$$  \hspace{1cm} \text{(B.88)}

where $(\psi')_{\alpha} = (\psi_{\alpha} + \mathcal{G} \eta_{\alpha})$. Note that when we set the sources to zero, we obtain our non-interacting partition function given by

$$Z_0 = \int D\psi D\psi^\dagger e^{-\int dx dy \psi^\dagger \mathcal{G}^{-1} \psi_{\alpha}}.$$  \hspace{1cm} \text{(B.89)}

Using this, we can write down the partition function as

$$Z[\eta, \eta^\dagger] = Z_0 e^{\int dx dy \eta^\dagger(\mathbf{x}) \mathcal{G} \eta_{\alpha}(\mathbf{y})}.$$  \hspace{1cm} \text{(B.90)}

### B.5.2 Interacting System

The interaction part of the Lagrangian can be generally denoted by $\mathcal{L}_I(\psi^\dagger, \psi)$. These fields can be conveniently removed in favour of derivatives with respect to the Grassmanian sources in the following manner.

$$\mathcal{L}_I(\psi^\dagger, \psi) \rightarrow \mathcal{L}_I \left( \frac{\partial}{\partial \eta}, -\frac{\partial}{\partial \eta^\dagger} \right).$$  \hspace{1cm} \text{(B.91)}
These follow from the following observations:

\[
\frac{\partial}{\partial \eta^\dagger \lambda} \ e^{-\int d\psi^\dagger \psi_\lambda} = e^{-\int d\psi^\dagger \psi_\lambda \psi^\dagger_\lambda (x)},
\]

\[
- \frac{\partial}{\partial \eta \lambda} \ e^{-\int d\psi^\dagger \psi_\lambda} = e^{-\int d\psi^\dagger \psi_\lambda \psi^\dagger_\lambda (x)}. \tag{B.92}
\]

Now, we can write the generating functional in the presence of sources as

\[
Z[\eta^\dagger, \eta] = \int D\psi D\psi^\dagger \ e^{-\int d\psi \bar{\psi} (G^0)_{\alpha\beta}^{-1} \psi_{\beta} + \int dx \mathcal{L}_s (\psi^\dagger, \psi) - \int dx \left[ \eta^\dagger_\alpha \psi_\alpha + \eta_\alpha \psi^\dagger_\alpha \right]}
\]

\[
= e^{\int dx \mathcal{L}_s \left( \frac{\delta}{\delta \eta^\dagger_\lambda}, -\frac{\delta}{\delta \eta^\dagger_\alpha} \right) \left( \frac{\delta}{\delta \eta^\dagger_\alpha}, -\frac{\delta}{\delta \eta^\dagger_\lambda} \right) \int d\psi D\psi^\dagger \ e^{-\int d\psi \bar{\psi} (G^0)_{\alpha\beta}^{-1} \psi_{\beta} - \int dx \left[ \eta^\dagger_\alpha \psi_\alpha + \eta_\alpha \psi^\dagger_\alpha \right]}
\]

\[
= Z_0 e^{\int dx \mathcal{L}_s \left( \frac{\delta}{\delta \eta^\dagger_\lambda}, -\frac{\delta}{\delta \eta^\dagger_\alpha} \right) \int d\psi \bar{\psi} (G^0)_{\alpha\lambda} (x, y) \eta_\alpha (y)}. \tag{B.93}
\]

After taking the derivatives with respect to the sources, the sources are set to zero of course.

In general in the finite temperature formalism, one can express the difference in the thermodynamic potential between the interacting and the non-interacting system in the following manner.

\[
\Omega - \Omega_0 = -T \ln \frac{Z}{Z_0}, \tag{B.94}
\]

where \( T \) denotes the temperature, and the Boltzmann’s constant has been set to unity since we are working in natural units. The thermodynamic potential for a system with \( A \) particles with energy \( E \) and entropy \( S \) at a temperature \( T \) is defined in the usual manner.

\[
\Omega (T, V, \mu) = E - TS - \mu A, \tag{B.95}
\]

where \( \mu \) is the chemical potential. In our case, we are at zero temperature. So we get

\[
E - E_0 = -\frac{1}{T} \left( \ln \frac{Z}{Z_0} \right), \tag{B.96}
\]

where \( T \) is the usual temporal volume factor.
B.5.3  Pure Contact Interaction

The corresponding interaction Lagrangian can be obtained from Eq. (3.13). It looks like

$$\mathcal{L}_{C_0} = -\frac{C_0}{2} \psi_\alpha^\dagger \psi_\beta^\dagger \psi_\beta \psi_\alpha.$$  \hspace{1cm} (B.97)

So, we get

$$E_{C_0} - E_0 = -\frac{1}{T} \ln \left[ e^{-\frac{C_0}{2} \int dx \left( \frac{\partial}{\partial \eta_\alpha} \frac{\partial}{\partial \eta_\beta} \frac{\partial}{\partial \eta_\beta^\dagger} \frac{\partial}{\partial \eta_\alpha^\dagger} \right) \left( \frac{1}{2T} \int \int \eta_\lambda^\dagger G^0_{\lambda \mu} \eta_\mu \int \int \eta_\gamma^\dagger G^0_{\gamma \delta} \eta_\delta \right) } \right],$$  \hspace{1cm} (B.98)

where it is understood that the sources will be ultimately set to zero. Contribution from the HF order is calculated by expanding the first exponent to linear order and the second to quadratic order. Noting that \( \ln(1 + \epsilon) = \epsilon \) for an infinitesimal \( \epsilon \), we can schematically write

$$E_{HF} = \frac{C_0}{2T} \int dx \left( \frac{\partial}{\partial \eta_\alpha} \frac{\partial}{\partial \eta_\beta} \frac{\partial}{\partial \eta_\beta^\dagger} \frac{\partial}{\partial \eta_\alpha^\dagger} \right) \left[ \frac{1}{2T} \int \int \eta_\lambda^\dagger G^0_{\lambda \mu} \eta_\mu \int \int \eta_\gamma^\dagger G^0_{\gamma \delta} \eta_\delta \right].$$  \hspace{1cm} (B.99)

Now, there are two distinct ways of hitting the sources with the derivatives. These two ways correspond to the direct and the exchange piece. These two different contractions schematically look like

$$\int dx \left( \frac{\partial}{\partial \eta_\alpha} \frac{\partial}{\partial \eta_\beta} \frac{\partial}{\partial \eta_\beta^\dagger} \frac{\partial}{\partial \eta_\alpha^\dagger} \right) \left[ \frac{1}{2T} \int \int \eta_\lambda^\dagger G^0_{\lambda \mu} \eta_\mu \int \int \eta_\gamma^\dagger G^0_{\gamma \delta} \eta_\delta \right]$$  \hspace{1cm} (B.100)

The contractions shown on top correspond to Hartree, and the bottom one is the exchange. The sign from anticommuting is trivially written down as \((-1)^c\) where \( c \) denotes the number of times the contraction lines cross each other. This gives rise to the negative sign in the Fock piece. Again, there are two ways of doing each of these
pieces so that we get a factor of two. Carrying out the derivatives, we get

\[
E_{\text{HF}} = \frac{C_0}{2T} \int dx \left[ G^0_{\alpha\alpha}(x, x^+) G^0_{\beta\beta}(x, x^+) - G^0_{\alpha\beta}(x, x^+) G^0_{\beta\alpha}(x, x^+) \right]
\]

\[
= \frac{C_0}{2} \left( \frac{1}{T} \int d\tau_x \right) \int d^3x \left[ \nu^2 - \nu \right] \frac{\rho(x) \rho(x)}{(-\nu)(-\nu)}
\]

\[
= \frac{C_0}{2} \left( 1 - \frac{1}{\nu} \right) \int d^3x \rho^2(x),
\]  

(\text{B.101})

where we have carried out spin sums over repeated indices.

### B.5.4 Contact Interaction with Derivatives

#### p-wave term

This term is the one with coefficient $C'_2$ given by (Eq. (3.13))

\[
\mathcal{L}_{C'_2} = \frac{C'_2}{8} (\psi_\alpha^\dagger \nabla_\beta \psi_\beta^\dagger) \cdot (\psi_\beta \nabla_\alpha \psi_\alpha).
\]  

(\text{B.102})

In order to keep track of where the derivatives act, we will write the four fields at four different space-time points and finally set them to the same co-ordinate $x$. Thus, the expression for HF energy becomes

\[
E_{\text{HF}} = -\frac{C'_2}{8T} \int dx \left( \frac{\partial}{\partial \eta_\alpha(x_1)} \nabla_\alpha \eta_\beta(x_2) \cdot \frac{\partial}{\partial \eta_\beta(x_3)} \nabla_\beta \eta_\alpha(x_4) \right)
\]

\[
\times \left[ \frac{1}{2} \int \int \eta_\lambda G^0_{\lambda\mu} \eta_\mu \int \int \eta_\gamma G^0_{\gamma\delta} \eta_\delta \right].
\]  

(\text{B.103})

It can be easily shown that

\[
(\psi(x_1) \nabla_\alpha \psi(x_2)) \cdot (\psi(x_3) \nabla_\beta \psi(x_4)) \equiv (\nabla_1 - \nabla_2) \cdot (\nabla_3 - \nabla_4) \psi_1 \psi_2 \psi_3 \psi_4,
\]  

