Static Response of Neutron Matter

by

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ABSTRACT

STATIC RESPONSE OF NEUTRON MATTER

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We investigate the problem of periodically modulated strongly interacting neutron matter. We carry out ab initio non-perturbative auxiliary-field diffusion Monte Carlo calculations using an external sinusoidal potential in addition to phenomenological two- and three-nucleon interactions. Several choices for the wave function ansatz are explored and special care is taken to extrapolate finite-sized results to the thermodynamic limit. We perform calculations at various densities as well as at different strengths and periodicities of the one-body potential. Our microscopic results are then used to constrain the isovector term from energy-density functional theories of nuclei at many different densities, while making sure to separate isovector contributions from bulk properties. Lastly, we use our results to extract the static density-density linear response function of neutron matter at different densities. Our findings provide insights into inhomogeneous neutron matter and are related to the physics of neutron-star crusts and neutron-rich nuclei.
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Today’s accomplishments were
yesterday’s impossibilities.

__________________________
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Chapter 1

Introduction

Neutron matter is integral to the study of neutron stars and neutron-rich nuclei [1]. The equation of state (EOS) of neutron matter has been studied extensively using \textit{ab initio} approaches [2, 3, 4, 5, 6, 7]. While neutron matter does not obtain in nature in pure form, its EOS is closely connected to that of physical systems. More specifically, it is direct input into Einstein's field equations (typically cast as the Tolman-Oppenheimer-Volkov equations) that lead to basic observable properties of a neutron star. On the other hand, the neutron-matter EOS is also connected to nuclei via the use of nuclear energy density functionals (EDFs). EDFs take on a variety of forms [8, 9, 10, 11] and are typically fit to empirical data such as nuclear masses and radii. Other constraints may include the EOS of neutron matter [12, 9, 13, 14, 15, 16, 17, 18], the neutron-matter pairing gap [19], the energy of a neutron impurity [20, 21], or the properties of a neutron drop [22, 23, 24, 25, 26]. The EDF approach is especially useful as it allows for predictions to be made across the nuclear chart. Investigating neutron matter is an excellent opportunity for benchmarking both phenomenological [27, 28, 29, 30, 31] and chiral [32, 33, 34, 35, 36, 37, 38, 39, 40, 41] nuclear interactions and many-body methods.
While homogeneous matter is an intriguing system, it is not fully representative of either finite systems or astrophysical settings, since nuclei and neutron-star matter are inhomogeneous systems. The matter in a neutron-star crust is rich with unbound neutrons and also contains a lattice of nuclei. Focusing only on the unbound neutrons, these experience the interaction with the lattice as a periodic modulation. Similarly, nuclei are finite systems: their density eventually drops off as one goes farther away from the center of the nucleus. Thus, as a first approximation, one can study the effects of a one-body external periodic potential on pure infinite neutron matter. This system, periodically modulated neutron matter, directly mimics the situation in a neutron star; also, if used as an input constraint to EDFs, it can inform us about the physics of neutron-rich nuclei. This problem of an external periodic modulation is known as the static response of neutron matter: it amounts to a comparison between externally modulated and unmodulated infinite neutron systems. This problem has been tackled using a variety of approximations in the literature [42, 43, 44, 45, 46, 47, 48, 49], see Ref. [50] for a recent review. The static response problem has also received a lot of attention in other areas of physics [51]. This includes pioneering quantum Monte Carlo calculations for strongly correlated systems such as liquid $^4$He at zero temperature and pressure [52] and the three-dimensional electron gas [53].

1.1 Nuclear Hamiltonian

Fundamentally nucleons are bodies resulting from strong interactions between quarks and gluons. Thus their behaviour can be deduced from quantum chromodynamics (QCD). Unfortunately the strong force is strong at large separation distances/low-energy) and weak at short distances/high-energy (asymptotic freedom). It is highly non-perturbative in the low-energy regime where nuclear physics occurs. Although
there exist methods like lattice QCD which can directly tackle the problem in terms of quarks and gluons, they are too computationally time-consuming to handle nuclear structure calculations. Most commonly nucleons are treated as the degrees of freedom that interact via the nuclear force. The nuclear force is none other than a residual colour interaction that is analogous to how van der Waals forces are residual electromagnetic interactions between molecules. Understanding/obtaining a model of the nuclear interaction is thus paramount for studying nuclear structure or any other aspect of nuclear physics. Our starting point is to consider a general non-relativistic nuclear Hamiltonian [28]:

\[ \hat{H} = -\frac{\hbar^2}{2m} \sum_i \nabla_i^2 + \sum_{i<j} v_{ij} + \sum_{i<j<k} v_{ijk} + \ldots \]  

(1.1)

This includes the kinetic energy, two-body (NN) interactions, three-body (NNN) interactions and higher order many-body interactions between particles if necessary. The development of good models of the nuclear interaction is a challenging ongoing process in nuclear physics. Models depend on the energy-regime of interest, data being fit to, and any constraints imposed by theoretical or practical considerations. Such a complicated endeavour has resulted in the emergence of various families and types of nuclear potentials. Of course, the physical predictions coming from these potentials ought to be unique but the difficulty of obtaining a decent form of the potential means we are left with a set of options to choose to make calculations from. Different potentials may yield different results.

In our calculations we work with interactions that belong to a phenomenological family of nuclear potentials. The NN potential in these was produced by imposing a set of symmetries on the operatorial structure of the Hamiltonian: translational invariance, Galilean invariance, rotational invariance, space reflection invariance, time
reversal invariance, invariance under the interchange of the particles, isospin symmetry, and hermiticity [54]. This resulted in a set of operators including central, spin-spin, tensor, and spin-orbit terms. Spin, isospin, and angular momentum dependence are some of the reasons why calculations with nucleons are so computationally demanding. Now, the phenomenological approach to these is to fit functions multiplying the operators to NN data. In 1993 the Nijmegen group analyzed all NN scattering data below 350 MeV published from 1955-1992. A family of nuclear potentials called Argonne were fit to the Nijmegen data with high precision. It is important to note that calculations with the Argonne potential, limited to NN interactions underestimate the triton binding energy. NNN interactions are included to take this into account. We employ the Argonne $v'_{8}$ (Av8') potential in our QMC calculations. The form of the Argonne NN potentials is:

$$v^{NN} = \sum_{i<j} v_{ij}, \quad v_{ij} = \sum_{p=1}^{n} v_{p}(r_{ij})\hat{O}^{p}_{ij}$$ \hspace{1cm} (1.2)

containing n operators which depend on the potential and are multiplied by radial functions where $r_{ij}$ is the distance between particles $i$ and $j$. Av8’ contains 8 operators given by:

$$\hat{O}^{p=1,8}_{ij} = (1, \sigma_{i} \cdot \sigma_{j}, S_{ij}, L_{ij} \cdot \sigma_{ij}) \otimes (1, \tau_{i} \cdot \tau_{j})$$ \hspace{1cm} (1.3)

where $\sigma_{i} \cdot \sigma_{j}$ is the spin-spin term, $S_{ij}$ is the tensor operator:

$$S_{ij} = 3(\sigma_{i} \cdot \hat{r}_{ij})(\sigma_{j} \cdot \hat{r}_{ij}) - \sigma_{i} \cdot \sigma_{j}$$ \hspace{1cm} (1.4)

$L_{ij}$ is the relative angular momentum:

$$L_{ij} = -i\hbar \textbf{r}_{ij} \times \nabla_{ij}$$
\( \sigma_{ij} \) is the total spin:

\[ \sigma_{ij} = \frac{\hbar}{2}(\sigma_i + \sigma_j) \]  

(1.6)

and \( \tau_i \cdot \tau_j \) is the isospin dependence. Studying pure neutron systems, we have \( \tau_i \cdot \tau_j = 1 \). \( \text{Av8'} \) is a simplified version of a more elaborate potential called Argonne \( v_{18} \) (Av18) which contains 18 operator terms [55]. \( \text{Av8'} \) is a reprojection of Av18. Calculations of light nuclei as well as nuclear matter with \( \text{Av8'} \) have given very similar results to Av18 [28]. Thus we have:

\[
v_{ij} = v_1(r_{ij}) + v_2(r_{ij}) + [v_3(r_{ij}) + v_4(r_{ij})] \sigma_i \cdot \sigma_j + [v_5(r_{ij}) + v_6(r_{ij})] S_{ij} + [v_5(r_{ij}) + v_6(r_{ij})] L_{ij} \cdot \sigma_{ij}
\]  

(1.7)

We employ Urbana IX (UIX) for the NNN interactions in our potential. It consists of spin dependent (SD) and spin independent (SI) parts:

\[ V_{ijk} = V_{ijk}^{SI} + V_{ijk}^{SD} \]  

(1.8)

Computationally intensive calculations of neutrons have been performed using the above potentials [56].

Pure neutron matter is homogeneous and not representative of most naturally occurring physics involving nucleons. Nuclei are bound systems and even the most neutron-rich nuclei must contain protons in order to exist. Some studies perform calculations on neutron drops (neutrons trapped in an external well) to probe physics of neutron-rich nuclei or other neutron-rich systems. The inclusion of a simple one-body external perturbation alongside the complicated nuclear Hamiltonian is meant to
encapsulate external influences from protons, nuclei etc. In the same spirit we consider an external periodic potential to help describe neutron-rich systems of interest. The periodicity of this modulation is especially motivated by the periodicity of nuclei found in neutron-star crusts which lie embedded inside of a sea of degenerate neutron matter. Whatever the form of external potential, the inhomogeneity that results is what we are interested in. Thus we are not too particular and pick a form that is not too difficult to implement. We add an external sinusoidal potential to the nuclear Hamiltonian:

\[ \hat{H} = -\frac{\hbar^2}{2m} \sum_i \nabla^2_i + \sum_{i<j} v_{ij} + \sum_{i<j<k} v_{ijk} + \sum_i v(r_i), \quad v(r) = 2v_q \cos q \cdot r \quad (1.9) \]

The direction of \( q \) is arbitrary as the non-modulated system of neutrons is homogeneous and isotropic in space. We take \( q \) to be in the \( z \) direction. The interaction terms make this into a very difficult problem with millions of coupled equations to solve. We employ a powerful computational method called Quantum Monte Carlo (QMC) to handle these difficulties. However, this method requires a smart choice of trial wave function to take in as input. Seeking to better understand our physical problem, we first consider a much simpler one: the Hamiltonian with the interaction terms turned off (i.e. set to 0).
Chapter 2

Non-interacting problem

2.1 Non-perturbed free-Fermi gas

Many of the concepts needed for an understanding of interacting particles require an understanding of a much simpler problem: the 3D non-interacting free-Fermi gas. We review the solutions and properties of this system prior to including the periodic potential that was introduced in the previous section. For a finite system of $N$ particles it is standard to restrict positions to a cubic box of volume $V = L^3$ and impose periodic boundary conditions on the wave function:

$$\Psi(x + n_1 L, y + n_2 L, z + n_3 L) = \Psi(x, y, z) \quad (2.1)$$

where $n_1$, $n_2$, and $n_3$ are integers. These restrictions allow us to work with normalizable Hilbert space eigenstates since plane-waves (the solutions to this Hamiltonian) are not normalizable over all of coordinate-space. We are interested in extended systems of particles. We envision such a system as a periodic array of identically occupied cubic boxes filling up all of space. We can do this because the system has translational invariance. The periodic boundary conditions satisfy this. Of course,
such a description isn’t perfect and finite-size effects creep into the solutions. We
show that these go away in the thermodynamic limit as required. In practice, the cal-
culations for the interacting system are limited in size so we must consider finite-size
effects and handle them somehow. The one-particle Hamiltonian and corresponding
time-independent Schrödinger equation are:

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2, \quad -\frac{\hbar^2}{2m} \nabla^2 \psi(r) = E \psi(r)$$ (2.2)

The solutions are given by plane waves:

$$\psi(r) = \frac{1}{\sqrt{V}} e^{i \mathbf{k} \cdot \mathbf{r}}, \quad E_k = \frac{\hbar^2}{2m} k^2, \quad \mathbf{k} = \frac{2\pi}{L} (n_x, n_y, n_z)$$ (2.3)

where $n_x$, $n_y$, $n_z$ are integers. For many fermions, the particles occupy the lowest
available $\mathbf{k}$ states in the ground-state. For a spin-1/2 system a maximum of two
particles with different spin-projection can occupy the same wave vector $\mathbf{k}$ due to
the Pauli exclusion principle. The wave function is ambiguous whenever an occupied
energy level is not completely filled because only a subset of degenerate states are
occupied and this subset is not unique. For this reason it is usually preferred to study
closed shells. Closed shell configurations for the free-Fermi gas occur at $N = 2, 14,$
38, 54, 66, 114....

Since a neutron star is a macroscopic system we are particularly interested in the
thermodynamic limit (TL) where $N \to \infty$, $V \to \infty$ and $n = N/V$ is constant. In
the TL the number density $n$ is related to $k_F$, the maximal wave vector magnitude by

$$k_F = (3\pi^2 n)^{1/3}.$$

The energy per particle is given by $E_{FG} = (3/5)\hbar^2 k_F^2/2m = (3/5)E_F$.

Differences in properties between the thermodynamic limit and a finite number of
particles are called finite-size (FS) effects. FS effects go to zero in the thermodynamic
limit. They are also largest at small $N$. This can be seen in Fig. 2.1 which plots FS
effects in the energy per particle versus particle number for the non-interacting free-Fermi gas. This result is density-independent. As mentioned earlier, we are primarily interested in shell closures. These appear at the cusps in the inset of Fig. 2.1. There is a minimum in FS effects occurring at 67 particles. The nearest closed shell cusp is at 66 particles. This is the particle number we will be making calculations for.

