Diffusion Monte Carlo study of strongly interacting two-dimensional Fermi gases

by
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ABSTRACT

DIFFUSION MONTE CARLO STUDY OF STRONGLY INTERACTING TWO-DIMENSIONAL FERMI GASES

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Ultracold atomic Fermi gases have been a popular topic of research, with attention being paid recently to two-dimensional (2D) gases. The interaction strength between spin-up and spin-down particles in two-component Fermi gases can be tuned in experiments, allowing for a strongly interacting regime where the gas properties are yet to be fully understood. We have probed this regime for 2D Fermi gases by performing $T = 0$ \textit{ab initio} diffusion Monte Carlo (DMC) calculations. In order to motivate our work, we first present an overview of 20th century breakthroughs relating to the discovery and understanding of quantum degeneracy and then we review the recent experimental advancements in cold atomic physics. The final topic in our introduction is a superfluid phase of nuclear matter, expected to exist in neutron stars, that can be compared to a Fermi gas of cold atoms. Following this, we describe our methods piece by piece. First we focus on the two-body problem, showing the partial wave expansion and its relation to scattering parameters for both 2D and 3D. After presenting the basics, we discuss our numerical methods for determining the scattering parameters. Solving for these allow us to define the interaction regime and guarantee diluteness of the many-body system. We build up to this many-body problem by first studying the non-interacting system with emphasis on finite size effects. The many-body wave functions we use for our QMC calculations are then introduced.
These contain variational parameters and are encoded with some knowledge of the interactions. Having discussed the problem and our methods, our numerical multi-dimensional integration techniques are explained. We use variational Monte Carlo (VMC) and diffusion Monte Carlo (DMC) to calculate ground state properties of the gas over a range of interaction strengths. We determine the energy per particle, Tan’s contact parameter, the chemical potential, and the pairing gap, all following from variationally optimized many-body wave functions.
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The devil is in the details.

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Chapter 1

Introduction

1.1 Historical overview

In 1925, Einstein predicted a phase transition for a dilute gas of integer-spin particles at very low temperature [1]. Inspired by Bose’s quantum-statistics interpretation of photons [2], he extended the theory to include massive particles and realized the possibility for a macroscopic occupation of the ground state. This occurs below the critical temperature $T_c$, where thermal fluctuations are sufficiently small. In this phase, the boson particles will condense as a large fraction occupy the ground-state momentum level. Relatively soon after the prediction, an intimately related phenomenon was seen. In 1938, $^4$He was cooled to $< 2.2$ K where a superfluid phase emerged [3, 4]. This quantum liquid has very small viscosity that decreases with temperature and, at $T = 0$, would allow a body to move through it without resistance. The first Bose Einstein condensate (BEC) gas was physically realized in 1995 when bosonic $^{87}$Rb atoms were cooled to $< 200$ nK [5].

Fermi gases, which consist of particles with half-odd spin, also undergo phase transitions at low temperatures. However in this case the Pauli exclusion principle leads
to dramatically different physics. In a classical gas, the properties are independent of whether or not the individual particles are fermions or bosons. This is the case because the thermal energy scale is large enough that particles are dispersed over a large number of high energy states and Pauli-exclusion need not be considered. Starting in this classical limit, as temperature is reduced, the particles lose momentum and low energy states become more densely populated. Here, the two fundamental types of matter have vastly different behaviour. In a Fermi gas, as $T \to 0$, the particles occupy low lying momentum states but are unable to condense to the lowest energy state. This is attributed to the Pauli exclusion principle, which states that two indistinguishable fermions cannot exist in the same state. As the lowest energy levels become occupied, they are said to be inaccessible due to Pauli blocking. Attractive pairing mechanisms between opposite momentum particles, called Cooper pairs, are responsible for a superfluid phase in this state. This was first understood in 1957, when Bardeen, Cooper, and Schrieffer developed their famous BCS theory to describe electrons in a superconductor [6]. In this case, the attractive pairing between fermion components (electrons) is brought about indirectly through lattice distortions (i.e., phonon interactions). The BCS theory has since been applied to a wide range of fermion systems. The phenomenon of superconductivity was first seen in 1911 when Hg was cooled to $< 4.2$ K [7]. In this experiment, the electrical resistance of a mercury wire suddenly became very small when cooled below the critical temperature using liquid $^4$He. Many years later, in 1972, Fermi $^3$He atoms were cooled until a superfluid phase emerged [8]. The temperatures required for this observation were $< 2.7$ mK, roughly 2000 times smaller than the $^4$He BEC discovered in 1938.