(\text{B.104})

where $x_k$ is replaced by $x$ finally, $\psi_k \equiv \psi(x_k)$ and $\nabla_k \equiv \nabla_{x_k}$. Using this, the HF energy term takes the form

\[
E_{\text{HF}} = -\frac{C'_2}{8T} (\nabla_1 - \nabla_2) \cdot (\nabla_3 - \nabla_4)
\]

\[
\int dx \left[ G^0_{\alpha\alpha}(x_4, x_2^+) G^0_{\beta\beta}(x_3, x_1^+) - G^0_{\alpha\beta}(x_4, x_2^+) G^0_{\beta\alpha}(x_3, x_1^+) \right].
\]  

(\text{B.105})

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and finally we set all \( x_k \) to \( x \) of course. The next steps are purely a matter of algebra, and we have already gone through them for most parts previously. The important thing to note is that in the Euclidean picture, the expression for density matrix is given by \( \gamma_\alpha(x, y) = -\nu G^0(x, y^+) \), without any factor of \( i \). Grinding through the algebra, we get the expected result.

\[
E_{\text{HF}} = \frac{C_2'}{4} \left( 1 + \frac{1}{\nu} \right) \int d^3x \left[ \rho(x) \tau(x) - \frac{1}{4} (\nabla \rho)^2 - j^2(x) \right]. \quad \text{(B.106)}
\]

**s–wave term**

The s–wave term in Eq. (3.13) is given by

\[
\mathcal{L}_{C_2} = \frac{C_2}{16} \left[ \psi_\alpha^\dagger \psi_\beta^\dagger (\psi_\beta \nabla \psi_\alpha) + (\psi_\alpha \nabla \psi_\beta) \psi_\beta \psi_\alpha \right]. \quad \text{(B.107)}
\]

We play the same game as before so that the expression for HF energy becomes

\[
E_{\text{HF}} = - \frac{C_2}{16T} \int dx \left( \frac{\partial}{\partial \eta_\alpha(x_1)} \frac{\partial}{\partial \eta_\beta(x_2)} \frac{\partial}{\partial \eta_\beta(x_3)} \frac{\partial}{\partial \eta_\alpha(x_4)} \nabla_x^2 \right) \times \left[ \frac{1}{2!} \int \int \eta_\lambda \eta_\mu \eta_\eta \int \int \eta_\gamma \eta_\delta \right]. \quad \text{(B.108)}
\]

As before, it can be easily shown that

\[
\psi_1^{\dagger 2} \nabla_x \psi_2 \equiv (\nabla_1 - \nabla_2)^2 \psi_1 \psi_2,
\]

where \( x_k \) is replaced by \( x \) finally. Using this, the HF energy term takes the form

\[
E_{\text{HF}} = - \frac{C_2}{16T} \left[ (\nabla_3 - \nabla_4)^2 + (\nabla_1 - \nabla_2)^2 \right] \int dx \left[ G^0_{\alpha\alpha}(x_4, x_2^+) G^0_{\beta\beta}(x_3, x_1^+) - G^0_{\alpha\beta}(x_4, x_1^+) G^0_{\beta\alpha}(x_3, x_2^+) \right]. \quad \text{(B.110)}
\]

Again, we grind through the algebra and get the following familiar expression.

\[
E_{\text{HF}} = \frac{C_2}{4} \left( 1 - \frac{1}{\nu} \right) \int d^3x \left[ \rho(x) \tau(x) + \frac{3}{4} (\nabla \rho)^2 - j^2(x) \right]. \quad \text{(B.111)}
\]

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APPENDIX C

VERIFYING FIERZ REARRANGEMENT FOR BOWTIE AND BEACHBALL DIAGRAM

In this appendix, we evaluate expressions for Bowtie and Beachball diagrams and then show how one gets the same results using modified vertex as dictated by Fierz rearrangement.

C.1 Verification for Bowtie (HF) Diagram

From the previous appendix (section B.4), we know that for spin-independent interactions, the two-body vertices for contact interactions have the spin structure $(\delta_{\lambda\alpha}\delta_{\mu\beta} + \delta_{\lambda\beta}\delta_{\mu\alpha})$ where $(\lambda, \mu)$ are the incoming spins and $(\alpha, \beta)$ are the outgoing ones. For a spin-dependent contact interaction, the interaction Lagrangian density has the form

$$\mathcal{L}_{C_0} = -\frac{C_0}{2} \left( \psi_\alpha^\dagger \sigma_{\alpha\lambda} \psi_\lambda \right) \cdot \left( \psi_\beta^\dagger \sigma_{\beta\mu} \psi_\mu \right),$$  \hspace{1cm} (C.1)

where the sum over repeated spin indices are implied. Hence, the two-body vertex structure gets modified to $(\sigma_{\alpha\lambda} \cdot \sigma_{\beta\mu} + \sigma_{\beta\lambda} \cdot \sigma_{\alpha\mu})$. The rest of the Feynman rules remain unchanged. Thus, the HF (bowtie) diagram contributes

$$E_{HF}^\sigma = \frac{1}{T} \left( \frac{i}{\xi} \right) \int d^4x \ iG(x,x^+)_{\lambda\alpha} \left[ -iC_0^\sigma (\sigma_{\alpha\lambda} \cdot \sigma_{\beta\mu} + \sigma_{\beta\lambda} \cdot \sigma_{\alpha\mu}) \right] iG(x,x^+)^\dagger_{\mu\beta}$$
\[ E_{HF} = - \left( \frac{3C_0^\sigma}{2\nu} \right) \int d^3 x \rho^2(x). \]  

We know from Eq. (B.101) that for a spin-independent interaction with coupling \( C_0 \), the contribution at HF order is

\[ E_{HF} = \frac{C_0}{2} \left( 1 - \frac{1}{\nu} \right) \int d^3 x \rho^2(x). \]

We note that Eq. (C.2) has the same structure as the above expression. So it is logical to think that if one has a Lagrangian with both spin-dependent piece and a spin-independent piece, it can be equivalently replaced by a single spin-independent contact term with a renormalised coupling \( \tilde{C}_0 \) such that

\[ \frac{\tilde{C}_0}{2} \left( 1 - \frac{1}{\nu} \right) = \frac{C_0}{2} \left( 1 - \frac{1}{\nu} \right) - \left( \frac{3C_0^\sigma}{2\nu} \right). \]

Solving for \( \tilde{C}_0 \), we get

\[ \tilde{C}_0 = C_0 - \frac{3C_0^\sigma}{\nu - 1} = C_0 - 3C_0^\sigma, \]

where we have used the fact that \( \nu = 2 \) for our case. The above is the exact same relation that we arrived at in section 5.2.4. This verifies Fierz rearrangement at the HF order.

### C.2 Verification for Beachball Diagram

For the spin-independent case, the expression for the beachball diagram is

\[ E_B = \frac{\Delta}{T} \left( i \right) \int d^4 x \int d^4 y \, iG(x, y)_{\lambda_1 \alpha_1} iG(x, y)_{\lambda_2 \alpha_2} iG(y, x)_{\lambda_3 \alpha_3} iG(y, x)_{\lambda_4 \alpha_4}, \]
where \( \Delta = (-iC_0)^2(\delta_{\lambda_1\alpha_2}\delta_{\lambda_2\alpha_4} + \delta_{\lambda_1\alpha_4}\delta_{\lambda_2\alpha_2})(\delta_{\lambda_3\alpha_1}\delta_{\lambda_4\alpha_2} + \delta_{\lambda_3\alpha_2}\delta_{\lambda_4\alpha_1}) \). 

(C.7)

The symmetry factor for the beachball is \( \xi = 8 \), but this is irrelevant to our present discussion. Let us generally denote the spin sum factor as \( \mathcal{J} \), so that for the spin-independent interaction case, \( \mathcal{J} = \delta_{\lambda_1\alpha_1}\delta_{\lambda_2\alpha_2}\delta_{\lambda_3\alpha_3}\delta_{\lambda_4\alpha_4} \Delta \). The expression for energy then reduces to

\[
E_B = \frac{\mathcal{J}}{T} \left( \frac{i}{\xi} \right) \int d^4x \int d^4y \, iG(x, y)iG(x, y)iG(y, x). \quad \text{(C.8)}
\]

The spin sum for this case is

\[
\mathcal{J} = \delta_{\lambda_1\alpha_1}\delta_{\lambda_2\alpha_2}\delta_{\lambda_3\alpha_3}\delta_{\lambda_4\alpha_4} \Delta \\
= (-iC_0)^2(\delta_{\lambda_1\alpha_1}\delta_{\lambda_2\alpha_2}\delta_{\lambda_3\alpha_3}\delta_{\lambda_4\alpha_4}(\delta_{\lambda_1\alpha_3}\delta_{\lambda_2\alpha_4} + \delta_{\lambda_1\alpha_4}\delta_{\lambda_2\alpha_3})(\delta_{\lambda_3\alpha_1}\delta_{\lambda_4\alpha_2} + \delta_{\lambda_3\alpha_2}\delta_{\lambda_4\alpha_1}) \\
= (-iC_0)^2(\delta_{\lambda_1\lambda_2}\delta_{\lambda_2\lambda_4} + \delta_{\lambda_1\lambda_4}\delta_{\lambda_2\lambda_3})(\delta_{\lambda_3\lambda_4}\delta_{\lambda_4\lambda_1} + \delta_{\lambda_3\lambda_1}\delta_{\lambda_4\lambda_4}) \\
= (-iC_0)^2(\delta_{\lambda_1\lambda_2}\delta_{\lambda_2\lambda_4} + \delta_{\lambda_1\lambda_4}\delta_{\lambda_2\lambda_3} + \delta_{\lambda_3\lambda_4}\delta_{\lambda_4\lambda_1} + \delta_{\lambda_3\lambda_1}\delta_{\lambda_4\lambda_4}) \\
= 2\nu(\nu - 1)(-iC_0)^2. \quad \text{(C.9)}
\]