### 2.2 Mathieu’s Equation

We now extend the above problem to include our external potential. We further restrict our potential to be periodic over the box containing the particles in order to preserve translational invariance. That is, $q = 2\pi/d$ where $L = nd$ and $n$ is a natural
number. The one-particle time-independent Schrödinger’s equation is:

\[-\frac{\hbar^2}{2m} \nabla^2 \psi(r) + 2v_q \cos(qz)\psi(r) = E\psi(r)\]  \hspace{1cm} (2.4)

Decomposing into Cartesian coordinates yields:

\[
\psi(r) = \psi_x(x)\psi_y(y)\psi_z(z) = \frac{1}{L} e^{i(k_xx + k_yy)}\psi_z(z),
\]

\[
E = \frac{\hbar^2}{2m}(k_x^2 + k_y^2) + E_z, \quad -\frac{\hbar^2}{2m}\frac{d^2\psi_z(z)}{dz^2} + 2v_q \cos(qz)\psi_z(z) = E_z\psi_z(z) \hspace{1cm} (2.5)
\]

Now consider the change of variables \(2s = qz\):

\[
-\frac{\hbar^2}{2m}\left(\frac{ds}{dz}\right)^2 \frac{d^2\psi_s(s)}{ds^2} + 2v_q \cos(2s)\psi_s(s) = E_z\psi_s(s)
\]

\[
-\frac{\hbar^2}{2m}\left(\frac{q}{2}\right)^2 \frac{d^2\psi_s(s)}{ds^2} + 2v_q \cos(2s)\psi_s(s) = E_z\psi_s(s)
\]

\[
\frac{d^2\psi_s(s)}{ds^2} + \left(\frac{8mE_z}{\hbar^2q^2} - 2\frac{8mv_q}{\hbar^2q^2} \cos(2s)\right)\psi_s(s) = 0
\]

\[
\frac{d^2\psi_s(s)}{ds^2} + (A - 2Q \cos(2s))\psi_s(s) = 0 \hspace{1cm} (2.6)
\]

where \(A = \frac{8mE_z}{\hbar^2q^2}\) is the eigenvalue and \(Q = \frac{8mv_q}{\hbar^2q^2}\). This recasting of Schrödinger’s equation is dimensionless. Since \(s = (\pi/d)z\), it also has \(\pi\) periodicity. Equation 2.6 is called Mathieu’s equation. The variable \(Q\) contains all the information about the interaction: i.e. the amplitude and periodicity. The eigenvalue \(A\) contains the energy of the particle. That is, for a given \(Q\), there will be an infinite spectrum of \(A\) values. A lot about the energy spectrum can be deduced from the nature of our potential. We know that periodic potentials result in Bloch wave functions. The same concept applied to ordinary differential equations is called Floquet theory. Given \(\pi\) periodicity, Floquet’s theorem states that there exist solutions to Mathieu’s equation
of the form:

\[ F_\nu(s) = e^{i\nu s} P(s) \]  \hspace{1cm} (2.7)

where \( P(s) \) is a function with the same periodicity as the potential and \( \nu \) is called the characteristic exponent. \( F_\nu \) is called a Floquet solution. Note that \( \nu \) is equivalent to \( \nu + 2 \) from the definition in 2.7 (for \( \pi \) periodicity). The mapping between \( \nu \) and physical states is thus a convention. For this problem we work in the extended zone scheme from solid-state physics. Notice how \( F_\nu(-s) = e^{-i\nu s} P(-s) \) is a Floquet solution of \(-\nu\): i.e. \( F_\nu(-s) = F_{-\nu}(s) \). This is true since both functions clearly satisfy Mathieu’s Equation for the same \( A \) and \( Q \). Whenever \( F_\nu(s) \) and \( F_\nu(-s) \) are linearly independent there is a double degeneracy at the energy level corresponding to \( A \) (ignoring additional degeneracies due to spin). This is true since they form a fundamental set of solutions for Mathieu’s differential equation. For a one-dimensional periodic potential these Floquet solutions will be linearly independent at all \( \nu \) except where band gaps occur. At the gaps \( F_\nu(s) \) is proportional to \( F_\nu(-s) \). Furthermore, the second linearly independent solution to Mathieu’s equation corresponding to \( F_\nu(s) \) is unbounded as \( |s| \to \infty \). Thus there is no degeneracy in energy at the band gap. From solid-state theory we know that band gaps occur at the Bragg planes. For our potential the reciprocal lattice vectors are simply \( 2m \) for any integer \( m \). Thus the Bragg planes are all the non-zero integer \( \nu \) values. So we know that the band gaps occur at integer \( \nu \) for non-zero \( v_q \). Compare this to \( v_q = 0 \) (free-Fermi gas) for which there are no band gaps and the dispersion relation is quadratic in \( \nu \). The band gaps for \( Q = 1 \) are shown in Fig. 2.2 where they can be seen as the discontinuities occurring at \( \nu = -2, -1, 1, 2 \).
In the mathematical literature, the integer values of $\nu$ (including $\nu = 0$) correspond to integer order Mathieu functions. The integer order Mathieu functions are the Mathieu cosine functions $Ce_n(s, Q), n \geq 0, n \in \mathbb{N}$ and Mathieu sine functions $Se_n(s, Q), n \geq 1, n \in \mathbb{N}$ which correspond to $A = a_n$ and $A = b_n$ respectively. $a_n$ and $b_n$ are called the integer order eigenvalues, the first few of which are shown in Fig. 2.3. $Ce_n(s, Q)$ are even functions and $Se_n(s, Q)$ are odd. These functions are real valued as well. It is clear from Eq. 2.7 that even-order ($n$ is even) Mathieu functions are $\pi$ periodic and odd-order Mathieu functions are $2\pi$ periodic/ $\pi$ anti-periodic. This is nicely illustrated in Fig. 2.4 for even integer-ordered Mathieu cosine functions. Plotted on the interval $[0, \pi/2]$, these functions are even and $\pi$-periodic.

It should be noted here that $a_n > b_n$ for $n > 0$. Thus $b_n$ corresponds to the bottom of the $n^{th}$ band gap and $a_n$ to the top. By convention, $Ce_n(s, Q)$ is associated with $\nu = n$ while $Se_n(s, Q)$ is associated with $\nu = -n$. The bands and gaps can be seen in Fig. 2.3 which plots the first few integer-order eigenvalues versus $Q$. The band gaps increase with $Q$ and are closed at $Q = 0$ as expected. Let’s denote the eigenvalue corresponding to characteristic exponent $\nu$ by $A = \lambda_\nu(Q)$ where (for real $\nu$):

$$
\lambda_\nu = \begin{cases} 
a_\nu, & \nu \geq 0, \nu \in \mathbb{N} 
b_{-\nu}, & \nu < 0, -\nu \in \mathbb{N} 
\lambda_{-\nu}, & \text{otherwise}
\end{cases}
$$

(2.8)

The allowed values of $\lambda$ for a given $Q$ are those that lie within the energy bands. The mathematical solutions to $\lambda$ that yield forbidden energies correspond to complex $\nu$ which don’t satisfy the boundary conditions and are thus unphysical. The energies at the edges of the bands correspond to integer $\nu$ (as was already discussed). The energies in the interior of the bands correspond to non-integer values of $\nu$. The states associated with non-integer $\nu$ and $-\nu$ are the degenerate Floquet solutions $F_\nu(s)$ and
Figure 2.2: Eigenvalues of Mathieu’s Equation versus the characteristic exponent $\nu$ for $Q = 1$.

$F_{\nu}(-s) = F_{-\nu}(s)$ mentioned earlier. Alternatively, we can define the non-integer order Mathieu cosine and sine functions by:

$$Ce_{\nu}(s,Q) = \frac{1}{2}[F_{\nu}(s) + F_{\nu}(-s)]$$

$$Se_{\nu}(s,Q) = -i\frac{1}{2}[F_{\nu}(s) - F_{\nu}(-s)]$$

(2.9)

The $F_{\nu}(s)$ satisfy the property $F_{\nu}^*(s) = F_{\nu}(-s)$. Thus $Ce_{\nu}(s,Q)$ and $Se_{\nu}(s,Q)$ are the real and imaginary parts of $F_{\nu}(s)$ respectively. Working with these components instead of Floquet solutions is simply a change of basis. We have:

$$\psi_{s,\nu}(s) = \begin{cases} 
  Ce_{\nu}(s,Q), \nu \geq 0 \\
  Se_{|\nu|}(s,Q), \nu < 0 
\end{cases}$$

(2.10)

Several of the non-integer order eigenvalues are shown in Fig. 2.3 and are seen to
Figure 2.3: Mathieu eigenvalues versus $Q$. The black curves denote the integer-order eigenvalues. The coloured curves show non-integer order eigenvalues [57, Fig. 28.13.1].

occur between $a_{n-1}$ and $b_n$ (in the bands). Imposing the same periodic boundary conditions as earlier and noting that $L = nd$ corresponds to $n\pi$ in the dimensionless Mathieu variable we have: $\nu n \pi = 2\pi n_z$, $n_z \in \mathbb{Z}$. Thus, $\nu = 2n_z/n$. The energy of $\psi_{z, \nu(n_z)}(z)$ is:

$$E_{z,n_z} = \frac{\hbar^2}{2m} \left( \frac{2\pi}{L} \right)^2 \left( \frac{n_z}{2} \right)^2 \lambda_{\nu(n_z)}$$  \hspace{1cm} (2.11)

Compare this with the energy in the $x$-direction:

$$E_{x,n_x} = \frac{\hbar^2}{2m} \left( \frac{2\pi}{L} \right)^2 n_x^2$$  \hspace{1cm} (2.12)

$n_x$ is an integer. The energy takes the same form in the $y$-direction. We mentioned earlier that the wave functions corresponding to these energies are plane-waves. However, since we will be working with real-valued wave functions in the $z$-direction,
makes sense to consider a real basis in $x$ and $y$ as well. Through the same types of linear combinations done in Eq. 2.9 we find that the real and imaginary components of plane-waves yield the alternative basis:

$$
\psi_{x,n_x}(x) = \begin{cases} 
\cos\left(\frac{2\pi n_x x}{L}\right), & n_x \geq 0 \\
\sin\left(\frac{2\pi n_x x}{L}\right), & n_x < 0
\end{cases} \quad (2.13)
$$

up to a normalization constant. The same thing holds for $y$. Note that our Mathieu functions are also good up to a normalization constant. We will show that the normalization does not matter in our QMC simulations because the wave function always appears in ratios that cancel out any constant factors. The orbitals can be denoted according to their energy quantum numbers: $(n_x, n_y, n_z)$. We are generally interested in the lowest energy orbitals (ground-state) and are able to compute these
2.3 Finite-size effects

Similarly to the free gas, intensive properties converge in the thermodynamic limit (TL). We calculate the energy per particle of the perturbed gas by filling up the lowest available energy states. Since we require an integer number of periods in the box we are forced to work with a discrete set of particle numbers when taking the TL. This is displayed in Fig. 2.5 where the density and amplitude are 0.1 fm$^{-3}$ and 21.363 MeV respectively. $q$ is fixed so that two periods fit in the box at $N = 66$. The energy per particle converges in the TL. We use the energy per particle of the non-interacting system to handle FS effects in the interacting problem (see also Ref. [58]).

FS effects in the energy per particle $E_I(N)$ of the interacting system will be handled by extrapolating to the TL:

$$E_I(\infty) = E_I(N) - E_{NI}(N) + E_{NI}(\infty)$$  \hspace{1cm} (2.14)

We tested Eq. (2.14) by applying it to energy calculations of homogeneous neutron matter. This was done for the SLy4 energies of 66 neutrons at various densities (see Section 3.6 below). The results are shown in Table 2.1. They agree with SLy4 energies of homogeneous neutron matter to within 0.5%. This boosts our confidence in Eq. (2.14). We further highlight the importance of FS corrections by comparing calculations of the response function to the analytically known response in the TL (see Section 4.1 below). The response function for 66000 particles at a density of 0.1 fm$^{-3}$ (circles in Fig. 2.6) matches the Lindhard function (solid line). This makes sense since 66000 particles is practically in the TL, as per Fig. 2.5. The response for
Figure 2.5: FS dependence of the non-interacting Fermi gas in the presence of a one-body potential of fixed strength $2v_q = 0.5E_F$ and periodicity $q = 1.4433\text{ fm}^{-1}$. $n$ is fixed at $0.1\text{ fm}^{-3}$.

66 particles at this density (squares) does not match the Lindhard function except at large $q$. This stresses that 66 particles is not in the TL so it is important that FS effects be handled in order to study infinite neutron matter. We note that the behavior exhibited by the 66-particle results in Fig. 2.6 is observed at other densities also: there is a dip as the $q$ is lowered, before the response goes back up for the lowest-$q$ point.
Figure 2.6: Static-response function of the non-interacting free-Fermi gas at a density of 0.1 fm$^{-3}$. The squares and circles are for 66 and 66000 particles respectively. The line is the Lindhard function describing the response in the TL.

Table 2.1: SLy4 energies of a free-Fermi gas of neutrons computed using the local density approximation. Eq. (2.14) was used to extrapolate to the TL and compare to SLy4 energies of homogeneous neutron matter.

<table>
<thead>
<tr>
<th>$n$ (fm$^{-3}$)</th>
<th>$E_I(66)$ (MeV)</th>
<th>$E_I(\infty)$ (MeV)</th>
<th>TL (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.04</td>
<td>7.15</td>
<td>7.22</td>
<td>7.23</td>
</tr>
<tr>
<td>0.06</td>
<td>8.62</td>
<td>8.71</td>
<td>8.73</td>
</tr>
<tr>
<td>0.08</td>
<td>9.99</td>
<td>10.10</td>
<td>10.13</td>
</tr>
<tr>
<td>0.10</td>
<td>11.40</td>
<td>11.53</td>
<td>11.58</td>
</tr>
</tbody>
</table>
Having set up the necessary ingredients for solving our problem, we now turn to the numerical methods that we employ to solve the Schrödinger equation. The strong interactions between particles makes this into a very difficult problem with millions of coupled equations to solve. There are many ways of approaching this problem and we have taken a computationally demanding one that is derived from first principles. The algorithms we use belong to the Monte Carlo family of computational algorithms. These are methods that take advantage of random sampling to find solutions to problems that are presented as stochastic in nature. Massive amounts of statistical data are acquired to produce numbers that are guaranteed to correspond to quantities of interest due to the laws of probability. Quantum Monte Carlo presents us with a non-perturbative method to perform dependable calculations of the ground-state energy of many-body systems. The method is exact but complications arising for fermions means it at least provides us with a good estimate of the ground-state energy for neutron systems. We first discuss the Variational Monte Carlo (VMC) method. This is used to initialize and optimize our simulations. Next we cover the principles of Diffusion Monte Carlo (DMC), important for understanding Auxiliary
Field Diffusion Monte Carlo (AFDMC) which we use to solve the problem.