Many properties of weakly interacting Bose gases are well described by mean field theory; specifically, the Gross-Pitaevskii equation. This explicitly takes each particle
to be in the ground state momentum level (and thereby have the same wave function). The same assumption cannot be made for the Fermi gas, which is generally more difficult to describe (at low temperatures). The mean-field BCS theory for fermions with tunable interactions is expected to yield accurate results when attraction is very strong or very weak. The intermediate regime, where gases are said to be strongly interacting, is not expected to be well described and beyond mean-field methods attempt to solve this problem. Among these are \textit{ab initio} quantum Monte Carlo (QMC) computational techniques, which offer a solution from first principles. These have been developed for over half a century, although the most important advancement has been in computational power. The Monte Carlo technique, built on the concept of Markov chains and the central limit theorem, was created in the 1940’s to address neutron transport in fusion reactions. This numerical method can evaluate multi-dimensional integrals of functions over complicated probability distributions. In the years following its invention, QMC was developed in a large part by quantum chemists in efforts to calculate electron orbital energy levels. It was also adopted by a number of nuclear and condensed matter physicists, interested in quantum gas applications. Some landmark results are the ground-state energy calculations for $^4\text{He}$ in 1965 [9] and $^3\text{He}$ in 1979 [10]. During these and the following years, QMC was applied to a large number of other problems including superconductivity and the description of increasingly complex atoms and molecules.

1.2 Modern developments

Following after the 1995 atomic BEC discovery at the University of Colorado Boulder, the first quantum degenerate atomic Fermi gas was engineered using $^{40}\text{K}$ in
1999 [11]. A few years later the same group, among others, created a BEC superfluid by inducing strong coupling between fermion components such that long lived bound states appeared [12, 13, 14]. These experiments were made possible due to Feshbach resonances, where the interaction between two low lying hyperfine atomic states can be controlled using a magnetic field. Sweeping across a resonance by increasing the magnetic field strength, pairing becomes weaker and the gas transitions from a state of tightly bound bosonic dimers to weakly interacting Cooper pairs; this is the BEC-BCS crossover. Among the first experimental evidence of this crossover was the in situ imaging of vortices across a Feshbach resonance, which was performed at MIT in 2005 [15]. These recent experiments are summarized quite nicely in Refs. [16, 17], which also give comprehensive reviews of 3D Fermi gas theory.

As experimentalists began studying atomic Fermi gases with tunable interactions, it became important to know the expected energy per particle at all coupling strengths. This energy depends on a product of the Fermi momentum $k_F$ (which is related to density, as seen in Section 3.1) and scattering length $a_d$, where $d$ is the dimensionality. In 3D, a very distinct interaction regime where $k_F a_{3D} \to \pm \infty$ became the initial focus. A question was formally posed to the many-body community by G. F. Bertsch in 1999: what are the ground state properties of a zero-range Fermi gas with infinite scattering length? Using QMC, the energy of such a system was first accurately estimated in 2003 as 0.44 times that of the noninteracting gas [18]. This finite-range result has since been improved by extrapolating to the limit of a contact interaction [19, 20]. These studies were carried out in the unitary limit, $k_F a_{3D} \to \pm \infty$, where the gas is dilute but also has very large scattering length. In this regime the gas properties are independent of the specific interaction details, which means that both dilute Fermi atoms with zero effective range and very dilute neutrons with finite
effective range should behave similarly. A QMC study in 2008 compared neutron matter and cold atoms on the BCS side of the crossover, where $k_Fa_{3D} < 0$, and found a trend towards increasingly similar energy per particle and pairing gap when approaching smaller couplings [21]. Meanwhile, some had shifted their attention to lower dimensional quantum gases.