When we have a spin-dependent interaction with a coupling \( C_0^\sigma \) along with the original spin-independent one, three distinct cases come in the picture. In the first case, both the vertices of the beachball have spin independence. In the second case, both the vertices have spin dependence. The third case is the one where one vertex is spin-dependent and the other is spin-independent. This case comes with a factor of two corresponding to two ways of choosing the spin-dependent vertex. Let us denote the corresponding spin sum factors as \( \mathcal{J}, \mathcal{J}_1, \) and \( \mathcal{J}_2 \) respectively. The expression for energy then takes the form

\[
E_B^\sigma = \frac{\mathcal{J} + \mathcal{J}_1 + 2\mathcal{J}_2}{T} \left( \frac{i}{\xi} \right) \int d^4x \int d^4y \, iG(x, y)iG(x, y)iG(y, x)iG(y, x), \quad \text{(C.10)}
\]

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where we already know the expression for $J$ from Eq. (C.9). When both the vertices have spin-dependence, the spin factor is of the form

$$J_1 = \delta_{\lambda_1 \alpha_1} \delta_{\lambda_2 \alpha_2} \delta_{\lambda_3 \alpha_3} \delta_{\lambda_4 \alpha_4} \Delta_1$$  \hspace{1cm} (C.11)

where $\Delta_1$ is given by

$$\Delta_1 = (-i C_0^\sigma)^2 (\sigma_{\lambda_1 \alpha_3} \cdot \sigma_{\lambda_2 \alpha_4} + \sigma_{\lambda_1 \alpha_4} \cdot \sigma_{\lambda_2 \alpha_3})(\sigma_{\lambda_3 \alpha_1} \cdot \sigma_{\lambda_4 \alpha_2} + \sigma_{\lambda_3 \alpha_2} \cdot \sigma_{\lambda_4 \alpha_1}). \hspace{1cm} (C.12)$$

Observe that $\sigma_{\alpha} \cdot \sigma_{\lambda} = (\sigma^a)_{\alpha_3} (\sigma^a)_{\lambda_{\mu}}$, where the index $a = \{1, 2, 3\}$ and sum over this index is implied. Acting through by the Kronecker deltas and using the above, the spin sum reduces to

$$J_1 = (-i C_0^\sigma)^2 \left[ (\sigma_{\lambda_1 \lambda_3} \cdot \sigma_{\lambda_2 \lambda_4}) (\sigma_{\lambda_3 \lambda_1} \cdot \sigma_{\lambda_4 \lambda_2}) + (\sigma_{\lambda_1 \lambda_4} \cdot \sigma_{\lambda_2 \lambda_3}) (\sigma_{\lambda_3 \lambda_2} \cdot \sigma_{\lambda_4 \lambda_1}) \right]
+ (-i C_0^\sigma)^2 \left[ (\sigma_{\lambda_1 \lambda_3} \cdot \sigma_{\lambda_2 \lambda_4}) (\sigma_{\lambda_3 \lambda_2} \cdot \sigma_{\lambda_4 \lambda_1}) + (\sigma_{\lambda_1 \lambda_4} \cdot \sigma_{\lambda_2 \lambda_3}) (\sigma_{\lambda_3 \lambda_1} \cdot \sigma_{\lambda_4 \lambda_2}) \right]
= (-i C_0^\sigma)^2 \left[ 2(\sigma^a \sigma^b)_{\lambda_1 \lambda_1} (\sigma^a \sigma^b)_{\lambda_2 \lambda_2} + (-i C_0^\sigma)^2 \left[ 2(\sigma^a \sigma^b)_{\lambda_1 \lambda_1} \right] \right]
= 2 (-i C_0^\sigma)^2 \left( \text{tr} (\sigma^a \sigma^b)^2 \right)^2 + \text{tr} \left[ (\sigma^a \sigma^b)^2 \right], \hspace{1cm} (C.13)$$

where $\text{tr}$ denotes a spin trace. Since $\text{tr} \sigma^a = 0$, we get

$$\text{tr} (\sigma^a \sigma^b) = \text{tr} (\delta_{ab} + i \epsilon_{abc} \sigma^c) = \delta_{\lambda \lambda} \delta_{ab} = -\nu \delta_{ab}. \hspace{1cm} (C.14)$$

Therefore, we get

$$[\text{tr} (\sigma^a \sigma^b)]^2 = \nu^2 \delta_{ab} = 3 \nu^2. \hspace{1cm} (C.15)$$

Next, we consider

$$\text{tr} \left[ (\sigma^a \sigma^b)^2 \right] = \text{tr} \left[ (\delta_{ab} + i \epsilon_{abc} \sigma^c)(\delta_{ab} + i \epsilon_{abd} \sigma^d) \right]$$

$$= \text{tr} \left[ (\delta_{ab})^2 - \epsilon_{abc} \epsilon_{abd} \sigma^c \sigma^d \right]$$

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\[ = \text{tr} (\delta_{aa}) - \epsilon_{abc} \epsilon_{abd} \text{tr} (\sigma^c \sigma^d) \]
\[ = -3 \nu + \nu \epsilon_{abc} \epsilon_{abd} \delta_{cd} = -3 \nu + (\epsilon_{abc})^2 = 3 \nu. \quad (C.16) \]

So, the spin factor \( J_1 \) becomes
\[ J_1 = 6 \nu (\nu + 1) (-i C_0^\sigma)^2. \quad (C.17) \]

Finally, we consider the case when one of the vertices is spin-dependent and the other is spin-independent. For this case, the spin factor is of the form
\[ J_2 = \delta_{\lambda_1 \alpha_1} \delta_{\lambda_2 \alpha_2} \delta_{\lambda_3 \alpha_3} \delta_{\lambda_4 \alpha_4} \Delta_2 \quad (C.18) \]
where \( \Delta_2 \) is given by
\[ \Delta_2 = (-i C_0^\sigma) (-i C_0) (\delta_{\lambda_1 \alpha_3} \delta_{\lambda_2 \alpha_4} + \delta_{\lambda_1 \alpha_4} \delta_{\lambda_2 \alpha_3}) (\sigma_{\lambda_3 \alpha_1} \cdot \sigma_{\lambda_4 \alpha_2} + \sigma_{\lambda_3 \alpha_2} \cdot \sigma_{\lambda_4 \alpha_1}). \quad (C.19) \]

Acting through the Kronecker deltas, the spin sum reduces to
\[ J_2 = (-i C_0^\sigma) (-i C_0) (\sigma_{\lambda_1 \lambda_2} \cdot \sigma_{\lambda_2 \lambda_1} + \sigma_{\lambda_3 \lambda_4} \cdot \sigma_{\lambda_4 \lambda_3}) \]
\[ = 2 (-i C_0^\sigma) (-i C_0) \sigma_{\lambda_1 \lambda_2} \cdot \sigma_{\lambda_2 \lambda_1} \]
\[ = 2 (-i C_0^\sigma) (-i C_0) (\sigma^a)_{\lambda_1 \lambda_2} (\sigma^a)_{\lambda_2 \lambda_1} = -6 \nu (-i C_0^\sigma) (-i C_0), \quad (C.20) \]
since \((\sigma^a)_{\lambda_1 \lambda_2} (\sigma^a)_{\lambda_2 \lambda_1} = (\sigma^a)_{\lambda_1 \lambda_1} = 3 \delta_{\lambda_1 \lambda_1} = -3 \nu\). So, we get the net spin factor to be
\[ J + J_1 + 2J_2 = -2 \nu (\nu - 1) (C_0)^2 - 6 \nu (\nu + 1) (C_0^\sigma)^2 + 12 \nu C_0 C_0^\sigma. \quad (C.21) \]

Now, if we replace these interactions by a single spin-independent contact term with a renormalised coupling \( \tilde{C}_0 = C_0 - 3C_0^\sigma \), the corresponding spin sum term would take the following form.
\[ \tilde{J} = -2\nu (\nu - 1) (C_0 - 3C_0^\sigma)^2. \quad (C.22) \]
For $\nu = 2$, it is easy to see that $\mathcal{J} + \mathcal{J}_1 + 2\mathcal{J}_2 = \tilde{\mathcal{J}}$. This verifies Fierz rearrangement for the beachball diagram. Based on the path integral formulation, we can make a general argument that Fierz rearrangement will hold for all orders.
APPENDIX D

SEMI-CLASSICAL EXPANSIONS

In a finite system, the eigenfunctions of the Hamiltonian are no longer plane waves, and thus the system has spatial variations of density. Therefore, the density matrices will have gradient terms that will capture the inhomogeneity of the system. The following are some of the approaches to density matrix expansions that one encounters in literature.