3.1 Variational Monte Carlo

Consider a typical quantum mechanical expectation value calculation. In many-body systems this will be an integral over a high-dimensional space. Direct integration techniques such as quadrature methods do not scale well with the number of dimensions. In these cases it is much preferred to sample the integrand statistically and average the samples. One can express an integral as an expectation value over a random variable $O(R)$ distributed according to a real, normalized, and positive weight function $P(R)$:

$$I = \int f(R)dR = \int \frac{f(R)}{P(R)}P(R)dR = \int O(R)P(R)dR$$

(3.1)

where $R$ denotes the coordinates/vectors of the space over which all functions are defined in. Then the mean value and variance of $O$ are given by:

$$\langle O \rangle = \int P(R)O(R)dR,$$

(3.2)

$$\sigma^2 = \int P(R)[O(R) - \langle O \rangle]^2dR$$

(3.3)

Monte Carlo integration works by drawing a large random sample of configurations $R_i$ distributed according to $P$. The central limit theorem of statistics tells us that the average value of $O(R)$ is a good approximation of $\langle O \rangle$. To be precise, if we define a new random variable:

$$X = \frac{\sum_{i=1}^{M} O(R_{i})}{M}$$

(3.4)
that comes from generating \( M \) independent samples, then the distribution of \( X \) approaches a normal distribution with mean \( \langle O \rangle \) and variance \( \sigma^2/M \) in the limit as \( M \) goes to infinity. Thus the standard deviation of the mean, i.e. the error in \( X \), is given by:

\[
\sigma_X = \frac{\sqrt{\sum_{j=1}^{M}(O_j) - \left(1/M\right)\sum_{i=1}^{M}O_i}^2}{M}
\]  

(3.5)

For our quantum system we are interested in the expectation value of the energy:

\[
E = \frac{\int \Psi_T^*(R) \hat{H} \Psi_T(R) dR}{\int |\Psi_T(R)|^2 dR}
\]  

(3.6)

where \( \Psi_T(R) \) is the trial wave function and \( \hat{H} \) is our Hamiltonian. Eq. 3.6 is valid assuming there are no spin components to the wave function. Note that \( R = (r_1, r_2, \ldots, r_N) \) is a \( 3N \)-dimensional vector corresponding to a \( 3 \)-dimensional \( N \) particle problem. To solve this in a Monte Carlo fashion we rewrite the energy as:

\[
E = \int P_T(R) E_L(R) dR
\]  

(3.7)

In this form it is clear that \( P_T(R) = |\Psi_T(R)|^2/(\int |\Psi_T(R)|^2 dR) \) is normalized and acts as the probability distribution in Monte Carlo integration. \( E_L(R) = (\hat{H} \Psi_T(R))/\Psi_T(R) \) is called the local energy. It is sampled from \( P_T(R) \) and averaged to estimate the energy corresponding to \( \Psi_T(R) \):

\[
E = \frac{\sum_{i=1}^{M}E_L(R_i)}{M}
\]  

(3.8)

The energy obtained is variational, i.e it is an upper bound on the ground-state energy.
of the system. We can prove the variational property by expressing the wavefunction as a linear combination of the energy basis states and evaluating $\langle \Psi_T | \hat{H} | \Psi_T \rangle$. $|\Psi_T\rangle = \sum_i c_i |\Psi_i\rangle$ where $\Psi_i$ are the energy eigenstates with coefficients $c_i$ in the trial wavefunction. The normalization of wavefunctions gives:

$$\langle \Psi_T | \Psi_T \rangle = \sum_{i,j} c_i^* c_j \langle \Psi_i | \Psi_j \rangle = \sum_i c_i^* c_i \langle \Psi_i | \Psi_i \rangle = \sum_i |c_i|^2 = 1 \quad (3.9)$$

where we’ve used the orthonormality of basis states to get to the third expression of Eq. 3.9. It follows that the expectation energy is given by:

$$\langle \Psi_T | \hat{H} | \Psi_T \rangle = \left( \sum_i c_i^* \langle \Psi_i | \right) \hat{H} \left( \sum_i c_i | \Psi_i \rangle \right)$$

$$= \left( \sum_i c_i^* \langle \Psi_i | \right) \left( \sum_i c_i E_i | \Psi_i \rangle \right)$$

$$= \sum_{i,j} c_i^* c_j E_j \langle \Psi_i | \Psi_j \rangle$$

$$= \sum_i |c_i|^2 E_i$$

$$= \sum_i |c_i|^2 (E_0 + \Delta E_i)$$

$$= \left( \sum_i |c_i|^2 \right) E_0 + \sum_i |c_i|^2 \Delta E_i$$

$$= E_0 + \sum_i |c_i|^2 \Delta E_i \quad (3.10)$$

where $\Delta E_i = E_i - E_0$ is the excitation energy of the $i_{th}$ energy level, and we used Eq. 3.9 in the last step of the derivation. The second term in the final expression is positive since the excitation energy terms are all positive. Thus, we have that $\langle \Psi_T | \hat{H} | \Psi_T \rangle \geq E_0$. VMC alone is usually not sufficient to determine the ground state energy since $E = E_0$ requires $|\Psi_T\rangle = |\Psi_0\rangle$. However, a variational procedure is nevertheless helpful for optimizing a trial wave function that is later used by other
The Monte Carlo method demands a large sample of walkers distributed according to $P_T(R)$. For a complicated $P_T(R)$ in a high dimensional space it can be extremely difficult to compute the normalization of $P_T(R)$. A sampling method that doesn’t require computation of a normalized $P_T(R)$ is most desirable. The Metropolis algorithm depends on $P_T(R)$ only as the ratio of $P$ at two points in space and is therefore independent of the normalization [59]. This algorithm uses random sampling to describe a random walk type process. It belongs to the class of stochastic processes known as Markov chains. These chains essentially involve a time evolution of states that only depend on the current state of the system. This independence of past history or “memorylessness” is called the Markov property. In VMC our Markov chain is an evolution of vectors $R$ in discrete steps that “walk” around the $3N$-configuration space according to $P_T(R)$. That is, over the course of the walk, the positions occupied by these “walkers” are distributed over the space with probability distribution $P_T(R)$. Markov chain Monte Carlo methods are largely preferable over direct sampling methods when the dimensionality is high. For example, rejection sampling becomes largely impractical because the rejection rate almost always explodes exponentially with increasing numbers of dimensions.

The caveat with Markov chain Monte Carlo methods is that subsequent samples are correlated. In order to obtain independent samples one must make many steps with the walker before taking the next sample. An equilibration stage also occurs at the beginning of the walk since the initial configuration of walkers does not follow the desired distribution. We typically initialize the walkers on a lattice and move them from there using the Metropolis algorithm.

The general concept of a Markov chain is that of a set of states with transition
probabilities connecting them. The state of the system evolves in discrete steps in the case of discrete-time Markov processes. Continuous-time Markov processes are possible as well. Diffusion is an example of a continuous-time Markov process. In VMC we evolve vectors $\mathbf{R}$ which represent possible states of the system. We move them in discrete steps in order to sample $P_T(\mathbf{R})$ making this an example of a discrete-time Markov process.

The most important property that our Markov chain must satisfy is called ergodicity. A Markov chain is ergodic if and only if:

1. It is irreducible: It is possible to get to any state from any state.

2. It is aperiodic: Let $T$ be the set of all $n$ where it is possible to return to a state in $n$ steps. The state is aperiodic if the greatest common divisor of $T$ is 1. The Markov chain is aperiodic if all its states are aperiodic.

3. It is positive recurrent: The average number of steps for any state to return to itself is finite.

This is important because an ergodic Markov chain has a unique stationary distribution of walkers occupying the states. Moreover, any initial distribution approaches the unique stationary distribution as the number of steps goes to infinity. This property is exploited in Monte Carlo methods to sample a probability distribution by using a Markov chain with stationary distribution equal to $P_T(\mathbf{R})$.

We now discuss the details of the Metropolis algorithm. We provide motivation for the transition probabilities $T(\mathbf{R}' \leftarrow \mathbf{R})$ for evolving a state from $\mathbf{R}$ to $\mathbf{R}'$. Note that $T(\mathbf{R}' \leftarrow \mathbf{R})$ is a probability density function. Since our state space is continuous, the probability of taking a step from $\mathbf{R}$ into a volume $d\mathbf{R}'$ containing $\mathbf{R}'$ is just $T(\mathbf{R}' \leftarrow \mathbf{R})d\mathbf{R}'$. We already discussed that an ergodic chain will approach a
stationary distribution. If we had \( T(R' \leftarrow R) = P(R') \) then we would be done and our transition probabilities would ensure that the fraction of walkers moving into any region is just the probability of being in that region according to \( P(R) \). But if life was this easy we would not even be using Metropolis to begin with as we would already have direct access to sampling \( T(R' \leftarrow R) = P(R') \). Rather, we choose our transition probabilities in such a way as to satisfy a detailed balance condition where the transition of walkers across any two states is exactly balanced when the walkers are distributed according to \( P \). This is equivalent to saying that \( P \) is a stationary distribution for our Markov process. Thus given that the Markov chain is ergodic, this detailed balance condition is sufficient to ensure that we obtain samples distributed according to \( P \) after equilibration. The detailed balance condition can be written as:

\[
P(R)dR T(R' \leftarrow R)dR' = P(R')dR' T(R \leftarrow R')dR
\]

\[
P(R)T(R' \leftarrow R) = P(R')T(R \leftarrow R')
\]

\[
\frac{P(R')}{P(R)} = \frac{T(R' \leftarrow R)}{T(R \leftarrow R')}
\]  

\[
(3.11)
\]

Next, we break up the transition probability as coming from some probability that a move is proposed times some probability that the move is accepted. The details of the move proposal probability density function \( g(R' \leftarrow R) \) are not important for the theory of the method but in practice are consequential to the efficacy of the process. If a move is proposed from \( R \) to \( R' \), then we accept that move with probability \( A(R' \leftarrow R) \). It is this acceptance probability that needs to be properly tuned to fulfill our detailed balance condition in Eq. 3.11. So we have that \( T(R' \leftarrow R) = A(R' \leftarrow R)g(R' \leftarrow R) \). Plugging this into Eq. 3.11 gives:

\[
\frac{P(R')}{P(R)} = \frac{A(R' \leftarrow R)g(R' \leftarrow R)}{A(R \leftarrow R')g(R \leftarrow R')}
\]

\[
\frac{A(R' \leftarrow R)}{A(R \leftarrow R')} = \frac{P(R')g(R \leftarrow R')}{P(R)g(R' \leftarrow R)}
\]  

\[
(3.12)
\]
A common choice for the acceptance probability is the Metropolis choice:

\[ A(R' \leftarrow R) = \min \left( 1, \frac{P(R')g(R \leftarrow R')}{P(R)g(R' \leftarrow R)} \right) \]

(3.13)

It is not hard to see that this satisfies Eq. 3.12. When one of the \( A(R' \leftarrow R) \), \( A(R \leftarrow R') \) is less than 1 then the other equals 1 and thus Eq. 3.12 is satisfied. This means that for any two states \( R \) and \( R' \), proposed transitions from one of them to the other will all be accepted while transitions going the opposite way will be rejected to a degree. If we set \( g(R' \leftarrow R) = g(R \leftarrow R') \) as is commonly done then we have:

\[ A(R' \leftarrow R) = \min \left( 1, \frac{P(R')}{P(R)} \right) \]

(3.14)

and we can see that transitions are always accepted towards regions where \( P(R') > P(R) \) and rejected otherwise.

It is common to use a uniform distribution of some distance for \( g(R' \leftarrow R) \). The size of the maximum jump for the transition is optimized so that \( \sim 50\% \) of moves are accepted. Too small of a jump will lead to very autocorrelated samples since the walkers will evolve very slowly (although the acceptance rate will be high). At the other end, too large of a jump being proposed will result in a lot of rejections since \( P(R) \) can change a lot more over a large distance so \( P(R')/P(R) \) may be a lot greater or a lot less than 1. This also leads to very autocorrelated samples since the walkers take many steps to move around at all. Thus the sweet spot of half acceptances and half rejections makes for less of an autocorrelation problem and faster convergence to the stationary distribution \( P(R) \). Note that we use a drifted Gaussian that has information about \( P_T(R) \) to propose transitions, for which the acceptance rate is very high.

In VMC we propagate many (\( \sim 1000 \)) walkers for thousands of steps to acquire
statistically acceptable samples of $P_T(R)$. VMC is primarily used prior to AFDMC to optimize $\Psi_T(R)$ as well as possible. It is also useful because the resulting distribution of walkers that are proportional to $P_T(R)$ are directly inputted into AFDMC.

### 3.2 Diffusion Monte Carlo

DMC is a projector method that extracts the ground-state from a trial wave function. The evolution process is a Markov process with transition probabilities depending on the Hamiltonian of the many-body system. The general solution for the time-evolution of the wave function is given by: $|\Psi(t)\rangle = \sum_j c_j e^{-iE_jt/\hbar} |\Psi_j\rangle$. Now consider imaginary values for $t$ such that $it$ is a real positive number. Let $\tau = it/\hbar$ be called imaginary time. Then the evolution of the wave function in imaginary time is $|\Psi(\tau)\rangle = \sum_j c_j e^{-E_j\tau} |\Psi_j\rangle$. The corresponding imaginary time Schrödinger equation is $(-\partial/\partial\tau)|\Psi\rangle = \hat{H}|\Psi\rangle$. The evolution in imaginary time consists of a linear combination of exponentially decaying energy eigenstates. The exponential decay is slowest for the ground-state which has the largest exponent at any given $\tau$. After normalizing the evolved wave function the higher energy states have decayed away and only the ground-state remains at infinite imaginary time. It is easy to see (both from Schrödinger’s equation and from the form of the wave function) that the imaginary time evolution operator is $e^{-\hat{H}\tau}$. The time evolution is typically carried out with an energy offset that controls the normalization of the wave function:

$$|\Psi(\tau)\rangle = e^{-(\hat{H}-E_T)\tau} |\Psi_T\rangle$$

$$= c_0 e^{-(E_0-E_T)\tau} |\Psi_0\rangle + c_1 e^{-(E_1-E_T)\tau} |\Psi_1\rangle + c_2 e^{-(E_2-E_T)\tau} |\Psi_2\rangle + \ldots$$

(3.15)

where $|\Psi_T\rangle$ is a trial wave function representing the state at zero imaginary time.
Thus \( \lim_{\tau \to \infty} |\Psi(\tau)\rangle = \lim_{\tau \to \infty} c_0 e^{-(E_0 - E_T)\tau} |\Psi_0\rangle \). Setting \( E_T = E_0 \) in Eq. 3.15 prevents the ground-state from decaying. \( E_T > E_0 \) results in exponential growth of the ground-state and \( E_T < E_0 \) in decay. The wave function in the position basis \( \Psi(R, \tau) = \langle R|\Psi(\tau)\rangle \) is represented by a sample of configuration vectors similarly to the representation of the probability distribution function in the VMC method. In practice the time evolution is carried out in small time steps \( \Delta \tau \). Given a random walk simulating the time evolution, one can adjust \( E_T \) to maintain a stable population size of configurations. The limiting value of \( E_T \) is \( E_0 \). This is one possible way to compute the ground-state energy of the system and is called the population growth estimator.