In 2D gases, the onset of a superfluid phase as the temperature is decreased is called the Berezinskii-Kosterlitz-Thouless (BKT) transition. As $T \to T_c$ from above, where $T_c$ is the BKT superfluid critical temperature, we approach the threshold for superfluidity from the normal state. This state is characterized by thermal vortices, responsible for destroying long range order in the gas. At $T = T_c$, in the strong-coupling crossover regime (i.e., the BEC-BCS crossover), the quantized angular momentum of each vortex is small enough to allow bound vortex-antivortex pairs with opposite momentum to form (see Ref. [22]). The ability to confine Fermi gases to 2D was seen about 10 years ago [23] and more successful experiments began to emerge only about 5 years ago [24, 25]. In these more recent studies, the 3D quantum degenerate gas is separated into a series of pancake shaped, quasi-2D gas clouds using a highly anisotropic trapping potential. While these studies were focused on observations of confined gases, even more recent experiments have determined the density distribution [26], pressure [27], equation of state [28], and phase diagram [29]. The quasi-2D nature of these gases makes comparison with theory complicated, and this is further compounded by finite temperature effects.

On the theoretical side, the BCS theory was first applied to 2D Fermi gases in the 1980’s [30, 31]. We discuss these results further in Chapter 4 and compare to our findings. Focusing now on more recent developments: a 2011 QMC study estimated the ground state energy and pairing gap for a range of interaction strengths [32]. This
was the first *ab initio* equation of state (EOS) prediction for the strongly interacting 2D Fermi gas. As well, other QMC methods have been used to tackle this problem, both at zero and at finite temperature [33, 34]. The special appeal of non-perturbative methods is their ability to provide dependable calculations of quantities in the center of the BEC-BCS crossover. In parallel, other many-body approaches have also emerged, leading to equations of state for the ground state of the 2D gas that are qualitatively similar to the QMC values [35, 36]. The recent finite temperature QMC study (Ref. [34], mentioned above) has already been compared to experiment [28], where the EOS was measured for various $T$. Interestingly, the critical temperature is expected to peak in the crossover region [37, 38]. Tan’s contact parameter, a universal quantity in the Fermi gas [39, 40], can be determined for various interaction regimes in the crossover (as done in Section 4.1.4 of this work). Currently the best measurements of the contact parameter in the limit $T \to 0$ were performed in 2012 [41].

1.2.1 The nuclear interaction

The nuclear force is complicated and the interaction details are, in general, very important. In some systems, however, we expect the interaction to be greatly simplified. A dilute gas of neutrons at low temperature has properties that are largely independent of the details of the interaction. For this phase, scattering can be modeled with purely attractive potentials that depend only on radial separation. A superfluid with this description is predicted to exist in the inner crust of neutron stars. For this state of nuclear matter we expect predominantly $s$-wave interactions between opposite spin particles. A duality is expected between this neutron matter and the cold atom experiments described above. In each case, the gas properties depend on the interaction strength (roughly a product of the density and scattering length). Unlike
the two-particle atomic system, neutron-neutron (NN) interactions cannot be tuned microscopically. In other words, the NN scattering length is fixed at $a_{\text{3D}} \approx -18.5$ fm. In this case the interaction strength, and associated gas properties, are determined by the density. In the cold atom experiments the effective range of the interaction is roughly zero and can be treated as a contact interaction, whereas the effective range of the NN interaction is finite and given by $r_e \approx 2.7$ fm.

A neutron star is very hot compared to terrestrial phenomena, however the Fermi momentum of the degenerate gas is very large. This means that the pairing remains largely unaffected by relatively big thermal fluctuations (i.e., by high temperatures). Of course, like cold atoms, pairing will dissipate for excited states where $T$ is larger than $T_c$. The critical temperature of dilute neutron matter is $\sim 10^{10}$ K. In contradistinction, the superfluid transition for cold atoms occurs at $\sim 200$ nK [42]. Despite this, the ratio of $T_c/T_F$, where $T_F$ is the Fermi temperature, is on the same order of magnitude for each system. This is consistent with the above discussion of similar pairing mechanisms between the two types of matter. Typical metallic superconductors (e.g., Hg, as discussed earlier) are said to have conventional pairing. In this case, the ratio of $T_c/T_F$ is many orders of magnitude smaller than dilute Fermi gases. High-temperature superconductors with complex constituents are said to have unconventional pairing [43]. The ratio of $T_c/T_F$ for these materials is roughly between that of conventional superconductors and cold Fermi gases. It is not unreasonable, therefore, to view ultracold atomic Fermi gases as high-temperature superfluids. An atomic Fermi gas with $T_F$ on the order of conventional superconductors would be a superfluid well above room temperature.
Chapter 2