D.1 Negele’s Density Matrix Expansion

Let us introduce the center-of-mass coordinate $R = (x + y)/2$ and relative coordinate $r = x - y$. The Dirac density matrix in terms of these coordinates looks like

$$
\gamma_s(R, r) = \nu \sum_k \psi_k(R + \frac{r}{2}) \psi_k^*(R - \frac{r}{2}) \theta(\epsilon_F - \epsilon_k).
$$

Observe that the above expression can be written as:

$$
\gamma_s(R, r) = \nu e^{i\frac{\pi}{2}(\nabla_1 - \nabla_2)} \sum_k \psi_k(R_1) \psi_k^*(R_2) \theta(\epsilon_F - \epsilon_k)
= e^{i\frac{\pi}{2}(\nabla_1 - \nabla_2)} \gamma_s(R_1, R_2),
$$

where $\nabla_j$ acts on $R_j$ and the expression is evaluated at $R_1 = R_2 = R$. Taking an angular average of the above expression [83] over the direction of $r$, one gets the
following result.

\[
\gamma_s(R, r) = \frac{\sinh \left[ \frac{\gamma (\nabla_1 - \nabla_2)}{2} \right]}{\frac{\gamma (\nabla_1 - \nabla_2)}{2}} \gamma_s(R_1, R_2).
\]  

(D.1)

Note that an angular average of a function \( F(x) \) in three spatial dimensions is defined as

\[
\bar{F}(x) = \frac{1}{4\pi} \int d\Omega F(x),
\]

where \( d\Omega \) is the differential solid angle element. We define variables \( a = k_F r \), \( b = \left( \frac{\nabla_1 - \nabla_2}{2k_F} \right) \), and use the plane wave expansion

\[
e^{i\chi x} = \sum_{\ell=0}^{\infty} (2\ell + 1)i^{\ell} j_\ell(z) P_\ell(\chi),
\]

(D.2)

to write

\[
\sinh(a\ b) = \frac{e^{ab} - e^{-ab}}{2} = \frac{e^{i(-a)(ib)} - e^{ia(ib)}}{2} = \frac{1}{2} \sum_{\ell=0}^{\infty} (2\ell + 1)i^{\ell} [j_\ell(-a) - j_\ell(a)] P_\ell(ib).
\]

Since \( j_\ell(-a) = (-1)^\ell j_\ell(a) \), only the odd \( \ell \) terms in the expansion survives. Indexing \( \ell = 2n + 1 \), the above expression takes the form

\[
\sinh(a\ b) = (-1) \sum_{n=0}^{\infty} (4n + 3)i^{2n+1} j_{2n+1}(a) P_{2n+1}(ib)
\]

Hence, we get the following Bessel function expansion :

\[
\frac{1}{a b} \sinh(a\ b) = \frac{1}{a} \sum_{n=0}^{\infty} (-1)^n (4n + 3) j_{2n+1}(a) Q_n(b^2)
\]

(D.3)

where \( Q_n(b^2) = P_{2n+1}(ib)/ib \), and this leads to the following expression for the density matrix.

\[
\tilde{\gamma}_s(R, r) = \frac{1}{k_F r} \left[ \sum_{n=0}^{\infty} (-1)^n (4n + 3) j_{2n+1}(k_F r) Q_n \left( \left( \frac{\nabla_1 - \nabla_2}{2k_F} \right)^2 \right) \right] \gamma_s(R_1, R_2).
\]

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Let us evaluate the first two terms in the expansion. Since $Q_0(b^2) = 1$, the leading order contribution to the density matrix is:

$$\langle \gamma_s(R, r) \rangle_{n=0} = 3 \rho(R) \frac{j_1(kF r)}{kF r},$$

the same result as obtained in Eq. (A.21), except for the fact that now the density is no longer a constant. Next, we note that $Q_1(b^2) = -\frac{1}{2}(3 + 5b^2)$. Explicitly writing $\gamma_s(R_1, R_2)$ in terms of the wavefunctions, and directly carrying out

$$\left(\frac{\nabla_1 - \nabla_2}{2kF} \right)^2 \gamma_s(R_1, R_2)$$
gives us $\frac{1}{\nu kF} \left( \frac{1}{4} \nabla^2 \rho(R) - \tau(R) \right)$, where we have used

$$\sum_k \left[ \psi_k(R) \nabla^2 \psi^*_k(R) + \psi^*_k(R) \nabla^2 \psi_k(R) \right] \theta(\varepsilon_F - \varepsilon_k) = \frac{1}{\nu} \left[ \nabla^2 \rho(R) - 2\tau(R) \right].$$

The above equation can be very easily shown to be true in the following fashion.

$$\frac{1}{\nu} \nabla^2 \rho(R) = \nabla^2 \sum_k \psi_k^*(R) \psi_k(R) \theta(\varepsilon_F - \varepsilon_k)$$

$$= \nabla \cdot \sum_k (\psi_k^*(R) \nabla \psi_k(R) + \psi_k(R) \nabla^* \psi_k(R)) \theta(\varepsilon_F - \varepsilon_k)$$

$$= \frac{2}{\nu} \tau(R) + \sum_k \left[ \psi_k(R) \nabla^2 \psi^*_k(R) + \psi^*_k(R) \nabla^2 \psi_k(R) \right] \theta(\varepsilon_F - \varepsilon_k),$$

where $\tau(R)$ is the kinetic energy density given by the following expression:

$$\tau(R) = \nu \sum_k \nabla \psi_k(R) \cdot \nabla^* \psi_k(R) \theta(\varepsilon_F - \varepsilon_k). \quad (D.4)$$

Thus, the next order contribution to the density matrix is

$$\langle \gamma_s(R, r) \rangle_{n=1} = \frac{35}{2} \frac{j_3(kF r)}{kF r} \left( \frac{1}{4} \nabla^2 \rho(R) - \tau(R) \right) + \frac{21}{2} \frac{j_3(kF r)}{kF r} \rho(R) \quad \text{(D.5)}$$

So, we have a density matrix expansion about the uniform system result.

### D.2 Wigner-Kirkwood Method

This is a very elegant method that carries out the semi-classical expansion scheme in a transparent and methodical fashion. We shall use this approach to derive the
expansion of the Bloch density matrix, and use the result to get expansions for the kinetic energy to illustrate the power of the method. The semi-classical expansion is essentially an expansion in powers of $\hbar$, and so in this section, we are going to keep the $\hbar$ dependence explicit so as not to mix up the various orders in the expansion.

D.2.1 Formalism

We start from the definition of the Bloch density matrix in $D$ spatial dimensions.

$$C(x, y, \beta) = \langle x| e^{-\beta \hat{H}}|y \rangle = e^{-\beta \hat{H}} \delta^D(x - y)$$

$$= \left( \frac{1}{(2\pi \hbar)^D} \right) \int d^D p e^{-\beta \hat{H}} e^{ip(x-y)/\hbar}$$

$$= \left( \frac{1}{\hbar} \right)^D \int d^D p e^{-ip \cdot y/\hbar} e^{-\beta \hat{H}} e^{ip \cdot x/\hbar}. \quad (D.6)$$

Now, $\hat{H} = \hat{T} + \hat{V}$ and $[\hat{T}, \hat{V}] \neq 0$, so that $e^{-\beta \hat{H}} \neq e^{-\beta \hat{T}} e^{-\beta \hat{V}}$. To set up the stage for a semiclassical expansion, we do the following trick [108]. From now on it is understood that $\hat{H}_x$ acts only on functions of $x$ and we therefore drop the suffix and write the following:

$$u(x, p, \beta) = e^{-\beta \hat{H}} e^{ip \cdot x/\hbar} = e^{-\beta H_C} e^{ip \cdot x/\hbar} w(x, p, \beta), \quad (D.7)$$

where $H_C = \frac{p^2}{2m} + v(x)$ is the classical Hamiltonian. Note that $\hat{H} e^{ip \cdot x/\hbar} = H_C e^{ip \cdot x/\hbar}$.

The quantum fluctuations of the system is captured by $w(x, p, \beta)$. For a classical system, this function would have been unity trivially. $u(x, p, \beta)$ satisfies Bloch’s equation (Eq. (A.7)). This can be easily verified by working with the first part of Eq. (D.7). Note that $u(x, p, \beta = 0) = e^{ip \cdot x/\hbar}$ so that $w(x, p, \beta = 0) = 1$. Substituting the second part of Eq. (D.7) in Bloch’s equation, we get

$$\partial_\beta u(x, p, \beta) = -H_C u + e^{-\beta H_C} e^{ip \cdot x/\hbar} \partial_\beta w(x, p, \beta). \quad (D.8)$$

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Using the fact that $\partial_\beta u = \hat{H} u$ leads to

$$
\begin{align*}
\partial_\beta w(x, p, \beta) &= e^{\beta HC} e^{-ip \cdot x/h} \left( H_C - \hat{H} \right) u(x, p, \beta) \\
&= H_C w(x, p, \beta) - e^{\beta HC} e^{-ip \cdot x/h} \hat{H} u(x, p, \beta) \\
&= H_C w - e^{\beta HC} e^{-ip \cdot x/h} \left( -\frac{\hbar^2}{2M} \nabla^2 u \right) - vw \\
&= \frac{i\hbar}{M} \left[ p \cdot \nabla w - \beta (p \cdot \nabla v) w \right] \\
&+ \frac{\hbar^2}{2M} \left[ \nabla^2 w - 2\beta \nabla v \cdot \nabla w - \beta w \nabla^2 v + \beta^2 w \nabla v \cdot \nabla v \right].
\end{align*}
$$

(D.9)

This result is exact for any spatial dimensions. Now we invoke the semiclassical expansion $w = (1 + \hbar w_1 + \hbar^2 w_2 + \cdots)$ so that $\partial_\beta w = (\hbar \partial_\beta w_1 + \hbar^2 \partial_\beta w_2 + \cdots)$. Comparing powers of $\hbar$, we get expressions for $\partial_\beta w_k$, and this allows us to solve for $w_k$. Since $w(x, p, \beta = 0) = 1$, the semiclassical expansion gives the condition

$$w_k(x, p, \beta = 0) = 0$$

for all $k$. This serves as the boundary condition while solving for $w_k$. To first order in $\hbar$, we get

$$
\partial_\beta w_1 = \frac{-i\beta}{M} p \cdot \nabla v \implies w_1 = \frac{-i\beta^2}{2M} p \cdot \nabla v. \quad \text{(D.10)}
$$