The imaginary time evolution can be expressed as an integral over the trial wave function multiplied by matrix elements of the time evolution operator:

\[
\langle R|\Psi(\tau)\rangle = \langle R|e^{-(\hat{H} - E_T)\tau}|\Psi_T\rangle \\
\Psi(R, \tau) = \langle R|e^{-(\hat{H} - E_T)\tau} \int |R\rangle\langle R'||\Psi_T\rangle dR' \\
\Psi(R, \tau) = \int \langle R|e^{-(\hat{H} - E_T)\tau}|R'\rangle |\Psi_T(R')\rangle dR' \tag{3.16}
\]

where we inserted the identity \( I = \int dR|R\rangle\langle R| \) to get to the second equality. \( \langle R|e^{-(\hat{H} - E_T)\tau}|R'\rangle \) is the time-evolution propagator. It is usually very difficult to compute unless the time steps are small enough that approximations can be made. Consider the time-evolution in small steps \( \Delta \tau = \tau/n \) and let \( G(R, R') = \langle R|e^{-(\hat{H} - E_T)\Delta \tau}|R'\rangle \). Then:

\[
\langle R_n|\Psi(\tau)\rangle = \langle R_n|\prod_n e^{-(\hat{H} - E_T)\Delta \tau}|\Psi_T\rangle \\
\Psi(R_n, \tau) = \int dR_{n-1} \ldots dR_1 dR_0 G(R_n, R_{n-1}) \ldots G(R_2, R_1) G(R_1, R_0) |\Psi_T(R_0)\rangle \tag{3.17}
\]

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Eq. 3.17 is derived analogously to Eq. 3.16 through the insertion of identities prior to every $\Delta \tau$ evolution. To calculate the small time propagator $G$ we use the Trotter-Suzuki formula for approximating the exponential of the sum of two operators:

$$e^{-\hat{H}\Delta \tau} = e^{-(\hat{T}+\hat{V})\Delta \tau} = e^{-\Delta \tau \hat{V}/2}e^{-\Delta \tau \hat{T}}e^{-\Delta \tau \hat{V}/2} + O[\Delta \tau^3]$$  \hspace{1cm} (3.18)

For small $\Delta \tau$ the error is proportional to $\Delta \tau^3$. Thus the approximate short-time propagator is:

$$G(R, R') = \langle R | e^{-(\hat{H} - \hat{E}_T)\Delta \tau} | R' \rangle$$

$$\approx \langle R | e^{-\hat{V}\Delta \tau/2}e^{-\hat{T}\Delta \tau}e^{-\hat{V}\Delta \tau/2} | R' \rangle$$

$$= e^{-(V(R)-\hat{E}_T)\Delta \tau/2}\langle R | e^{-\hat{T}\Delta \tau} | R' \rangle e^{-(V(R')-\hat{E}_T)\Delta \tau/2}$$

$$= \langle R | e^{-\hat{T}\Delta \tau} | R' \rangle e^{-\Delta \tau(V(R)+V(R')-2\hat{E}_T)/2}$$

$$= G_d(R, R')G_b(R, R')$$  \hspace{1cm} (3.19)

Where $G_d(R, R') = \langle R | e^{-\hat{T}\Delta \tau} | R' \rangle$ and $G_b(R, R') = e^{-\Delta \tau(V(R)+V(R')-2\hat{E}_T)/2}$ come from the kinetic and potential terms of the Hamiltonian respectively. The kinetic energy propagator is readily derived by inserting the identity resolved in momentum eigenstates $\langle R | \mathbf{P} \rangle = e^{i\mathbf{P} \cdot \mathbf{R}/\hbar}(2\pi\hbar)^{3N/2}$:

$$G_d(R, R') = \langle R | e^{-\hat{T}\Delta \tau} | R' \rangle$$

$$= \langle R | e^{-\hat{T}\Delta \tau} \int | \mathbf{P} \rangle \langle \mathbf{P} | R' \rangle d\mathbf{P}$$

$$= \frac{1}{(2\pi\hbar)^{3N/2}} \int d\mathbf{P} \langle R | e^{-\hat{T}\Delta \tau} | \mathbf{P} \rangle e^{-i\mathbf{P} \cdot \mathbf{R}'/\hbar}$$

$$= \frac{1}{(2\pi\hbar)^{3N}} \int e^{-\mathbf{P}^2\Delta \tau/2m + i\mathbf{P} \cdot (\mathbf{R}-\mathbf{R}')/\hbar} d\mathbf{P}$$

$$= \frac{1}{(2\pi\hbar)^{3N}} \sqrt{\frac{2m\pi}{\Delta \tau}} e^{-m(\mathbf{R}-\mathbf{R}')^2/2\Delta \tau^2}$$
\[ = \sqrt{\frac{m}{2\pi \hbar^2 \Delta \tau}} e^{-\frac{m(R - R')^2}{2\Delta \hbar^2}} \]  

(3.20)

where \( \hat{T}|P\rangle = \frac{P^2}{2m}|P\rangle \) is used to get to the fourth equality. The Gaussian integral \( \int_{-\infty}^{\infty} e^{-ax^2+bx} dx = \sqrt{\frac{\pi}{a}} e^{b^2/4a} \) is used to evaluate every dimension of the \( 3N \)-dimensional integral. We will show that the propagators represent transition probabilities in the evolution of the trial wave function. \( G_d \) is called the diffusion Green’s function (note that the kinetic part of the Schrödinger Equation is a diffusion equation). It is a normal distribution with standard deviation \( \sqrt{\hbar^2 \Delta \tau/m} \). \( G_b \) is called the branching Green’s function. In practice the evolution is computed using a modified version of the Green’s function. The sampling is achieved using the Gaussian to determine points along the walk and the branching term as a weight on the walkers. This is discussed in more detail below.

The most common way of computing expectation values in DMC is to take the mixed estimator. The mixed estimator for an operator \( \hat{O} \) is defined as:

\[ \langle \hat{O} \rangle_M = \frac{\langle \Psi(\tau)|\hat{O}|\Psi_T \rangle}{\langle \Psi(\tau)|\Psi_T \rangle} \]  

(3.21)

Where of course we are interested in the limit of infinite imaginary time where

\[ \lim_{\tau \to \infty} \langle \hat{O} \rangle_M = \frac{\langle \Psi_0|\hat{O}|\Psi_T \rangle}{\langle \Psi_0|\Psi_T \rangle} \]  

(3.22)

This works out nicely for the Hamiltonian which commutes with the time-evolution operator \( e^{-\hat{H}\tau} \):

\[ \langle \hat{H} \rangle_M = \frac{\langle \Psi(\tau)|\hat{H}|\Psi_T \rangle}{\langle \Psi(\tau)|\Psi_T \rangle} = \frac{\langle \Psi(\tau/2)|\hat{H}|\Psi(\tau/2) \rangle}{\langle \Psi(\tau/2)|\Psi(\tau/2) \rangle} = E(\tau/2) \]  

(3.23)

Thus the mixed estimator for the Hamiltonian converges to the ground-state energy.
at infinite imaginary time. For operators that do not commute with the Hamiltonian a combination of mixed and variational estimators approximate the expectation value for that quantity. Inserting the integral form of $\Psi(R, \tau)$ from Eq. 3.17 gives:

$$\langle \hat{H} \rangle_M = \frac{\int dR_n \ldots dR_0 G(R_n, R_{n-1}) \ldots G(R_2, R_1) G(R_1, R_0) \Psi_T(R_0) \hat{H} \Psi_T(R_n)}{\int dR_n \ldots dR_0 G(R_n, R_{n-1}) \ldots G(R_2, R_1) G(R_1, R_0) \Psi_T(R_0) \Psi_T(R_n)}$$

$$\int dP_n G(R_n, R_{n-1}) \ldots G(R_2, R_1) G(R_1, R_0) \Psi_T(R_0) \Psi_T(R_n)$$

$$= \frac{\int dP_n G(R_n, R_{n-1}) \ldots G(R_2, R_1) G(R_1, R_0) \Psi_T(R_0) \hat{H} \Psi_T(R_n)}{\int dP_n G(R_n, R_{n-1}) \ldots G(R_2, R_1) G(R_1, R_0) \Psi_T(R_0) \Psi_T(R_n)}$$

$$= \frac{\int dP_n \left( \frac{G(R_n, R_{n-1}) \ldots G(R_2, R_1) G(R_1, R_0) \Psi_T(R_0) \hat{H} \Psi_T(R_n)}{\mathcal{W}(P_n)} \right)}{\int dP_n \left( \frac{G(R_n, R_{n-1}) \ldots G(R_2, R_1) G(R_1, R_0) \Psi_T(R_0) \Psi_T(R_n)}{\mathcal{W}(P_n)} \right)} \left( \frac{\mathcal{W}(P_n)}{\int dP_n \mathcal{W}(P_n)} \right)$$

(3.24)

where $P_n = (R_0, R_1, \ldots, R_{n-1}, R_n)$ is a path coordinate. The final expression in Eq. 3.24 presents both numerator and denominator in the form of a Monte Carlo integration (see Eqs. 3.1-3.5) that is evaluated by sampling paths $P_n^i$ from a weight function $\mathcal{W}(P_n)$, where $i$ denotes the path sampled. The weight function is commonly taken to be $\mathcal{W}(P_n) = \Psi_T(R_n) G(R_n, R_{n-1}) \ldots G(R_2, R_1) G(R_1, R_0) \Psi_T(R_0)$. It should be clear from Eq. 3.17 that $\int dR_{n-1} \ldots dR_0 \mathcal{W}(P_n) = \Psi(R_n, \tau) \Psi_T(R_n)$ which is normalizable. In fact we can rewrite the weight function as:

$$\mathcal{W}(P_n) = \left[ \prod_{i=0}^{n-1} \Psi_T(R_{i+1}) G(R_{i+1}, R_i) \frac{1}{\Psi_T(R_i)} \right] \Psi_T^2(R_0)$$

$$= \left[ \prod_{i=0}^{n-1} \tilde{G}(R_{i+1}, R_i) \right] \Psi_T^2(R_0)$$

(3.25)

so that we have:

$$\Psi(R_n, \tau) \Psi_T(R_n) = \int dR_{n-1} \ldots dR_1 dR_0 \tilde{G}(R_n, R_{n-1}) \ldots \tilde{G}(R_2, R_1) \tilde{G}(R_1, R_0) \Psi_T^2(R_0)$$

(3.26)
The mixed estimator for \( \hat{H} \) using our choice of \( \mathcal{W}(\mathbf{P}_n) \) is:

\[
\langle \hat{H} \rangle_M = \int d\mathbf{P}_n \frac{\hat{H}\Psi_T(R_n)}{\Psi_T(R_n)} \frac{\mathcal{W}(\mathbf{P}_n)}{d\mathbf{P}_n \mathcal{W}(\mathbf{P}_n)}
\]

\[
= \int d\mathbf{R}_n \frac{\hat{H}\Psi_T(R_n)}{\Psi_T(R_n)} \frac{\Psi(R_n, \tau)\Psi_T(R_n)}{d\mathbf{R}_n \Psi(R_n, \tau)\Psi_T(R_n)}
\]

\[
= \sum_{i=1}^{M} \frac{\hat{H}\Psi_T(R^i_n)}{\Psi_T(R^i_n)} = \sum_{i=1}^{M} E_L(R^i_n)
\]  

Comparing the first and second expressions in Eq. 3.27 shows that the sampled paths \( \mathbf{P}_n \) distributed according to \( \mathcal{W}(\mathbf{P}_n) \), have \( \mathbf{R}_n \) components distributed according to \( \Psi(R_n, \tau)\Psi_T(R_n) \). Thus, there is an equivalence between sampling path points \( \mathbf{P}_n \) and evolving the trial wave function. It is statistically preferable to sample the evolution of \( f(\mathbf{R}, \tau) = \Psi_T(\mathbf{R})\Psi(\mathbf{R}, \tau) \) over \( \Psi(\mathbf{R}, \tau) \). This approach of using distributions other than \( \Psi(\mathbf{R}, \tau) \) to calculate some property of \( \Psi(\mathbf{R}, \tau) \), in this case the ground-state energy, is known as importance sampling. The \( \mathbf{R} \) vectors along the paths are sampled using the propagator \( \tilde{G} \). We begin the time evolution with an initial distribution \( \Psi_T^2(\mathbf{R}_0) \). Note that this distribution is obtained from the Metropolis algorithm in VMC. We sample an \( \mathbf{R}_1 \) vector from each \( \mathbf{R}_0 \) vector so as to obtain path vectors distributed as \( \tilde{G}(\mathbf{R}_1, \mathbf{R}_0)\Psi_T^2(\mathbf{R}_0) \). Sampling the rest of the path vectors in this manner results in a set of samples of \( \mathbf{P}_n \) distributed according to \( \mathcal{W}(\mathbf{P}_n) \). The \( \mathbf{R}_j \) vectors along the path are distributed as \( \Psi(\mathbf{R}_j, j\Delta \tau)\Psi_T(\mathbf{R}_j) \). The small time importance sampled propagator is \( \tilde{G}(\mathbf{R}, \mathbf{R}') \approx \tilde{G}_d(\mathbf{R}, \mathbf{R}')\tilde{G}_b(\mathbf{R}, \mathbf{R}') \) where (see Appendix B for derivation):

\[
\tilde{G}_d(\mathbf{R}, \mathbf{R}') = \sqrt{\frac{m}{2\pi\hbar^2 \Delta \tau}} e^{-\frac{m(\mathbf{R} - \mathbf{R}' - \frac{\hbar}{m} \nabla \psi_T(\mathbf{R}'))^2}{2\Delta \tau \hbar^2}}
\]

\[
\tilde{G}_b(\mathbf{R}, \mathbf{R}') = e^{-\Delta \tau (E_L(\mathbf{R}) + E_L(\mathbf{R}') - 2E_T)/2}
\]  