Two-body interactions

The two-body problem is the starting point for our many-body study. Scattering theory has been well studied and documented, especially for 3D systems. It is standard for quantum mechanics textbooks to broach the subject, however the vast majority discuss only the 3D case. We begin with the 3D scattering problem, then concentrate on the scattering physics in 2D and differences between the two theories. We also study the details of our wave function and scattering parameter determination techniques.

2.1 3D Scattering Theory

Describing the interaction of two particles in their center of mass reference frame, the two-body problem is reduced to that of one body with mass $m_r$ in the presence of a potential that represents the interaction. $m_r$ is the reduced mass of the two-body system, and simplifies to $m/2$ if the particles have equal mass. The problem is further simplified by assuming the interaction has no angular dependence. In this case, the potential is spherically symmetric: $V(\mathbf{r}) \rightarrow V(r)$, where $r = |\mathbf{r}| = \sqrt{r_x^2 + r_y^2 + r_z^2}$.
is the separation distance between particles. The time-dependent wave functions for such a system can be written as \( \psi(r, t) = \psi(r)e^{-iEt/\hbar} \), where \( \psi(r) \) is an eigenfunction of the time-independent Schrödinger equation:

\[
-\frac{\hbar^2}{2m_r} \nabla^2 \psi(r, \theta, \phi) + V(r) \psi(r, \theta, \phi) = E \psi(r, \theta, \phi),
\]

(2.1)

and the scattering energy \( E \) is the eigenvalue. Using the separation of variables technique, the wave function is expanded into partial waves:

\[
\psi(r, \theta, \phi) = \sum_{l,m} \alpha_l R_l(r) Y^m_l(\theta, \phi),
\]

(2.2)

where we sum over quantized values of the total angular momentum \( l \) and the magnetic projection \( m \). The partial waves consist of radial functions \( R_l(r) \) that depend only on the particle separation and spherical harmonics \( Y^m_l(\theta, \phi) \) that include the angular dependence of the wave function. The spherical harmonics of interest are those where \( m = 0 \) due to the azimuthal symmetry of our scattering potential. These functions satisfy the property \( Y^0_l(\theta) = \sqrt{(2l+1)/4\pi} P_l(\cos \theta) \), where \( P_l(\cos \theta) \) are Legendre polynomials. Making the partial waves substitution and inserting the 3D spherical coordinate Laplacian, Eq. (2.1) becomes

\[
\left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) \right] \sum_l \alpha'_l R_l(r) P_l(\cos \theta) \\
+ \left[ k^2 - \frac{2m_r}{\hbar^2} V(r) \right] \sum_l \alpha'_l R_l(r) P_l(\cos \theta) = 0,
\]

(2.3)

where \( k^2 = 2m_r E/\hbar^2 \) and \( \alpha'_l = \alpha_l \sqrt{(2l+1)/4\pi} \). This equation must be satisfied for each \( l \) as can be determined by the linear independence of the Legendre polynomials. We remove the summations and solve the equation for each angular momentum.
channel separately:

\[
\left[ P_l(\cos \theta) \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial R_l(r)}{\partial r} \right) + R_l(r) \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial P_l(\cos \theta)}{\partial \theta} \right) \right] a'_l \\
+ \left[ k^2 - \frac{2m_r}{\hbar^2} V(r) \right] a'_l R_l(r) P_l(\cos \theta) = 0.
\]  

(2.4)

It’s clear to see that we can divide out the \(a'_l\) coefficients. The \(\theta\) dependent derivative term can be simplified using the Legendre differential equation:

\[
- l(l+1) P_l(\cos \theta) = \frac{\partial^2 P_l(\cos \theta)}{\partial \theta^2} + \frac{\cos \theta \partial P_l(\cos \theta)}{\sin \theta \partial \theta},
\]

(2.5)

where we have used the chain rule to modify the derivatives from \(\partial / \partial (\cos \theta) \rightarrow \partial / \partial \theta\).