At the next order,

$$
\begin{align*}
\partial_\beta w_2 &= \frac{i}{M} p \cdot \nabla w_1 - \frac{i\beta}{M} (p \cdot \nabla v) w_1 - \frac{\beta}{2M} \nabla^2 v + \frac{\beta^2}{2M} (\nabla v)^2 \\
&= \frac{\beta^2}{2M^2} (p \cdot \nabla)^2 v - \frac{\beta^3}{2M^2} (p \cdot \nabla v)^2 - \frac{\beta}{2M} \nabla^2 v + \frac{\beta^2}{2M} (\nabla v)^2.
\end{align*}
$$

Integrating, we get

$$w_2 = \frac{\beta^3}{6M^2} (p \cdot \nabla)^2 v - \frac{\beta^4}{8M^2} (p \cdot \nabla v)^2 - \frac{\beta^2}{4M} \nabla^2 v + \frac{\beta^3}{6M} (\nabla v)^2. \quad \text{(D.11)}$$
Observe that the power of momentum \( p \) in \( w_k \) is \( k \), so that terms involving odd powers of \( \hbar \) have odd powers of \( p \). Using Eq. (D.6) and Eq. (D.7),

\[
C(x, x, \beta) = \left( \frac{1}{\hbar} \right)^D \int d^D p e^{-ip \cdot x/\hbar} \left[ e^{-\beta H_C} e^{ip \cdot x/\hbar} w(x, p, \beta) \right] \\
= \left( \frac{1}{\hbar} \right)^D \int d^D p e^{-\beta H_C} \left[ 1 + \hbar w_1 + \hbar^2 w_2 + \cdots \right] \\
\equiv \left[ C_0 + \hbar^2 C_2 + \hbar^4 C_4 + \cdots \right]. \tag{D.12}
\]

We have used the fact that odd powers of \( p \) do not contribute to the integral. The density is easily obtained once we know \( C(x, x, \beta) \).

\[
\rho(x) = \nu \mathcal{L}_{\nu}^{-1} \left[ \frac{1}{\beta} C(x, x, \beta) \right] \\
\equiv \left[ \rho_0 + \hbar^2 \rho_2 + \hbar^4 \rho_4 + \cdots \right]. \tag{D.13}
\]

The kinetic energy density is obtained as [104]

\[
\tau(x) = -\nu \mathcal{L}_{\nu}^{-1} \left[ \frac{1}{\beta} (\partial_\beta + v(x)) C(x, x, \beta) \right] \\
= -\nu \mathcal{L}_{\nu}^{-1} \left[ \frac{1}{\beta} \partial_\beta C(x, x, \beta) \right] - v(x) \rho(x) \\
\equiv \left[ \tau_0 + \hbar^2 \tau_2 + \hbar^4 \tau_4 + \cdots \right]. \tag{D.14}
\]

We also define the following for future notational brevity.

\[
\Xi_D = \frac{\nu}{\hbar D}. \tag{D.15}
\]

Finally, the partition function is given by

\[
Z(\beta) = \nu \int d^D x C(x, x, \beta) = \nu \int d^D x \left[ C_0 + \hbar^2 C_2 + \hbar^4 C_4 + \cdots \right]. \tag{D.16}
\]

### D.2.2 Application: One Dimension

Let us apply the formalism to work out a density expansion for a one dimensional system with a classical Hamiltonian \( H_C = \frac{p^2}{2m} + v(x) \). The leading order term in the
expansion of $C(x, x, \beta)$ is given by

$$C_0(x, x, \beta) = \left( \frac{1}{\hbar} \right) \int_{-\infty}^{\infty} dp \, e^{-\beta H_C} = \left( \frac{1}{\hbar} \right) e^{-\beta \nu(x)} \sqrt{\frac{2M\pi}{\beta}}. \quad (D.17)$$

The next order contribution is given by

$$C_2 = \left( \frac{1}{\hbar} \right) \int_{-\infty}^{\infty} dp \, e^{-\beta H_C} \left[ \frac{\beta^3}{6M^2} p^2 \left( \frac{dv}{dx} \right)^2 - \frac{\beta^4}{8M^2} \left( \frac{dv}{dx} \right)^2 + \frac{\beta^2}{4M \frac{dv}{dx}} + \frac{\beta^3}{6M} \left( \frac{dv}{dx} \right)^2 \right]$$

$$= \left( \frac{1}{\hbar} \right) \sqrt{\frac{2M\pi}{\beta}} \left[ \frac{\beta^3}{24M} \left( \frac{dv}{dx} \right)^2 - \frac{\beta^2}{2M} \frac{d^2 v}{dx^2} \right]. \quad (D.18)$$

We use the above to evaluate the terms in the semiclassical expansion of $\rho(x)$. Using

$$\epsilon_F - \nu(x) = \frac{\hbar^2 \nu(x)}{2M},$$

we get

$$\rho_0(x) = \nu \mathcal{L}^{-1}_{\epsilon_F} \left[ \frac{1}{\beta} C_0(x, x, \beta) \right] = \left( \frac{2\nu}{\hbar} \right) p_F(x). \quad (D.19)$$

The next order is

$$\rho_2(x) = \nu \mathcal{L}^{-1}_{\epsilon_F} \left[ \frac{1}{\beta} C_2(x, x, \beta) \right] = \left( \frac{\nu}{\hbar} \right) \left[ \frac{1}{16p_F^5} \left( \frac{dp_F^2}{dx} \right)^2 - \frac{1}{12p_F^3} \left( \frac{dp_F^2}{dx} \right)^2 \right]. \quad (D.20)$$

Thus, to second order, the expression for density is

$$\rho(x) = \Xi_1 \left[ 2p_F(x) - \hbar^2 \left( \frac{1}{12p_F^3} \frac{d^2 p_F^2}{dx^2} - \frac{1}{16p_F^5} \left( \frac{dp_F^2}{dx} \right)^2 \right) \right]. \quad (D.21)$$

Since the dimension of $p_F/\hbar$ is $L^{-1}$, the above can easily be verified as to be dimensionally correct. The above expression can be helpful if inverted. While evaluating Hugenholtz diagrams, one normally works in the uniform system limit and gets analytic answers in terms of the Fermi momentum $p_F$. If we know $p_F[\rho]$, that provides us a chance to go beyond the local density approximation. To a first approximation, $p_F(x) = \frac{\rho(x)}{2\Xi_1}$. Using this in Eq. (D.21),

\[
(2 \Xi_1) p_F = \rho + \Xi_1 \hbar^2 \left( \frac{1}{12} \left( \frac{2 \Xi_1}{\rho} \right)^3 \frac{d^2 \rho}{dx^2} - \frac{1}{16} \left( \frac{2 \Xi_1}{\rho} \right)^5 \left( \frac{d}{dx} \left( \frac{\rho}{2 \Xi_1} \right)^2 \right)^2 \right).
\]

$$\Rightarrow p_F[\rho] = \frac{\rho}{2 \Xi_1} + \Xi_1 \hbar^2 \left( \frac{1}{12\rho^3} \frac{d^2 \rho^2}{dx^2} - \frac{1}{16\rho^5} \left( \frac{d\rho^2}{dx} \right)^2 \right). \quad (D.22)$$

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Next, let us determine the semiclassical expansion of the kinetic energy density. In the Kohn-Sham system, the kinetic part is always dealt with exactly, so we will not have any use of the expression, but it is instructive to go ahead with the derivation. Firstly, it can be shown that at any order $k$, $\partial_\beta C_k(x, x, \beta)$ has the form

$$\partial_\beta C_k(x, x, \beta) = -v(x) C_k(x, x, \beta) - f_k(x, \beta).$$

From Eq. (D.14), we get for any order,

$$\tau_k(x) = \nu \mathcal{L}_{\varepsilon_F}^{-1} \left[ \frac{1}{\beta} \partial_\beta C_k(x, x, \beta) \right] - v(x) \rho_k(x)$$

$$= \nu \mathcal{L}_{\varepsilon_F}^{-1} \left[ \frac{1}{\beta} v(x) C_k(x, x, \beta) \right] + \nu \mathcal{L}_{\varepsilon_F}^{-1} \left[ \frac{1}{\beta} f_k(x, \beta) \right] - v(x) \rho_k(x)$$

$$= \nu \mathcal{L}_{\varepsilon_F}^{-1} \left[ \frac{1}{\beta} f_k(x, \beta) \right]. \quad (D.23)$$

Evaluation $f_k(x, \beta)$ for the first few $k$ gives:

$$f_0(x, \beta) = \frac{1}{2\beta} C_0(x, x, \beta),$$

$$f_2(x, \beta) = \frac{\beta}{8M} \left[ \frac{d^2v}{dx^2} - \frac{5}{6} \beta \left( \frac{dv}{dx} \right)^2 \right] C_0(x, x, \beta).$$

From Eq. (D.23), we get for $k = 0$:

$$\tau_0(x) = \nu \mathcal{L}_{\varepsilon_F}^{-1} \left[ \frac{1}{\beta} f_0(x, \beta) \right] = \Xi_1 \frac{p_{\varepsilon}^2(x)}{3M}. \quad (D.24)$$