\( E_L(\mathbf{R}) = \frac{\hat{H}\Psi_T(\mathbf{R})}{\Psi_T(\mathbf{R})} \) is the local energy. \( \mathbf{v}_D(\mathbf{R}) = \nabla \psi_T(\mathbf{R})/\Psi_T(\mathbf{R}) \) is called the drift.
velocity. It carries the evolving walkers in the direction of increasing $|\Psi_T|$. This makes sense because $\Psi_T$ is essentially a weight on our distribution that we use in order to guide the evolution along nicely. Thus it is desirable for $\Psi_T$ to be as similar to the ground-state wave function as possible. As for the time evolution algorithm: for each walker randomly sample a $3N$-dimensional vector $\chi$ of normally distributed numbers with mean 0 and variance $\hbar^2\Delta \tau/m$. Also, generate a random number $\eta$ from the uniform distribution on the interval $[0, 1]$. Propagate $\text{floor}[\eta + G_b(R, R')]$ copies of the walker from the original position $R'$ to $R = R' + \chi + \frac{\hbar^2\Delta \tau}{m}v_D(R')$. Notice how the copying of walkers is governed by the branching term. We use the Gaussian to generate new points since it is normalized and the branching term as a weight to determine how many walkers to place at the new position. In importance sampling the branching term depends on the local energy at the coordinates $R$ and $R'$. A good choice of $\Psi_T$ will have low variance in $E_L$ resulting in much lower fluctuations in walker populations compared to $G_b$ which depends on $V$ in the exponent.

In Fermionic systems the anti-symmetry of the wave function results in nodal surfaces where $\Psi_T = 0$. This is known as the Fermion sign problem. An attempt to remedy this may involve both positive and negative weights on walkers to try and cancel out symmetric components of the wave function. However this results in an exponentially decaying signal to noise ratio that has only been remedied for some simple systems. An effective method for tackling the time evolution of an anti-symmetric wave function is to fix the nodal surface and evolve the various nodal pockets independently of each other. This is called the fixed-node approximation. If a walker ever attempts to cross the nodal surface it is removed from the calculation. This results in the least energy wave function sharing the same nodal surface as $\Psi_T$. This means that the nodal surface must be the same as the true ground-states’ in
order for DMC to be exact for Fermions. The drift velocity almost always prevents walkers from trying to cross the nodal surface because it biases their evolution in the direction of increasing $|\Psi_T|$, thus increasing the efficiency of the algorithm.

### 3.3 Auxiliary Field Diffusion Monte Carlo

The DMC formalism above does not describe the evolution of any spin or isospin components of the wave function. As we have seen, the nuclear potential contains spin-dependent components. We use a nuclear parametrization (AV8) containing quadratic spin, tensor, and spin-orbit terms. There is also isospin but this does nothing to pure neutron systems. The quadratic spin operator is $\mathbf{\sigma}_j \cdot \mathbf{\sigma}_k$. The tensor term is similar but also contains angular dependence: $3(\hat{r}_{jk} \cdot \mathbf{\sigma}_j)(\hat{r}_{jk} \cdot \mathbf{\sigma}_k) - \mathbf{\sigma}_j \cdot \mathbf{\sigma}_k$. These are two-body terms so $jk$ indices sum over all particle pairs. A consequence of these operators is that we must consider all possible spin-states. The number of spin-states is $2^N$ so it is not computationally feasible to consider the states separately. AFDMC is an extension of the DMC formalism that treats the spin degrees of freedom as another component of walkers to be sampled.

The key to incorporating spin interactions in the Monte Carlo algorithm is re-expressing the propagator using the Hubbard-Stratonovich transformation:

$$e^{-\lambda \hat{O}^2/2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-x^2/2} e^{x\sqrt{-\lambda \hat{O}}}$$  \hspace{1cm} (3.29)$$

In order to do this we must cast our two-body potential in the form of the left hand side of Eq. 3.29. In Appendix C we show that the quadratic and tensor components
of the interaction can be rewritten as:

\[
V_{SD} = \frac{1}{2} \sum_{n=1}^{3N} \lambda_n \hat{O}_n^2,
\]

\[
\hat{O}_n = \sum_{i\alpha} \sigma_{i\alpha} \psi_{i\alpha}^n
\] (3.30)

where Roman subscripts denote particle labels and Greek subscripts denote Cartesian components. The \(\lambda_n\) and \(\psi_n\) depend on the walker coordinate \(\mathbf{R}\) and are the eigenvalues and eigenvectors of a 3Nx3N real symmetric matrix containing spin coefficients of the interaction. This yields the propagator:

\[
e^{-V_{SD} \Delta \tau} = e^{-\frac{1}{2} \sum_n \lambda_n \hat{O}_n^2 \Delta \tau} \approx \prod_{n=1}^{3N} e^{-\frac{1}{2} \lambda_n \hat{O}_n^2 \Delta \tau}
\] (3.31)

where the approximation is first order in \(\Delta \tau\). The \(\hat{O}_n\) operators in the final expression can be linearized using the Hubbard-Stratonovich transformation:

\[
e^{-V_{SD} \Delta \tau} = \prod_{n=1}^{3N} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx_n e^{-x_n^2/2} e^{\sqrt{-\lambda_n \Delta \tau} x_n \hat{O}_n}
\] (3.32)

The important consequence of this is that the operator in the exponent is a sum of one-body spinors. Since the spinors of difference particles commute we have:

\[
e^{\sqrt{-\lambda_n \Delta \tau} x_n \hat{O}_n} = \prod_{j=1}^{N} e^{\sqrt{-\lambda_n \Delta \tau} x_n \sigma_j \cdot \psi_{j\alpha}^n}
\] (3.33)

where \(\psi_{j\alpha}^n = (\psi_{jx}^n, \psi_{jy}^n, \psi_{jz}^n)\). The \(x_n\) are called auxiliary fields and are sampled from the standard normal distribution \(\frac{1}{\sqrt{2\pi}} e^{-x_n^2/2}\). The operator term in the integrand has the effect of rotating the spin state of every single one of the particles (see Appendix C for details on the rotation): i.e. every walker consists of a coordinate vector \(\mathbf{R}\) and a set of up and down spin amplitudes for every particle. We denote a walker by \(|\mathbf{R}, S\rangle\).
It is these spin states that are acted upon by \( e^{\sqrt{-\lambda_n \Delta \tau} x_n \hat{O}_n} \). This must be done for \( 3N \) auxiliary fields \( x_n \). The net difference in computation is a reduction in the number of operations from exponential (direct evaluation of the non-linearized propagator on all the spin states) to linear (spin rotations for every nucleon). The eigenvalues \( \lambda_n \) and eigenvectors \( \psi_n \) must also be computed prior to evolving the walker as well. A similar linearization of operators is required for the spin-orbit and 3-body interaction terms in the Hamiltonian.

Similarly to DMC, importance sampling is implemented in practice. The importance distribution is weighed using \( \Psi_T^* (R, S) = \langle \Psi_T | R, S \rangle \). At infinite imaginary time the ground-state is represented by: \( \sum_{R,S} \frac{1}{\langle \Psi_T | R, S \rangle} | R, S \rangle \). In addition the auxiliary field integrals are shifted by a constant \( \bar{x} = -\sqrt{-\lambda_n \Delta \tau} \langle \Psi_T | \hat{O}_n | R, S \rangle \langle \Psi_T | R, S \rangle \). Implementing these results in a weight factor of \( e^{-\Delta \tau \langle \Psi_T | V_{SD} | R, S \rangle \langle \Psi_T | R, S \rangle / \langle \Psi_T | R, S \rangle} \) which we compute in the local energy \( \tilde{G}_b (R, R') = e^{-\Delta \tau (E_L (R) + E_L (R') - 2E_r) / 2} \). The nuclear wave function can be complex as should be clear from the Pauli spin matrices. This results in a phase problem analogous to the sign problem in the real-valued case. Thus it is important to apply constraints to the walker evolution. We enforce \( \text{Re} [\langle \Psi_T | R, S \rangle / \langle \Psi_T | R', S \rangle] > 0 \) along the walk, dropping the walker whenever it does not satisfy the constraint. We take the real part of the local energy \( E_L (R, S) = \langle \Psi_T | \hat{H} | R, S \rangle / \langle \Psi_T | R, S \rangle \) as well as the drift velocity \( v_D (R, S) = \nabla \langle \Psi_T | R, S \rangle / \langle \Psi_T | R, S \rangle \) in our calculations. The energy estimate is computed by averaging the local energy over all walkers.

The auxiliary field method works for any operator that can be linearized using the Hubbard-Stratonovich transformation. We can actually use it to reproduce the action of the diffusion Green’s function propagator on the walkers:

\[
e^{-\Delta \tau} = e^{-\frac{\hat{p}_n^2 \Delta \tau}{2m}} = e^{-\frac{1}{2} \sum_{n=1}^{3N} \frac{\hat{p}_n^2 \Delta \tau}{m}}
\]
So that each \( p_n \) acts like:

\[
\begin{align*}
&\quad e^{-\frac{1}{2} \frac{\hbar \Delta \tau}{m}} \Psi(R) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx_n e^{-\frac{x_n^2}{2}} e^{-\frac{i}{\hbar} \hat{p}_n \sqrt{\frac{\hbar \Delta \tau}{m} x_n}} \\
&\quad = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx_n e^{-\frac{x_n^2}{2}} \Psi \left( r_1, r_2, \ldots, r_n - \sqrt{\frac{\hbar \Delta \tau}{m} x_n}, r_{n+1}, \ldots, r_{3N} \right)
\end{align*}
\]  

(3.35)

where the final expression of Eq. 3.35 is obtained using the fact that the momentum operator is the generator of translations. The transformation is a translation of the function \( \Psi(R) \) a distance of \( \sqrt{\frac{\hbar \Delta \tau}{m} x_n} \) in the \( r_n \) direction: i.e. we can just shift the individual walkers by that amount. The contribution of the translated function to the integral is proportional to \( \frac{1}{\sqrt{2\pi}} e^{-\frac{x_n^2}{2}} \). So the fraction of walkers that should be translated an \( \sqrt{\frac{\hbar \Delta \tau}{m} x_n} \) amount is \( \frac{1}{\sqrt{2\pi}} e^{-\frac{x_n^2}{2}} dx_n \). Thus we sample \( x_n \) from the standard normal distribution for each walker and then shift its \( r_n \) coordinate by \( \sqrt{\frac{\hbar \Delta \tau}{m} x_n} \). Eq. 3.34 says we need to do this for every \( x_n \), i.e. for all \( 3N \) coordinates. This is exactly the same as \( G_d \) from Eq. 3.20 which is a product of \( 3N \) one dimensional gaussians with standard deviation \( \sqrt{\frac{\hbar \Delta \tau}{m}} \).

### 3.4 Trial wave function

The form of the trial-wave function has great ramifications on the outcome of our Quantum Monte Carlo simulations. Since we are limited in time and computational resources we want our imaginary time propagation to equilbrate in a timely manner: i.e., we want small variance in our energy estimator. This requires choosing a trial-wave function that is tailored to the Hamiltonian of our system. The nodal pockets
of the trial wave function have an even greater significance on the accuracy of the results. The method is only exact when the nodes match those of the ground-state wave function.

\[ \Psi_T(R, S) = F_J(R)D(R, S) \]  

(3.36)

This is a product of a Jastrow factor and a Slater determinant of single-particle orbitals. The Jastrow factor is a nodeless function containing central correlations.

\[ F_J(R) = \prod_{i<j} f(r_{ij}) \]  

(3.37)

where \( f(r) \) satisfies (for \( r < d \)):

\[ -\frac{\hbar^2}{m} \nabla^2 f(r) + v(r)f(r) = \lambda f(r) \]  

(3.38)

where \( v(r) \) is the spin-independent component of the interaction. \( d < L/2 \) is called the healing distance. \( f(r \geq d) = 1 \). Thus particles that are farther than \( d \) distance apart are not correlated under the Jastrow function. The Jastrow factor is node-less so it only influences the variance of the calculation, by giving the wave function some information about where the particles should be based on the interaction.

The Slater determinant is the anti-symmetric part of the wave function. This is the trickier object to work with because it contains all the information about the nodal surface. A common choice is to take the ground-state of the non-interacting neutrons. We previously discussed the single-particle orbitals for our non-interacting Hamiltonian. They are products of plane-waves with Mathieu functions. We also mentioned that the number of particles we calculate for is 66. Due to spin-degeneracy and no preferred spin direction, there are 33 spin up orbitals and 33 spin down orbitals.
Let’s denote an orbital ket by $|\phi_n\rangle$. Then we have:

$$D(R, S) = \begin{vmatrix}
\langle r_1, s_1 | \phi_1 \rangle & \langle r_2, s_2 | \phi_1 \rangle & \cdots & \langle r_{66}, s_{66} | \phi_1 \rangle \\
\langle r_1, s_1 | \phi_2 \rangle & \langle r_2, s_2 | \phi_2 \rangle & \cdots & \langle r_{66}, s_{66} | \phi_2 \rangle \\
\vdots & \vdots & \ddots & \vdots \\
\langle r_1, s_1 | \phi_{66} \rangle & \langle r_2, s_2 | \phi_{66} \rangle & \cdots & \langle r_{66}, s_{66} | \phi_{66} \rangle 
\end{vmatrix}$$

(3.39)

where $|\phi_n\rangle$ for $n \leq 33$ are orbitals with spin up only. For $n > 33$ we use the same orbitals but with spin down only. Note that this form of the trial wave function as a function of $R$ and $S$ is the projection of the trial wave function ket onto a walker: $\Psi_T(R, S) = \langle R, S | \Psi_T \rangle$. In VMC we focus on $s_1 \cdots s_{33}$ being spin up and $s_{34} \cdots s_{66}$ being spin down. We do this because we know that every permutation of 33 spin up and 33 spin down will yield the same VMC energy by symmetry. Note that $S$ is free to evolve in AFDMC and that the quantity of interest for computing estimators is $\langle \Psi_T | R, S \rangle$.