The next order contribution is

$$\tau_2(x) = \nu \mathcal{L}_{\varepsilon_F}^{-1} \left[ \frac{1}{\beta} f_2(x, \beta) \right] = \left( \Xi_1 \frac{5}{8M} \right) \left[ \frac{5}{12p_{\varepsilon}^3} \left( \frac{dp_{\varepsilon}^2}{dx} \right)^2 - \frac{1}{p_{\varepsilon}} \frac{d^2p_{\varepsilon}^2}{dx^2} \right]. \quad (D.25)$$

Thus, to second order, the expression for kinetic energy density is

$$\tau(x) = \Xi_1 \left[ \frac{p_{\varepsilon}^2(x)}{3M} + \hbar^2 \left( \frac{1}{8M} \right) \left( \frac{5}{12p_{\varepsilon}^3} \left( \frac{dp_{\varepsilon}^2}{dx} \right)^2 - \frac{1}{p_{\varepsilon}} \frac{d^2p_{\varepsilon}^2}{dx^2} \right) \right]. \quad (D.26)$$

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In order to write $\tau(x)$ in terms of $\rho(x)$ and its gradients, we use Eq. (D.22) in the above expression. Retaining only terms up to order $\hbar^2$, we find that

$$
\tau_0[\rho] = \frac{\Xi_1}{3M} \left[ \left( \frac{\rho}{2\Xi_1} \right)^3 + 3 \left( \frac{\rho}{2\Xi_1} \right)^2 \Xi_1 \hbar^2 \left( \frac{1}{12\rho^3} \frac{d^2\rho^2}{dx^2} - \frac{1}{16\rho^5} \left( \frac{d\rho^2}{dx} \right)^2 \right) \right]
$$

$$
= \frac{1}{24M} \left[ \frac{\rho^3}{\Xi_1^2} \hbar^2 + \hbar^2 \left( \frac{1}{2\rho} \frac{d^2\rho}{dx^2} - \frac{3}{8\rho^3} \left( \frac{d\rho^2}{dx} \right)^2 \right) \right].
$$

Since $\tau_2(x)$ is of order $\hbar^2$, we use only the leading contribution to $p_F[\rho]$ in Eq. (D.22).

$$
\tau_2[\rho] = \frac{\Xi_1}{8M} \left[ \frac{5}{12} \left( \frac{2\Xi_1}{\rho} \right)^3 \left( \frac{d\rho^2}{dx} \left( \frac{\rho}{2\Xi_1} \right)^2 \right)^2 - \left( \frac{2\Xi_1}{\rho} \right) \frac{d^2\rho}{dx^2} \left( \frac{\rho}{2\Xi_1} \right)^2 \right]
$$

$$
= \frac{1}{24M} \left[ -\frac{3}{2\rho} \frac{d^2\rho}{dx^2} + \frac{5}{8\rho^3} \left( \frac{d\rho^2}{dx} \right)^2 \right].
$$

Using the above, the final expression for $\tau[\rho]$ reduces to [22]

$$
\tau[\rho] = \frac{1}{24M} \left[ \frac{\rho^3}{\Xi_1^2} - \hbar^2 \left( \frac{1}{\rho} \frac{d^2\rho}{dx^2} - \frac{1}{4\rho^3} \left( \frac{d\rho^2}{dx} \right)^2 \right) \right]
$$

$$
= \frac{\hbar^2}{24M} \left[ \frac{4\pi^2\rho^3}{\nu^2} - \frac{1}{\rho} \frac{d^2\rho}{dx^2} + \frac{1}{4\rho^3} \left( \frac{d\rho^2}{dx} \right)^2 \right]
$$

$$
= \frac{\hbar^2}{24M} \left[ \frac{4\pi^2\rho^3}{\nu^2} - \frac{2}{\rho} \frac{d^2\rho}{dx^2} - \frac{1}{\rho} \left( \frac{d\rho}{dx} \right)^2 \right]. \quad (D.27)
$$

Note that the factor of $\nu$ is explicit only in the leading term. What we are really want for our purposes is a to express $p_F$ as a functional of $\rho$ and $\tau$. We have expressed $p_F$ as a functional of $\rho$ and its derivatives (Eq. (D.22)), and now we use the above expression of the kinetic energy density functional to make the expression for $p_F$ more robust. First, we observe that

$$
\left[ \frac{d^2\rho^2}{dx^2} - \frac{1}{4\rho^2} \left( \frac{d\rho^2}{dx} \right)^2 \right] = \frac{4\pi^2\rho^4}{\nu^2} \frac{h^2}{24M} \rho^\tau.
$$

Next, we find from Eq. (D.22) that $p_F$ can be written as

$$
p_F = \frac{\hbar\pi\rho}{\nu} + \frac{\hbar\nu}{24\pi\rho^3} \left[ \frac{d^2\rho^2}{dx^2} - \frac{1}{4\rho^2} \left( \frac{d\rho^2}{dx} \right)^2 \right] - \frac{1}{2\rho^2} \left( \frac{d\rho^2}{dx} \right)^2.
$$

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Simplifying, we get the following expression

$$
\frac{1}{\hbar} p_F[\rho, \tau] = \frac{7\pi \rho}{6\nu} - \frac{\nu}{\pi \rho^2} \left[ \frac{M}{\hbar^2} + \frac{1}{12\rho} \left( \frac{dp}{dx} \right)^2 \right].
$$

It is instructive to note that all functional elements of $p_F[\rho, \tau]$ scale the same way.

### D.2.3 Application: Three Dimensions

Now we deal with a three dimensional system with a classical Hamiltonian $H_C = \frac{p^2}{2M} + v(x)$. The leading order term in the expansion of $C(x, x, \beta)$ is given by

$$
C_0(x, x, \beta) = \left( \frac{1}{\hbar} \right)^3 \int d^3p e^{-\beta H_C} = \left( \frac{1}{\hbar} \right)^3 e^{-\beta v(x)} \left( \frac{2M\pi}{\beta} \right)^{3/2}.
$$

The next order contribution is given by

$$
C_2 = \left( \frac{1}{\hbar} \right)^3 \int d^3p e^{-\beta H_C} \left[ \frac{\beta^3}{6M^2} (p \cdot \nabla)^2 v - \frac{\beta^4}{8M^2} (p \cdot \nabla v)^2 - \frac{\beta^2}{4M} \nabla^2 v + \frac{\beta^3}{6M} (\nabla v)^2 \right].
$$

Let us consider the above integral one term at a time. Firstly, evaluating the last two terms is easy, one just gets the $C_0$ factor from the $p$ integral. Thus, the last two terms contribute

$$
\left[ -\frac{\beta^2}{4M} \nabla^2 v + \frac{\beta^3}{6M} (\nabla v)^2 \right] C_0(x, x, \beta).
$$

Now, consider the first term. Observe that $(p \cdot \nabla)^2 v = p_i p_j \partial_i \partial_j v$. When $i \neq j$, the integral is odd and vanishes. But for the $i = j$ case, the first term of the above integral reduces to the following form:

$$
\left( \frac{1}{\hbar} \right)^3 \frac{\beta^3}{6M^2} e^{-\beta v(x)} \left[ \partial_x^2 v \int_{-\infty}^{\infty} dp_x p_x^2 e^{-\frac{\beta p_x^2}{2M}} \int_{-\infty}^{\infty} dp_y e^{-\frac{\beta p_y^2}{2M}} \int_{-\infty}^{\infty} dp_z e^{-\frac{\beta p_z^2}{2M}} + \text{y and z terms} \right]
$$

Let us define the following integral:

$$
I(D) = \left( \int_{-\infty}^{\infty} dq q^2 e^{-\beta\frac{q^2}{2M}} \right) \left( \int_{-\infty}^{\infty} dq e^{-\beta\frac{q^2}{2M}} \right)^{D-1}
$$
\[
\frac{1}{2} \sqrt{\pi} \left( \frac{2M}{\beta} \right)^{3/2} \left( \sqrt{\pi} \left( \frac{2M}{\beta} \right)^{1/2} \right)^{D-1} = \left( \frac{2M \pi}{\beta} \right)^{D/2} \left( \frac{M}{\beta} \right). \tag{D.30}
\]

Using this, the first term reduces to
\[
\left( \frac{1}{\hbar} \right)^3 \frac{\beta^3}{6M^2} e^{-\beta v(\mathbf{x})} \left( \sum_{i=1}^3 \partial_i^2 v \right) I(3)
= \frac{\beta^2}{6M} (\nabla^2 v) C_0(\mathbf{x}, \mathbf{x}, \beta).
\]

Finally, consider the second term. Observe that \((\mathbf{p} \cdot \nabla v)^2 \equiv p_i p_j \partial_i v \partial_j v\). Again, the \(i = j\) case survives. At this stage, let us assume that \(v(\mathbf{x}) = v(r)\). So, \(\partial_k v = \frac{x_k}{r} (\partial_r v)\), and hence \((\partial_k v)^2 \equiv \frac{x_k^2}{r^2}(\nabla v)^2\). Now, the second term reduces to
\[
- \left( \frac{1}{\hbar} \right)^3 \frac{\beta^4}{8M^2} e^{-\beta v(\mathbf{x})} \left( \nabla v \right)^2 \frac{1}{r^2} \left( \sum_{k=1}^3 x_k^2 \right) I(3)
= - \frac{\beta^3}{8M} (\nabla v)^2 C_0(\mathbf{x}, \mathbf{x}, \beta).
\]

Adding these contributions, we finally get
\[
C_2(\mathbf{x}, \mathbf{x}, \beta) = \left[ \frac{\beta^3}{24M} (\nabla v)^2 - \frac{\beta^2}{12M} (\nabla^2 v) \right] C_0(\mathbf{x}, \mathbf{x}, \beta). \tag{D.31}
\]

Now, we are in a position to evaluate the terms in the semiclassical expansion of \(\rho(\mathbf{x})\).

Using \(\varepsilon_F - v(\mathbf{x}) = \frac{\varepsilon_F(\mathbf{x})}{2M}\), we get
\[
\rho_0(\mathbf{x}) = \nu \mathcal{L}_{\varepsilon_F}^{-1} \left[ \frac{1}{\beta} C_0(\mathbf{x}, \mathbf{x}, \beta) \right] = \left( \frac{4\pi}{3} \right) \Xi_3 \varepsilon_F^3(\mathbf{x}). \tag{D.32}
\]

The next order is
\[
\rho_2(\mathbf{x}) = \nu \mathcal{L}_{\varepsilon_F}^{-1} \left[ \frac{1}{\beta} C_2(\mathbf{x}, \mathbf{x}, \beta) \right] = -\Xi_3 \left[ \frac{\pi}{24\varepsilon_F^3} \left( \nabla \varepsilon_F^2 \right)^2 - \frac{\pi}{6\varepsilon_F^3} \nabla^2 \varepsilon_F^2 \right]. \tag{D.33}
\]

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Thus, to second order, the expression for density is

$$\rho(x) = \Xi_3 \left[ \frac{4\pi}{3} p_F^2(x) - \hbar^2 \left( \frac{\pi}{24p_F^2} \left( \nabla p_F^2 \right)^2 - \frac{\pi}{6p_F} \nabla^2 p_F^2 \right) \right]. \quad (D.34)$$

Next, let us find out $p_F[\rho]$. To a first approximation, $p_F^3(x) = \frac{3\rho(x)}{4\Xi_3}$. Using this in Eq. (D.34), we get

$$p_F^3 = \left( \frac{3}{4\Xi_3} \right)^{1/3} \left[ 1 + \frac{\hbar^2}{8} \left( \frac{1}{4\rho^2} \left( \nabla p^2 \right)^2 - \frac{1}{\rho^{4/3}} \nabla^2 p^{2/3} \right) \right]. \quad (D.35)$$

Next, we do binomial expansion and get the following:

$$p_F[\rho] = \left( \frac{3\rho}{4\Xi_3} \right)^{1/3} \left[ 1 + \frac{\hbar^2}{24} \left( \frac{4\Xi_3}{3} \right)^{2/3} \left( \frac{1}{4\rho^2} \left( \nabla p^2 \right)^2 - \frac{1}{\rho^{4/3}} \nabla^2 p^{2/3} \right) \right]. \quad (D.36)$$

Now, let us see how the kinetic energy looks like as a functional of density. As before, at any order $k$, $\partial_\beta C_k(x, x, \beta)$ has the form

$$\partial_\beta C_k(x, x, \beta) = -v(x) C_k(x, x, \beta) - f_k(x, \beta),$$

so that for any order, the kinetic energy density is given by

$$\tau_k(x) = v \mathcal{L}_{\epsilon_F}^{-1} \left[ \frac{1}{\beta} f_k(x, \beta) \right]. \quad (D.37)$$

Evaluation $f_k(x, \beta)$ for the first few $k$ gives:

$$f_0(x, \beta) = \frac{3}{2\beta} C_0(x, x, \beta),$$

$$f_2(x, \beta) = \frac{\beta}{24M} \left[ \nabla^2 v - \frac{3}{2\beta} (\nabla v)^2 \right] C_0(x, x, \beta).$$

From Eq. (D.37), we get for $k = 0$:

$$\tau_0(x) = v \mathcal{L}_{\epsilon_F}^{-1} \left[ \frac{1}{\beta} f_0(x, \beta) \right] = 2\pi \Xi_3 \frac{p_F^5(x)}{5M}. \quad (D.38)$$
The next order contribution is

\[ \tau_2(x) = \nu L^{-1}_{xF} \left[ \frac{1}{\beta} f_2(x, \beta) \right] = - \left( \frac{\pi \Xi_3}{16M} \right) \left[ \frac{1}{p_F} \left( \nabla p_F^2 \right)^2 + \frac{4}{3} p_F \nabla^2 p_F^2 \right]. \tag{D.39} \]

Thus, to second order, the expression for kinetic energy density is

\[ \tau(x) = \pi \Xi_3 \left[ \frac{2p_F^2(x)}{5M} - \hbar^2 \left( \frac{1}{16M} \right) \left( \frac{1}{p_F} \left( \nabla p_F^2 \right)^2 + \frac{4}{3} p_F \nabla^2 p_F^2 \right) \right]. \tag{D.40} \]

Now we wish to write \( \tau \) as a functional of \( \rho \) by using Eq. (D.36) in the above expression. Retaining only terms up to order \( \hbar^2 \), we find that

\[
\tau_0[\rho] = \frac{2\pi \Xi_3}{5M} \left( \frac{3\rho}{4\pi \Xi_3} \right)^{5/3} \left[ 1 + 5 \times \frac{\hbar^2}{24} \left( \frac{4\pi \Xi_3}{3} \right)^{2/3} \left( \frac{1}{4\rho^2} \left( \nabla \rho^{2/3} \right)^2 - \frac{1}{\rho^{4/3}} \nabla^2 \rho^{2/3} \right) \right].
\]

\[
= \frac{2\pi \Xi_3}{5M} \left( \frac{3\rho}{4\pi \Xi_3} \right)^{5/3} + \frac{\hbar^2}{16M} \left( \frac{1}{4\rho^{1/3}} \left( \nabla \rho^{2/3} \right)^2 - \rho^{1/3} \nabla^2 \rho^{2/3} \right).
\]

Since \( \tau_2(x) \) is of order \( \hbar^2 \), we use only the leading contribution to \( p_F[\rho] \) in Eq. (D.36).

\[
\tau_2[\rho] = - \left( \frac{\pi \Xi_3}{16M} \right) \left( \frac{3}{4\pi \Xi_3} \right) \left[ \frac{1}{\rho^{1/3}} \left( \nabla \rho^{2/3} \right)^2 + \frac{4}{3} \rho^{1/3} \nabla^2 \rho^{2/3} \right].
\]

Using the above, the expression for \( \tau[\rho] \) reduces to

\[
\tau[\rho] = \frac{2\pi \Xi_3}{5M} \left( \frac{3\rho}{4\pi \Xi_3} \right)^{5/3} - \frac{\hbar^2}{16M} \left( \frac{1}{2\rho^{1/3}} \left( \nabla \rho^{2/3} \right)^2 + 2\rho^{1/3} \nabla^2 \rho^{2/3} \right)
\]

\[
= \frac{\hbar^2}{10M} \left[ 3 \left( \frac{6\pi^2}{\nu} \right)^{2/3} \rho^{5/3} - \frac{5}{8} \left( \frac{1}{2\rho^{1/3}} \left( \nabla \rho^{2/3} \right)^2 + 2\rho^{1/3} \nabla^2 \rho^{2/3} \right) \right]
\]

\[
= \frac{\hbar^2}{10M} \left[ 3 \left( \frac{6\pi^2}{\nu} \right)^{2/3} \rho^{5/3} - \frac{5}{4} \left( \frac{2}{3} \nabla^2 \rho - \frac{1}{9\rho} \left( \nabla \rho \right)^2 \right) \right]. \tag{D.41}
\]

We have used the following identity in simplifying the above.

\[ \rho^a \nabla^2 \rho^b = b \rho^{a+b-1} \left[ \nabla^2 \rho + \frac{b-1}{\rho} \left( \nabla \rho \right)^2 \right]. \]

Now, a way to handle the last term is to realize that

\[
\int d^3x \rho^a \nabla^2 \rho^b = - (a b) \int d^3x \rho^{a+b-2} \left( \nabla \rho \right)^2.
\]
Using the above, the equivalent expression for $\tau[\rho]$ reduces to [104]

$$
\tau[\rho] = \frac{h^2}{10M} \left[ 3 \left( \frac{6\pi^2}{\nu} \right)^{2/3} \rho^{5/3} + \frac{5}{36\rho} (\nabla \rho)^2 \right].
$$

(D.42)

It is extremely interesting to actually compare the numerical performance of these two theoretically equivalent formula for $\tau[\rho]$. As before, the factor of $\nu$ is explicit only in the leading term. Fig. 5.4 illustrates how Eq. (D.42) behaves compared to the computed $\tau$ for a particular system.