The idea is that even though we have ignored the interactions in our Slater determinant, by including the external potential we hope that the nodal surface will be something like that of the full problem. To further optimize the trial wave function, one can include variational parameters and minimize the VMC energy. We tried this out by directly varying the orbital wave functions but did not find an appreciable change.

### 3.5 Equation of state

We computed the equation of state of 66 neutrons both with and without an external potential. We first present results that do not include NNN interactions. The NN interactions are given by the Argonne v8’ potential [60]. Calculations were
performed for densities in the range of \(0.02 \text{ fm}^{-3}\) to \(0.12 \text{ fm}^{-3}\) since these are similar to the densities found in the crust and outer-core of a neutron star. Setting up our wave function as described in Sec. 3.4, we perform VMC+AFDMC calculations to get the ground-state energy of the system. The AFDMC results for these are the squares in Fig. 3.1. The energy increases with increasing density. The energies agree with known values [56]. We computed energies using plane-wave orbitals for a one-body potential of strength \(2v_q = 0.5E_F\) and two periods of the potential in the box.
(diamonds). This yields lower energies than the unperturbed problem. However, we discussed in Sec. 3.4 that we’d use Mathieu functions for our trial wave function in this case. The energies for the Mathieu single-particle orbitals (circles) are up to 1 MeV different from the plane-wave results, emphasizing the importance of choosing a good trial wave function (note that VMC energies are lower with Mathieu functions than plane-waves). Overall, the AFDMC energies with an external potential are several MeV smaller than those without an external potential. This reflects the particles’

tendency to stay away from the repulsive regions of the potential and collect in the wells of the potential. Note that the amplitude of the external potential used is density

Figure 3.2: Neutron-matter VMC energy per particle as a function of the variational parameter $\beta$ using NN interactions. $n_0 = 0.1 \text{fm}^{-3}$, $2v_q = 0.5E_F = 21.363$ MeV, and $q = 4\pi/L$. 

41
dependent. Also, the period of the potential decreases with increasing density. This
is consistent with what happens in a neutron-star crust where the lattice spacing
decreases with increasing density.

We now describe the optimization procedure of our trial wave functions mentioned
at the end of Sec. 3.4. Since this is a variational optimization the goal is to minimize
the VMC energy. Firstly, Mathieu functions yield lower VMC energies than plane-
waves in the Slater determinant (note: we only use Mathieu functions for the z
component of the wave function). This supports our decision to use the orbitals of
the non-interacting problem in our trial wave function. We further optimize these
using a variational parameter $\beta$ where we vary the orbitals by choosing Mathieu
functions corresponding to the external potential $v(r) = \beta \cos q \cdot r$ [52]. For the
case $\beta = 2v_q$ these are the orbitals corresponding to the non-interacting problem:
i.e. with no further optimization. Consider a density of 0.1 fm$^{-3}$ for the case where
$2v_q = 0.5E_F$ and two periods of the potential fit in the box. The minimum VMC
energy that we simulated occurs at $\beta = 18$ MeV (Fig. 3.2). The AFDMC energy for
$\beta = 18$ MeV is 8.19 MeV. The AFDMC energy for $\beta = 2v_q$ is 8.15 MeV. Thus, the
difference in energy due to the $\beta$ optimization procedure is much smaller than the
difference due to using plane-waves vs Mathieu functions. Therefore, it is safe to set
$\beta = 2v_q$ for practical purposes.

We are primarily interested in the static response of neutron matter. This requires
us to perform calculations across a set of strengths of the external potential. It
is important that the strengths are large enough so that the energy is statistically
different from homogeneous neutron matter. At the same time the filling of the
single particle orbitals changes at larger $v_q$ in comparison to the free non-interacting
orbital filling. We performed simulations for various orbital fillings and found no
significant change in the energy. We did this for $2v_q = 0.5E_F$ at $n = 0.08\text{ fm}^{-3}$ for two different fillings and found AFDMC energies of 7.072 and 7.062 MeV. The same was done for $2v_q = 0.75E_F$ at $n = 0.04\text{ fm}^{-3}$ yielding 1.818 and 1.822 MeV. We decided to calculate energies for $2v_q = 0.25, 0.3, 0.35, 0.5, 0.75 E_F$. NNN interactions were included in these simulations. Specifically, the Urbana IX potential was used, as is appropriate for neutron-rich matter [61]. Turning up the potential strength results in a decrease in energy. This is seen in the circles in Fig. 3.3 for 66 particles at a density of 0.1 fm$^{-3}$ and two periods of the potential in the box. We have also applied
Eq. (2.14) to extrapolate to the TL (squares). We extract the response function from such results. We present those results in the next chapter.

### 3.6 Energy-density functionals

Another method for computing the energy of this system comes from density functional theory (DFT). In this case, the nuclear force takes a phenomenological form of the Skyrme type. The many-body wave function takes the form of a Slater determinant of single-particle orbitals $\psi_i(r)$. The ground-state energy is given by:

$$ E = \int \mathcal{H}(r)d^3r, \quad (3.40) $$

where $\mathcal{H}$ is the energy density energy functional (EDF) [8]:

$$ \mathcal{H} = \frac{\hbar^2}{2m} \tau + 2v_q \cos(q \cdot r)n + \mathcal{E}_{Sk} \quad (3.41) $$

and

$$ n(r) = \sum_i [\psi_i(r)]^2 \quad n(\mathbf{r}) = \sum_i [\nabla \psi_i(\mathbf{r})]^2 \quad (3.42) $$

are the nucleon and kinetic energy densities. The Skyrme interaction terms of the EDF in the isospin representation are:

$$ \mathcal{E}_{Sk} = \sum_{T=0,1} \left[ (C_T^{n,a} + C_T^{n,b} n_0^2) n_T^2 + C_T^{\Delta n} (n_T n_T^*)^2 + C_T^{\tau} n_T \tau_T \right] \quad (3.43) $$

For pure neutron matter $n_0 = n_1 = n$ and the same is true for $\tau$. We have done
calculations for the SLy4, SLy7, and SkM* parametrizations. \( C_1^{\Delta n} \) is known as the isovector gradient term. \( C_1^{\Delta n} = -16, -6, \) and \(-17 \text{ MeV fm}^5 \) in SLy4, SLy7, and SkM* respectively [9]. In what follows, we will adjust this parameter based on our AFDMC results. Eq. (3.40) provides us with a method to approximate the energy using the density functions. This is called the local-density approximation (LDA).

Our method of computing the LDA energy is similar to the VMC optimization of the trial wave function. The \( \psi_i \)'s are the orbitals of the non-interacting Hamiltonian with our external potential. Reviewing the contents of Chapter 2, the orbitals are plane-waves in \( x \) and \( y \). For non-zero \( v_q \) the orbitals in \( z \) are given by Mathieu’s equation:

\[
\frac{d^2 \psi_z(s)}{ds^2} + (A - 2\beta \cos (2s)) \psi_z(s) = 0 \tag{3.44}
\]

\( s = \pi/d \). We allowed \( \beta \) to be a free/variational parameter: i.e. we minimized Eq. (3.40) as a function of \( \beta \) to produce the LDA energies. Each orbital is doubly degenerate due to spin. So when we study 66 particles we select 33 unique orbitals which we enumerate twice. Another degree of freedom is the selection of orbitals defined by: \( (n_x, n_y, n_z) \). It was found that the minimum energy did not always correspond to the traditional lowest energy orbitals of the non-interacting problem. In the non-perturbed case \( (v_q = 0) \) the LDA energy occurred at \( \beta = 0 \) and a traditional selection of plane-waves. For non-zero \( v_q \) the LDA energy occurred at non-zero \( \beta \) (Mathieu functions) but that \( \beta \) did not have to equal \( Q \) corresponding to \( v_q \). In the case of non-closed shells the interchange of equivalent energy orbitals had no effect on the LDA energy.
3.6.1 Constraining the isovector gradient coefficient

We have also used the response of neutron matter to constrain energy density functionals. The energy in Eq. (3.40) is minimized with respect to the variational parameter $\beta$ and different orbital fillings. This is done for a range of potential strengths. Fig. 3.4 displays the results of this procedure for SLy4 (solid line) for a 66 particle system at a density of $0.10\text{fm}^{-3}$ and two periods of the potential in the box. The 66 particle AFDMC NN+NNN energies (circles) are more repulsive than the SLy4 energies. The separation between the AFDMC and SLy4 energies is largest at $v_q = 0$. 

Figure 3.4: Neutron-matter energy per particle for 66 particles as a function of the one-body potential strength at a density of $n_0 = 0.10\text{fm}^{-3}$, using NN+NNN interactions and a one-body potential periodicity $q = 4\pi/L$. Circles denote AFDMC results, and the solid line follows from the SLy4 energy-density functional. The dashed line corresponds to SLy4 results with a modified isovector gradient term.
The separation decreases as $v_q$ increases. $\nabla n = 0$ at homogeneity so the isovector gradient term does not contribute to the $v_q = 0$ energy. Thus the difference between the AFDMC and SLy4 energies at homogeneity is due to the bulk energy of the system. This homogeneous mismatch in energy must be respected in fitting the EDF to AFDMC results. The isovector gradient term has the effect of bringing the SLy4 energies closer to the AFDMC energies at larger $v_q$. Thus, our fitting of the isovector gradient term maintains the $v_q = 0$ difference between the EDF and QMC energies.

We fit to low strengths $2v_q = 0.25$ and $0.3E_F$, in order to ensure that the density perturbation magnitude is not comparable to the unperturbed density. We found a modified isovector gradient term of $C_1^{\Delta n} = -29$ MeV fm$^5$ at this density (dashed line...
Figure 3.6: Neutron-matter energy per particle for 66 particles as a function of the one-body potential strength at a density of \(n_0 = 0.04 \text{ fm}^{-3}\), using NN+NNN interactions and a one-body potential periodicity \(q = 4\pi/L\). Circles denote AFDMC results, and the solid line follows from the SLy4 energy-density functional. The dashed line corresponds to SLy4 results with a modified isovector gradient term.

The homogeneous energy difference between AFDMC and SLy4 impacts how the isovector gradient term should be modified. Above \(n = 0.06 \text{ fm}^{-3}\) the homogeneous AFDMC energy (circles in Fig. 3.5) is more repulsive than the homogeneous SLy4 energy (solid line in Fig. 3.5). Below this density the AFDMC is more attractive than the SLy4 energy. We see this at \(n = 0.04 \text{ fm}^{-3}\) where the AFDMC NN+NNN energies (circles in Fig. 3.6) are smaller than SLy4 (solid line in Fig. 3.6) for small enough \(v_q\). The separation between AFDMC and SLy4 decreases with increasing \(v_q\) at
both densities larger and smaller than $0.06 \text{ fm}^{-3}$. This means that the fitted isovector gradient term is density dependent. This result is also found using the density-matrix expansion [62, 63]. For $n > 0.06 \text{ fm}^{-3}$ the isovector gradient fit must make the SLy4 energies more attractive if they are to be equidistant from the AFDMC energies. This requires a decrease in the isovector gradient term. For $n < 0.06 \text{ fm}^{-3}$ an increase in the isovector gradient term is required. At a density of $0.04 \text{ fm}^{-3}$ we find a modified isovector term of $C_1^{\Delta n} = 9 \text{ MeV fm}^5$ (dashed line in Fig. 3.6). Since we fit the isovector term to low strengths, the modified SLy4 still approaches the AFDMC results at some large $v_q$.

We have carried out calculations such as those in Fig. 3.4 and Fig. 3.6 for several other densities. They exhibit qualitatively the same trends as discussed above. We then used these AFDMC results to constrain the isovector coefficient for several functionals. Specifically, Fig. 3.7 lists the isovector gradient term of modified SLy4, SLy7, and SkM*. All of these were done using two periods of the potential in the box. The errors were determined by fitting to different strengths and examining the spread of the modified isovector gradient term. Note that the density dependent energy versus $v_q$ behaviour described above does not hold for SkM*. Nevertheless, our fitting prescription yields the same density dependence in the modification of the isovector term for all three parameterizations. We see a decrease is required at large densities. At low densities there is an increase in the isovector term. The isovector term is least modified at $n = 0.06 \text{ fm}^{-3}$, where in the homogeneous case the AFDMC and SLy4 results agree reasonably well, as per Fig. 3.5.