Let us now express $p_F$ as a functional of $\rho$ and $\tau$. From Eq. (D.41), we observe

$$
\left[ \frac{1}{\rho^{1/3}} (\nabla \rho^{2/3})^2 + 4\rho^{1/3} \nabla^2 \rho^{2/3} \right] = \frac{48}{5} \left( \frac{6\pi^2}{\nu} \right)^{2/3} \rho^{5/3} - \frac{32M}{h^2} \tau.
$$

Next, we note that $p_F$ can be written as

$$
p_F = \left( \frac{3\rho}{4\pi\Xi_3} \right)^{1/3} \left[ 1 + \frac{h^2}{24} \left( \frac{4\pi\Xi_3}{3} \right)^{2/3} \frac{1}{4\rho^{5/3}} \left( \frac{1}{\rho^{1/3}} (\nabla \rho^{2/3})^2 - 4\rho^{1/3} \nabla^2 \rho^{2/3} \right) \right].
$$

Simplifying, we get the following expression:

$$
\frac{1}{h} p_F[\rho, \tau] = \frac{11\pi}{5} \left( \frac{3\rho}{4\pi\nu} \right)^{1/3} - \frac{1}{24\pi} \left( \frac{4\pi\nu}{3} \right)^{1/3} \frac{1}{\rho^{4/3}} \left( \frac{4M}{h^2} \tau + \rho^{1/3} \nabla^2 \rho^{2/3} \right)
\begin{align*}
&= \frac{11\pi}{5} \left( \frac{3\rho}{4\pi\nu} \right)^{1/3} - \frac{1}{12\pi\rho^{4/3}} \left( \frac{4\pi\nu}{3} \right)^{1/3} \left( \frac{2M}{h^2} \tau + \frac{1}{3} \left[ \nabla^2 \rho - \frac{1}{3}\rho (\nabla \rho)^2 \right] \right).
\end{align*}
$$

(D.43)

Again we note that all functional elements of $p_F[\rho, \tau]$ scale the same way.

**D.2.4 Application: D Dimensions**

Finally, we deal with a system in $D$ spatial dimensions. The leading order term in the expansion of $C(x, x, \beta)$ is given by

$$
C_0(x, x, \beta) = \left( \frac{1}{h} \right)^D \int d^D p e^{-\beta H_C} = \left( \frac{1}{h} \right)^D e^{-\beta \nu(x)} \left( \frac{2M\pi}{\beta} \right)^{D/2}.
$$

(D.44)
The next order contribution is given by

\[ C_2 = \left( \frac{1}{\hbar} \right)^D \int d^D \mathbf{p} e^{-\beta H_C} \left[ \frac{\beta^3}{6 M^2} (\mathbf{p} \cdot \nabla)^2 v - \frac{\beta^4}{8 M^2} (\mathbf{p} \cdot \nabla v)^2 - \frac{\beta^2}{4 M} \nabla^2 v + \frac{\beta^3}{6 M} (\nabla v)^2 \right]. \]

As before, the last two terms contribute

\[ \left[ -\frac{\beta^2}{4 M} \nabla^2 v + \frac{\beta^3}{6 M} (\nabla v)^2 \right] C_0(\mathbf{x}, \mathbf{x}, \beta). \]

The first term is given by

\[
\left( \frac{1}{\hbar} \right)^D \frac{\beta^3}{6 M^2} e^{-\beta v(\mathbf{x})} \left( \sum_{i=1}^{D} \partial_i^2 v \right) I(D) \\
= \left( \frac{1}{\hbar} \right)^D \frac{\beta^3}{6 M^2} e^{-\beta v(\mathbf{x})} \nabla^2 v \left( \frac{2 M \pi}{\beta} \right)^{D/2} \left( \frac{M}{\beta} \right) \\
= \frac{\beta^2}{6 M} (\nabla^2 v) C_0(\mathbf{x}, \mathbf{x}, \beta).
\]

Assuming that \( v(\mathbf{x}) = v(r) \), the second term reduces to

\[
- \left( \frac{1}{\hbar} \right)^D \frac{\beta^4}{8 M^2} e^{-\beta v(\mathbf{x})} (\nabla v)^2 \frac{1}{r^2} \left( \sum_{k=1}^{D} x_k^2 \right) I(D) \\
= -\frac{\beta^3}{8 M} (\nabla v)^2 C_0(\mathbf{x}, \mathbf{x}, \beta).
\]

Adding these contributions, we get

\[
C_2(\mathbf{x}, \mathbf{x}, \beta) = \left[ \frac{\beta^3}{24 M} (\nabla v)^2 - \frac{\beta^2}{12 M} (\nabla^2 v) \right] C_0(\mathbf{x}, \mathbf{x}, \beta).
\] (D.45)

Now, let us evaluate the terms in the semiclassical expansion of \( \rho(\mathbf{x}) \).

\[
\rho_0(\mathbf{x}) = \nu \mathcal{L}_{\epsilon_F}^{-1} \left[ \frac{1}{\beta} C_0(\mathbf{x}, \mathbf{x}, \beta) \right] = \Xi_D \left[ \frac{\pi^{D/2}}{\Gamma(D/2 + 1)} \right] p_F^D(\mathbf{x}).
\] (D.46)

The next order is

\[
\rho_2(\mathbf{x}) = \nu \mathcal{L}_{\epsilon_F}^{-1} \left[ \frac{1}{\beta} C_2(\mathbf{x}, \mathbf{x}, \beta) \right] \\
= \Xi_D \pi^{D/2} \left[ \frac{p_F^{D-6}}{12 \Gamma(D/2 - 2)} (\nabla p_F^2)^2 + \frac{p_F^{D-4}}{6 \Gamma(D/2 - 1)} \nabla^2 p_F^2 \right].
\] (D.47)
Next, let us find out \( p_F[\rho] \). Proceeding in the usual fashion, we get

\[
\Xi_D \left[ \frac{\pi^{D/2}}{\Gamma(D/2 + 1)} \right] p_F^D = \rho - \hbar^2 \pi \Xi_D^{2/D} \left[ \Gamma(D/2 + 1) \right]^{1-2/D} \times \left[ \frac{\rho^{1-6/D}}{12 \Gamma(D/2 - 2)} (\nabla \rho^{2/D})^2 + \frac{\rho^{1-4/D}}{6 \Gamma(D/2 - 1)} \nabla^2 \rho^{2/D} \right].
\]

At this stage, let us define a few constants for notational brevity.

\[
d = \frac{2}{D},
A_{1,D} = \Gamma(\frac{1}{d} - 2),
A_{2,D} = \Gamma(\frac{1}{d} - 1),
A_{3,D} = \Gamma(\frac{1}{d}),
A_{4,D} = \Gamma(\frac{1}{d} + 1),
A_{5,D} = \Gamma(\frac{1}{d} + 2),
\]

Thus, we get the following :

\[
p_F[\rho] = \frac{1}{\sqrt{\pi}} \left( \frac{A_{4,D} \rho}{\Xi_D} \right)^{d/2} \left[ 1 - \frac{\hbar^2 \pi}{6D} \Xi_D^d A_{4,D}^{1-d} \left( \frac{1}{2 A_{1,D}} \frac{(\nabla \rho^d)^2}{\rho^{3d}} + \frac{1}{A_{2,D}} \frac{\nabla^2 \rho^d}{\rho^{2d}} \right) \right]. \tag{D.48}
\]

Now, let us see how the kinetic energy looks like as a functional of density. Evaluation \( f_k(x, \beta) \) for the first few \( k \) gives :

\[
f_0(x, \beta) = \frac{D}{2\beta} C_0(x, x, \beta),
\]

\[
f_2(x, \beta) = \frac{\beta}{24M} \left[ (4 - D) \nabla^2 v - \frac{(6 - D)}{2} \beta (\nabla v)^2 \right] C_0(x, x, \beta).
\]

Proceeding as usual, we get for \( k = 0 \):

\[
\tau_0(x) = \nu \mathcal{L}_{\epsilon_F}^{-1} \left[ \frac{1}{\beta} f_0(x, \beta) \right] = \pi^{D/2} \Xi_D \left( \frac{D}{A_{5,D}} \right) \frac{p_F^{2+D}(x)}{4M}. \tag{D.49}
\]
The next order contribution is

\[ \tau_2(x) = \nu \mathcal{L}_{\xi_F}^{-1} \left[ \frac{1}{\beta} f_2(x, \beta) \right] \]

\[ = \left( \frac{\pi^{D/2} \Xi_D}{24M} \right) \left[ \left( \frac{D-6}{2A_{2,D}} \right) p_F^{D-4} (\nabla p_F^d)^2 + \left( \frac{4 - D}{A_{3,D}} \right) p_F^{D-2} \nabla^2 p_F^d \right] \] \quad \text{(D.50)}

Next, we write \( \tau \) as a functional of \( \rho \). Retaining only terms upto order \( \hbar^2 \),

\[ \tau_0[\rho] = \frac{\Xi_D}{4M\pi} \left( \frac{D}{A_{5,D}} \right) \left( \frac{A_{4,D} \rho}{\Xi_D} \right)^{2+d} \]

\[ - \quad \hbar^2 \left( \frac{D+2}{24M} \right) \left( \frac{A_{4,D}^2}{A_{5,D}} \right) \left[ \frac{1}{2A_{1,D}} \frac{(\nabla \rho^d)^2}{\rho^{2d-1}} + \frac{1}{A_{2,D}} \frac{\nabla^2 \rho^d}{\rho^{d-1}} \right]. \quad \text{(D.51)}

Since \( \tau_2(x) \) is of order \( \hbar^2 \), we use only the leading contribution to \( p_F[\rho] \).

\[ \tau_2[\rho] = \left( \frac{A_{4,D}}{24M} \right) \left[ \left( \frac{D-6}{2A_{2,D}} \right) \frac{(\nabla \rho^d)^2}{\rho^{2d-1}} + \left( \frac{4 - D}{A_{3,D}} \right) \frac{\nabla^2 \rho^d}{\rho^{d-1}} \right]. \quad \text{(D.52)}

The expression for \( \tau[\rho] \) is thus given by \( \tau[\rho] = \tau_0[\rho] + \hbar^2 \tau_2[\rho] \). We refrain from writing out the expression to avoid clutter. In principle, one can proceed exactly as we have done for the 1 and 3 dimensional cases to obtain \( p_F \) as a functional of \( \rho \) and \( \tau \). The above formulae of course reproduce the results of the previous sections.
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