Note that the isovector coefficient fits discussed above were all carried out by focusing on the EDF and QMC results for $L = 2d$, i.e., using two periods of the potential in the box. As we will see in the following subsection, our attempt to
Figure 3.7: Isovector gradient coefficients for the modified SLy4, SLy7, and SkM* Skyrme potentials. All calculations were done with two periods of the potential in the box. Coefficients were modified to make Skyrme responses match the QMC responses.

make the QMC and EDF results equidistant essentially amounts to trying to match (not QMC energies to EDF energies, but) the EDF response function to the QMC response function. In other words, we are attempting to modify the SLy4 response from Fig. 4.1 below to match that in Fig. 4.2 below. All this, for the specific case of \( L = 2d \). As the difference between SLy4 and modified SLy4 in Fig. 4.1 shows, for \( L = 2d \) we would need a more attractive modification, whereas for \( L = d \) we would need a more repulsive one (and for \( L = 3d \) we would need a modification that is more attractive than that for \( L = 2d \)). Thus, the optimal thing to do is to try to optimize
results for as many periodicities as possible simultaneously. We have done this at the two densities of $n = 0.10\,\text{fm}^{-3}$ and $n = 0.04\,\text{fm}^{-3}$, where we have produced AFDMC results for many different periodicities, as discussed below.
Chapter 4

Static Response

4.1 Static-response theory

Our AFDMC calculations can be used to calculate the static response functions for neutron matter. Let $\hat{H}_0$ denote the unperturbed Hamiltonian. The static perturbation may be expressed as:

$$\hat{H}_v = \hat{H}_0 + \int d\mathbf{r} \hat{n}(\mathbf{r})v(\mathbf{r})$$

(4.1)

where $\hat{n}(\mathbf{r}) = \sum_{i=1}^N \delta(\mathbf{r} - \mathbf{r}_i)$ is the one-body density operator. The natural question that arises is how do the ground-state properties shift due to such a potential. We express the ground-state density of the system as a functional of the external potential: $n_v(\mathbf{r}) = n_0(\mathbf{r}, [v])$. $n_0(\mathbf{r}, [0]) = n_0$ as the unperturbed system is homogeneous and isotropic in space. The density-density response functions are defined as the functional derivatives of density with respect to $v$ [64]:

$$n_v(\mathbf{r}) = n_0 + \sum_{k=1}^{\infty} \frac{1}{k!} \int d\mathbf{r}_1 \ldots d\mathbf{r}_k \chi^{(k)}(\mathbf{r}_1 - \mathbf{r}, \ldots, \mathbf{r}_k - \mathbf{r})v(\mathbf{r}_1) \ldots v(\mathbf{r}_k),$$

(4.2)

where the $\chi^{(k)}$'s are called response functions. $\chi^{(1)}(\mathbf{r})$ is the linear density-density
response function. Likewise, the ground state energy can also be expressed as a functional of \( v \): \( E_v = E_0([v]) \). We know from first-order perturbation theory that 
\[
\frac{dE_0[λv]}{dλ} = \int drn_0(r,[λv])v(r) \quad \text{(see Appendix C for derivation)}.
\]
From this it follows that:
\[
E_v - E_0[0] = \int_0^1 dλ \int drn_0(r,[λv])v(r)
\quad \text{(4.3)}
\]
Inserting Eq. 4.2 into Eq. 4.3 yields:
\[
E_v - E_0 = n_0 \int drv(r) + \sum_{k=1}^{∞} \frac{1}{(k+1)!} \int drdr_1...dr_k \chi^{(k)}(r_1-r,...,r_k-r) \times 
\quad v(r)v(r_1)...v(r_k)
\quad \text{(4.4)}
\]
The density change can be expressed in terms of the Fourier components of the potential \( v(r) = \sum_q v_q \exp(iq\cdot r) \) and the Fourier transforms of the response functions with respect to their spatial arguments \( \chi^{(k)}(q_1,...,q_k) \):
\[
n_v(r) - n_0 = \sum_{k=1}^{∞} \frac{1}{k!} \sum_{q_1,...,q_k} \chi^{(k)}(q_1,...,q_k)v_{q_1}...v_{q_k} \exp[i(q_1+...+q_k)\cdot r]
\quad \text{(4.5)}
\]
Likewise the change in energy per particle is:
\[
\frac{E_v}{N} - \frac{E_0}{N} = v_0 + \frac{1}{n_0} \sum_{k=1}^{∞} \frac{1}{(k+1)!} \sum_{q_1+q_2+...+q_k=0} \chi^{(k)}(q_1,...,q_k)v_qv_{q_1}...v_{q_k}
\quad \text{(4.6)}
\]
For the one-body external potential \( v(r) = 2v_q \cos(q\cdot r) \) the density is given by:
\[
n_q - n_0 = 2n_q \cos(q\cdot r)
\quad n_q = \chi^1(q)v_q + \frac{\chi^3(q,q_3-q)}{2}v_q^3 + ...
\quad \text{(4.7)}
\]
The change in the density $n_v(r) - n_0$ depends only on odd powers of $v_q$. The change in energy is:

$$\frac{E_v}{N} - \frac{E_0}{N} = \frac{\chi^1(q)}{n_0} v_q^2 + \frac{\chi^3(q, q, -q)}{4n_0} v_q^4 + \ldots$$  \hspace{1cm} (4.8)

The energy change only depends on even powers of $v_q$. If the energy per particle is known at several different values of $v_q$ then Eq. (4.8) gives a method to calculate lower-order response functions by fitting to a polynomial of even powers. The coefficient of the quadratic term gives the linear density-density response function. The coefficient of the quartic term is very small in our calculations, on the order of $10^{-4}$ MeV$^{-3}$ or smaller. Higher-order fits, with more points, are required to reliably extract the third-order response function.

The response of a non-interacting Fermi gas can be computed analytically. It is given by the Lindhard function [65]:

$$\chi_L = -\frac{mq_F}{2\pi^2\hbar^2} \left[ 1 + \frac{q_F}{q} \left( 1 - \left( \frac{q}{2q_F} \right)^2 \right) \ln \left| \frac{q + 2q_F}{q - 2q_F} \right| \right]$$  \hspace{1cm} (4.9)

We compare our results in the next sections with this response.

### 4.2 Response functions

Using calculations like those discussed above, we extracted linear density-density response functions at both 0.04 fm$^{-3}$ and 0.10 fm$^{-3}$ for AFDMC, SLy4 and modified SLy4 results. (To do this, we fit to even-powered polynomials up to fourth order in Eq. (4.8).) Since we are studying neutron matter we use Eq. (2.14) to extrapolate energies to the TL. It was previously mentioned that we only consider $q$ such that
Figure 4.1: Static-response functions of neutron-matter at a density of $0.10 \, \text{fm}^{-3}$. The circles are the SLy4 response extrapolated to the TL limit. The diamonds are for the modified SLy4 with $C_1^{\Delta n} = -29 \, \text{MeV fm}^5$ extrapolated to the TL. The response was extracted by fitting to $2v_q = 0.25, 0.3, 0.35, 0.5$, and $0.75 \, E_F$. The dashed curve is the SLy4 response produced in the TL [66]. The solid line is the Lindhard function describing the response of a non-interacting Fermi gas.

an integer number of periods of the potential fit in the box. We have performed simulations for $q = 2, 4, 6, 8, 12, 16, 20$ times $\pi/L$ corresponding to 1, 2, 3, 4, 6, 8, and 10 periods of the potential inside the box.

We have also taken advantage of the compressibility sum rule: this provides us with a way to calculate $\chi(0)$ starting from the energy per particle as a function of density of the unperturbed system:

$$\frac{1}{\chi(0)} = -\frac{\partial^2(n_0E/N)}{\partial n_0^2}$$  \hspace{1cm} (4.10)
Figure 4.2: Static-response functions of neutron-matter at a density of 0.10 fm$^{-3}$. Produced using AFDMC results. Circles are with NN+NNN interactions extrapolated to the TL limit. Diamonds are for NN interactions extrapolated to the TL. The response was extracted by fitting to: $2\nu_q = 0.25, 0.3, 0.35, 0.5, \text{ and } 0.75 E_F$. The square is the response at $q = 0$ predicted by the compressibility sum rule for the NN+NNN case. The curve is the Lindhard function describing the response of a non-interacting Fermi gas.

We used Eq. (4.10) to compute $\chi(0)$ for the various response functions that we extracted and checked for consistency with our modulated results.

We first present results at $n_0 = 0.10 \text{ fm}^{-3}$. We have found that the SLy4 response (circles in Fig. 4.1) does not match the Lindhard function (solid line in Fig. 4.1) although there are similarities. Both responses have a finite $\chi(0)$ and go to 0 at large $q$. We compare to the SLy4 response function in the TL [66] (dashed line in Fig. 4.1). Our response agrees with it pretty well for all except the smallest $q$ values.
The compressibility sum rule gives a value of \(-\chi(0)/n_0 = 0.057\,\text{MeV}^{-1}\) for SLy4 which matches the TL SLy4. We are also interested in the modified SLy4 response (diamonds in Fig. 4.1). This response is similar in shape but larger in magnitude than the SLy4 response we extracted. This makes sense since the modified SLy4 is more attractive than SLy4. The compressibility sum rule gives the same \(\chi(0)\) for modified SLy4 as SLy4 since the unperturbed system is independent of the gradient term.

In Fig. 4.2 we show updated AFDMC NN+NNN results (circles): note that these include the corrected FS handling and therefore differ (in the lowest-\(q\) response value) from the circles in Fig. 3 of Ref. [67]. The diamonds in Fig. 4.2 show the AFDMC NN response function in the TL. Our results in the TL are similar in shape to the Lindhard function (line in Fig. 4.2). At larger \(q\) the response goes to zero and matches the Lindhard function. At smaller \(q\) the NN+NNN response is smaller than the Lindhard function. The NN response is larger than the Lindhard function at the lowest \(q\) value, but other than that it is very similar to the NN+NNN response. The compressibility sum rule gives a value of \(-\chi(0)/n_0 = 0.14\,\text{MeV}^{-1}\) for neutron matter with our NN+NNN interactions (square in Fig. 4.2) and a value of 0.089 MeV\(^{-1}\) for NN interactions only. These are larger than the corresponding value of 0.035 MeV\(^{-1}\) for the Lindhard function. Note that Fermi liquid theory yields \(-\chi(q)/n_0 \approx 0.035\,\text{MeV}^{-1}\) at \(n_0 = 0.10\,\text{fm}^{-3}\) [42, 68].

We now examine some of the responses at a density of 0.04 fm\(^{-3}\). We have found that the AFDMC results do not follow the Lindhard function (solid line in Fig. 4.3) as well as the 0.10 fm\(^{-3}\) AFDMC results do. Both the AFDMC NN response (diamonds in Fig. 4.3) and the AFDMC NN+NNN response (circles in Fig. 4.3) are larger than the Lindhard function at small \(q\). The compressibility sum rule gives a value of \(-\chi(0)/n_0 = 0.14\,\text{MeV}^{-1}\) for neutron matter with our NN+NNN
Figure 4.3: Static-response function of neutron-matter at a density of 0.04 fm$^{-3}$. The circles are with NN+NNN interactions extrapolated to the TL. Diamonds are for NN interactions extrapolated to the TL. The AFDMC responses were extracted by fitting to: $2\nu_q = 0.25, 0.3, 0.35,$ and $0.5 E_F$. The solid line is the Lindhard function describing the response of a non-interacting Fermi gas.

interactions and 0.19 MeV$^{-1}$ for NN interactions only. These are larger than the $-\chi(0)/n_0 = 0.065$ MeV$^{-1}$ of the Lindhard function. Fermi liquid theory yields $-\chi(q)/n_0 \approx 0.083$ MeV$^{-1}$ at $n_0 = 0.04$ fm$^{-3}$ [42, 68].

For all results it was found that the response function goes to zero as $q$ goes to infinity and $\chi(0)$ is finite. In addition, the response functions extracted from AFDMC and the Lindhard functions show more similarity to one another than to the SLy4 responses. Overall, the SLy4 responses are narrower and steeper than the other responses. It is also interesting to contrast these to the response functions of $^4$He [52].
and the 3D electron gas [53] both of which have $\chi(0) = 0$.

Similarly to what was shown in Figs. 4.2 & 4.3, one can extract the response function of neutron matter for other densities. We have carried out precisely such an extraction and show the results in Fig. 4.4. These correspond to AFDMC calculations using NN+NNN interactions for the case where two periods fit inside the box. They are compared to the free-gas result, which follows from the Lindhard function. Overall, we see that the microscopic results are roughly similar to the free-gas results regardless of the density. At a more fine-grained level, we observe that the answer to whether or not the microscopic response is higher or lower than the free-gas one
depends on the density. One could say that this behavior is similar to what is seen in Fig. 3.5, but such a comparison is misleading for two reasons: a) there we were comparing AFDMC results to EDF results, not to free-gas values, and b) our new results in Fig. 4.4 show the answer for the response, i.e. at finite one-body potential strength. Thus, these responses cannot be simply extracted from the homogeneous-gas answers and constitute microscopic benchmarks.
Chapter 5

Summary & Conclusion

To summarize, in this thesis we have investigated the properties of periodically modulated neutron matter, using a combination of large-scale simulations and qualitative insights. We started from the non-interacting problem, examining in detail finite-size effects: since 66 is the number of particles commonly used for homogeneous neutron matter, we studied the adjustments that need to be carried out in order to use that particle number for the inhomogeneous problem. We then reported on our auxiliary-field diffusion Monte Carlo simulations, underlining the importance of optimizing the trial wave function by minimizing the VMC energy. This depended on a detailed understanding of the single-particle orbitals. AFDMC allowed us to compute the ground-state energy of neutron matter at various densities, potential strengths, and periodicities of the potential. In particular we studied the inhomogeneous problem by increasing the strength of the potential starting from homogeneity.

We then examined several consequences of our ab initio results. We first saw the impact that they have on energy density functionals. We used the response of neutron matter to constrain the isovector term while carefully disentangling the contributions of bulk and gradient terms. We found a density-dependent isovector
term and provided our estimate for its magnitude at each density. Next, we extracted the linear density-density static response function of neutron matter from AFDMC and EDF results at two different densities. This required a set of *ab initio* results for each of the periodicities that we studied. We then compared and contrasted the response function of neutron matter to that of other systems. More than a proof-of-principle, this work provides detailed benchmarks that other *ab initio* calculations can compare to, or EDF approaches can use as input.
Appendix A

The importance sampled propagator

A differential equation describing the time evolution for a distribution \( f(R, \tau) \) takes the form:

\[
- \frac{\partial}{\partial \tau} f(R, \tau) = \hat{E} f(R, \tau) \tag{1}
\]

with corresponding time evolution propagator \( e^{-\hat{E} \Delta \tau} \). This is valid whenever \( \hat{E} \) and \( \frac{\partial}{\partial \tau} \) commute. The non-importance time evolution in DMC is given by \( -\frac{\partial}{\partial \tau} \Psi(R, \tau) = \hat{H} - E_T \Psi(R, \tau) \). We derive the corresponding importance equation describing the evolution of \( f(R, \tau) = \Psi_T(R) \Psi(R, \tau) \):

\[
\begin{align*}
- \frac{\partial}{\partial \tau} f(R, \tau) &= -\frac{\partial}{\partial \tau} (\Psi_T(R) \Psi(R, \tau)) \\
&= \Psi_T(R) \left[ -\frac{\partial}{\partial \tau} \Psi(R, \tau) \right] = \Psi_T(R) (\hat{H} - E_T) \Psi(R, \tau) \\
&= \Psi_T(R) \left[ -\frac{\hbar^2}{2m} \nabla^2 \Psi(R, \tau) + V(R) \Psi(R, \tau) \right] - E_T f(R, \tau) \\
&= -\frac{\hbar^2}{2m} \left[ \Psi_T(R) [\nabla^2 \Psi(R, \tau)] + 2[\nabla \Psi_T(R)] [\nabla \Psi(R, \tau)] + [\nabla^2 \Psi_T(R)] \Psi(R, \tau) \right] \\
&\quad + \frac{\hbar^2}{m} \left[ [\nabla \Psi_T(R)] [\nabla \Psi(R, \tau)] + [\nabla^2 \Psi_T(R)] \Psi(R, \tau) \right] \\
&\quad + \left[ -\frac{\hbar^2}{2m} \nabla^2 \Psi_T(R) + V(R) \Psi_T(R, \tau) \right] \Psi(R, \tau) - E_T f(R, \tau) \\
&= -\frac{\hbar^2}{2m} \nabla^2 [\Psi_T(R) \Psi(R, \tau)] + \frac{\hbar^2}{m} \nabla \cdot [\nabla \Psi_T(R) \Psi(R, \tau)] + [\hat{H} \Psi_T(R)] \Psi(R, \tau) - E_T f(R, \tau) \\
&= -\frac{\hbar^2}{2m} \nabla^2 f(R, \tau) + \frac{\hbar^2}{m} \nabla \cdot \left[ \frac{\nabla \Psi_T(R)}{\Psi_T(R)} f(R, \tau) \right] + \left[ \frac{\dot{\Psi}_T(R)}{\Psi_T(R)} - E_T \right] f(R, \tau)
\end{align*}
\]
\[ -\frac{\hbar^2}{2m} \nabla^2 f(R, \tau) + \frac{\hbar^2}{m} \nabla \cdot [v_D(R) f(R, \tau)] + [E_L(R) - E_T] f(R, \tau) \]  

(2)

where we added and subtracted \((\hbar^2/m)\left[ [\nabla \Psi_T(R)] [\nabla \Psi(R, \tau)] + [\nabla^2 \Psi_T(R)] \Psi(R, \tau) \right]\) to get from equality 4 to 5. \(v_D(R) = \frac{\nabla \Psi_T(R)}{\Psi_T(R)}\) is called the drift velocity. \(E_L(R) = \frac{\hbar \Psi_T(R)}{\Psi_T(R)}\) is the local energy. Thus the importance propagator is given by:

\[
e^{-\hat{T} \Delta \tau - i \frac{\hbar^2 \Delta \tau}{m} \hat{P} \cdot v_D(R) - \frac{\Delta \tau}{2} \hat{E}_L(E_T)} \approx e^{-\Delta \tau [E_L - E_T]/2} e^{-\hat{T} \Delta \tau} e^{-i \frac{\hbar^2 \Delta \tau}{m} \hat{P} \cdot v_D(R)} e^{-\Delta \tau [E_L - E_T]/2} \]

(3)

Notice that we write \(v_D(\hat{R})\), where the \(R\) has been promoted to an operator. The approximation in Eq. 3 is \(O[\Delta \tau^2]\). The matrix elements are given by:

\[
\tilde{G}(R, R') \approx \langle R | e^{-\Delta \tau [E_L - E_T]/2} e^{-i \frac{\hbar^2 \Delta \tau}{m} \hat{P} \cdot v_D(R)} e^{-\Delta \tau [E_L - E_T]/2} | R' \rangle
\]

(4)

\[
= \langle R | e^{-\hat{T} \Delta \tau} e^{-i \frac{\hbar^2 \Delta \tau}{m} \hat{P} \cdot v_D(R)} | R' \rangle e^{-\Delta \tau [E_L(\hat{R}) + E_L(\hat{R}') - 2E_T]/2}
\]

\[
\approx \langle R | e^{-\hat{T} \Delta \tau} e^{-i \frac{\hbar^2 \Delta \tau}{m} \hat{P} \cdot v_D(R')} | R' \rangle e^{-\Delta \tau [E_L(\hat{R}) + E_L(\hat{R}') - 2E_T]/2}
\]

\[
= \langle R | e^{-\hat{T} \Delta \tau} | R' + \frac{\hbar^2 \Delta \tau}{m} v_D(R') \rangle e^{-\Delta \tau [E_L(\hat{R}) + E_L(\hat{R}') - 2E_T]/2}
\]

\[
= \sqrt{\frac{m}{2\pi \hbar^2 \Delta \tau}} e^{-\frac{m |R - R'|^2 + \hbar^2 \Delta \tau v_D(R')^2}{2\Delta \tau \hbar^2}} e^{-\Delta \tau [E_L(\hat{R}) + E_L(\hat{R}') - 2E_T]/2}
\]

\[
= \tilde{G}_d(R, R') \tilde{G}_b(R, R')
\]

where \(\tilde{G}_d(R, R') = \sqrt{\frac{m}{2\pi \hbar^2 \Delta \tau}} e^{-\frac{m |R - R'|^2 + \hbar^2 \Delta \tau v_D(R')^2}{2\Delta \tau \hbar^2}}\) and \(\tilde{G}_b(R, R') = e^{-\Delta \tau [E_L(\hat{R}) + E_L(\hat{R}') - 2E_T]/2}\).

The third and fourth lines in Eq. 4 were obtained using \(e^{-i \frac{\hbar^2 \Delta \tau}{m} \hat{P} \cdot v_D(R)} | R' \rangle \approx e^{-i \frac{\hbar^2 \Delta \tau}{m} \hat{P} \cdot v_D(R')} | R' \rangle + \frac{\hbar^2 \Delta \tau}{m} v_D(R') \rangle\) since both operators acting on \(| R' \rangle\) are equivalent up to first order in \(\Delta \tau\) and the momentum operator is the generator of translations. The expression for \(\tilde{G}_d(R, R')\) can be found by recognizing that it is the same as Eq. 3.20 but with \(R' + \frac{\hbar^2 \Delta \tau}{m} v_D(R') \rangle\) replacing \(R'\).
Appendix B

Derivation of the spin propagator for AFDMC

The spin terms of the AV8 interaction excluding spin-orbit are:

\[ V_{SD} = \sum_{j<k} \left( [v_3(r_{jk}) + v_4(r_{jk})] \sigma_j \cdot \sigma_k + [v_5(r_{jk}) + v_6(r_{jk})]\right) \]

\[ = \frac{1}{2} \sum_{j,k,j \neq k} \left( [v_3(r_{jk}) + v_4(r_{jk})] \sigma_j \cdot \sigma_k + [v_5(r_{jk}) + v_6(r_{jk})]\right) \]

\[ = \frac{1}{2} \sum_{j,k} \left( [v_3(r_{jk}) + v_4(r_{jk})] \sigma_j \cdot \sigma_k + [v_5(r_{jk}) + v_6(r_{jk})]\right) \]

\( \sigma_j \cdot \sigma_k = \sigma_k \cdot \sigma_j \) and \( \hat{r}_{jk} = -\hat{r}_{kj} \). So

\[ V_{SD} = \frac{1}{2} \sum_{j,k} \left( [v_3(r_{jk}) + v_4(r_{jk})] (\sigma_{jz} \sigma_{kz} + \sigma_{jy} \sigma_{ky} + \sigma_{jz} \sigma_{kz}) + [v_5(r_{jk}) + v_6(r_{jk})]\right) \]

\[ = \frac{1}{2} \sum_{j,\alpha,k,\beta,j \neq k} \sigma_{j\alpha} \left( [v_3(r_{jk}) + v_4(r_{jk})]\delta_{\alpha\beta} + [v_5(r_{jk}) + v_6(r_{jk})]\right) \sigma_{k\beta} \]

\[ = \frac{1}{2} \sum_{j,\alpha,k,\beta} \sigma_{j\alpha} A_{j\alpha,k\beta} \sigma_{k\beta} \]

where \( A_{j\alpha,k\beta} = 0 \) when \( j = k \). \( A \) can be treated as a 3Nx3N real symmetric matrix.
It can be diagonalized with real eigenvalues and eigenvectors defined by:

\[
\sum_{k,\beta} A_{j\alpha, k\beta} \psi_n^{k\beta} = \lambda_n \psi_{j\alpha}^n
\]  

(7)

It follows from the properties of real symmetric matrices with distinct eigenvalues that the \( \psi_n \) can be chosen to be orthogonal. Thus \( A \) can be diagonalized as \( D = U^{-1}AU \) where \( D_{jj} = \lambda_j, \ U_{jk} = \psi_j^k, \) and \( U^{-1} = U^T. \) From this we can express \( A_{jk} \) using \( A = UDU^{-1}: \)

\[
A_{jk} = (UDU^{-1})_{jk} = \sum_n \psi_n^j \sum_m \lambda_n \delta_{nm} \psi_m^k
\]

\[
= \sum_n \psi_n^j \lambda_n \psi_n^k
\]  

(8)

Substituting this result into Eq. 6 yields:

\[
V_{SD} = \frac{1}{2} \sum_{j\alpha, k\beta, n} \sigma_{j\alpha} \psi_n^{j\alpha} \lambda_n \psi_n^{k\beta} \sigma_{k\beta} = \frac{1}{2} \sum_n \left( \sum_{j\alpha} \sigma_{j\alpha} \psi_n^{j\alpha} \right)^2 \lambda_n
\]

\[
= \frac{1}{2} \sum_{n=1}^{3N} \lambda_n \hat{O}_n^2, \ \hat{O}_n = \sum_{j\alpha} \sigma_{j\alpha} \psi_n^{j\alpha}
\]  

(9)

**Spin rotations in AFDMC**

The AFDMC propagator in Eq. 3.32 has the effect of rotating the spin state of each particle in the walker configuration. The walkers contain up and down spin amplitudes for each particle. Let \( |k\rangle = a_k |\uparrow\rangle_k + b_k |\downarrow\rangle_k \) denote the spin state for particle \( k. \) The general form of the spin operators in the AF integral is \( e^{\sigma_k \cdot \hat{n}}. \) Now, \( e^{-i\theta \sigma_k \cdot \hat{n}} = (\cos \theta)I - i \sin \theta (\sigma_k \cdot \hat{n}) \) where \( \hat{n} \) has real components. If \( \hat{n} \) has complex amplitudes then the vector in the equation must satisfy \( \sum_{\alpha} n_{\alpha}^2 = 1 \) in order for the equality to be true (as opposed to \( \sum_{\alpha} |n_{\alpha}|^2 = 1 \) which defines a normalized vector).
\( e^{\sigma_k \cdot \hat{n}} = e^{-i(\theta)\sigma_k \cdot \hat{n}} = (\cosh \theta) \mathbf{I} + (\sinh \theta) \sigma_k \cdot \hat{n} \). The rotation on particle k then is:

\[
e^{\sigma_k \cdot \hat{n}} |k\rangle = [(\cosh \theta) \mathbf{I} + (\sinh \theta)(\sigma_{kx} \hat{n}_x + \sigma_{ky} \hat{n}_y + \sigma_{kz} \hat{n}_z)] |k\rangle
\]

and in matrix form:

\[
\begin{align*}
e^{\sigma_k \cdot \hat{n}} |k\rangle &= \begin{pmatrix} \cosh \theta + (\sinh \theta) \hat{n}_z \\ (\sinh \theta)(\hat{n}_x + i\hat{n}_y) \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}
\end{align*}
\]

\[
\begin{pmatrix} \cosh \theta + (\sinh \theta) \hat{n}_x \\ \sinh \theta (\hat{n}_x - i\hat{n}_y) \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}
\]

\[
\begin{pmatrix} \cosh \theta - (\sinh \theta) \hat{n}_z \\ \sinh \theta (\hat{n}_x + i\hat{n}_y) \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}
\]

\[
\begin{pmatrix} \cosh \theta + (\sinh \theta) \hat{n}_z \\ (\sinh \theta)(\hat{n}_x - i\hat{n}_y) \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}
\]

\[
\begin{pmatrix} \cosh \theta - (\sinh \theta) \hat{n}_z \\ \sinh \theta (\hat{n}_x + i\hat{n}_y) \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}
\]

(10)
Appendix C

Turning on a one-body potential

Let $E_0[v]$ and $\Psi(R, [v])$ denote the ground-state energy and wave-function of some original system perturbed by a general one-body potential $v(r)$. We are interested in how the energy behaves as the potential is turned on/strengthened. Consider the perturbation resulting from scaling the potential up from $\lambda' v(r)$ to $\lambda^* v(r)$: $\lambda^*, \lambda' \in \mathbb{R}$, $\lambda^* > \lambda'$. To first order in perturbation-theory we have:

$$E_0[\lambda^* v] - E_0[\lambda' v] = \int dR \Psi^*(R, [\lambda v]) \left[ (\lambda^* - \lambda') \sum_i v(r_i) \right] \Psi(R, [\lambda v])$$

$$= (\lambda^* - \lambda') \sum_i \int dR |\Psi(R, [\lambda v])|^2 v(r_i)$$

$$= (\lambda^* - \lambda') \sum_i \int dr_i \left( \int dr_1 \ldots dr_{i-1} dr_{i+1} \ldots dr_N |\Psi(R, [\lambda v])|^2 \right) v(r_i)$$

$$= (\lambda^* - \lambda') \sum_i \int dr_i \frac{n_0(r_i, [\lambda v])}{N} v(r_i)$$

$$= (\lambda^* - \lambda') \int d\mathbf{n}_0(r, [\lambda v]) v(r)$$

(11)

where we used the one-body density $n_0(r_1, [\lambda v]) = N \int dr_2 \ldots dr_N |\Psi(R, [\lambda v])|^2$ to get from equality 3 to 4. Dividing both sides by $(\lambda^* - \lambda')$ and taking the limit $\lambda^* \to \lambda'$ yields:

$$\lim_{\lambda^* \to \lambda'} \frac{E_0[\lambda^* v] - E_0[\lambda' v]}{(\lambda^* - \lambda')} = \frac{dE_0[\lambda v]}{d\lambda} \bigg|_{\lambda=\lambda'}$$

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\[ = \int drn_0(r, [\lambda v]v(r) \]  

Note that this derivation works for wave-functions containing spin-dependence as well because our external potential contains no spin operators.
Bibliography