As we will see, this equation allows us to cancel out all \(\theta\) dependence. In the first line below, we have divided Eq. (2.4) by \(R_l(r) P_l(\cos \theta)\) on each side. In line 3, we make the substitution \(R_l(r) \rightarrow u_l(r)/r\) and use Eq. (2.5).

\[
- \left[ k^2 - \frac{2m_r}{\hbar^2} V(r) \right] = \left[ \frac{1}{R_l(r)} \frac{\partial}{\partial r} \left( r^2 \frac{\partial R_l(r)}{\partial r} \right) + \frac{1}{P_l(\cos \theta) r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial P_l(\cos \theta)}{\partial \theta} \right) \right] \\
= \frac{1}{R_l(r)} \left[ \frac{2 \delta R_l(r)}{\partial r} + \frac{\partial^2 R_l(r)}{\partial r^2} \right] + \frac{1}{P_l(\cos \theta) r^2} \left[ \frac{\partial^2 P_l(\cos \theta)}{\partial \theta^2} + \frac{\cos \theta \partial P_l(\cos \theta)}{\sin \theta \partial \theta} \right] \\
= \frac{1}{u_l(r)} \left[ 2 \left( \frac{1}{r} \frac{\partial u_l(r)}{\partial r} - \frac{u_l(r)}{r^2} \right) + r \frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial u_l(r)}{\partial r} - \frac{u_l(r)}{r^2} \right) \right] \\
+ \frac{1}{r^2 P_l(\cos \theta)} \left[ - l(l+1) P_l(\cos \theta) \right] \\
= \frac{1}{u_l(r)} \frac{\partial^2 u_l(r)}{\partial r^2} - \frac{l(l+1)}{r^2}.
\]

(2.6)

After rearranging, we are left with the Schrödinger equation for the reduced radial wave function \(u_l(r)\):

\[
- \frac{\partial^2 u_l(r)}{\partial r^2} = u_l(r) \left[ k^2 - \frac{2m_r}{\hbar^2} V(r) - \frac{l(l+1)}{r^2} \right].
\]

(2.7)
The angular functions \( Y_l^0(\theta) \) have reduced to the \( l(l+1)/r^2 \) term, which is called the centrifugal barrier.

In the asymptotic regime, outside the range of the potential, Eq. (2.7) has a solution that can be written in terms of spherical Bessel functions of the first \((j_l)\) and second \((n_l)\) kind [44]:

\[
 u_l(r) \propto kr[j_l(kr) \cos \delta_l - n_l(kr) \sin \delta_l], \tag{2.8}
\]

where \( \delta_l \) are the phase shifts of \( u_l(r) \) compared to the non-scattered wave functions. For the case of a fully attractive square well potential, phase shifts generally become larger as the depth is increased. With knowledge of \( u_l(r) \) at two radial separations \( r_1 \) and \( r_2 \) outside the range of the potential, we are able to calculate \( \delta_l \) using

\[
 \cot \delta_l = \frac{\tilde{K} n_l(kr_1) - n_l(kr_2)}{\tilde{K} j_l(kr_1) - j_l(kr_2)}, \tag{2.9}
\]

where \( \tilde{K} = r_1 u_l(r_2)/r_2 u_l(r_1) \). The wave function can be found by numerically solving Eq. (2.7), as will be discussed in Section 2.3. The size of \( \delta_l \) is a good measure of the scattering influence for a given \( V(r) \). In other words, \( \delta_l \) represents by how much \( V(r) \) effects \( u_l(r) \) for a given angular momentum channel \( l \). As \( l \to \infty \) the phase shifts \( \delta_l \to 0 \) as is manifest in the centrifugal barrier term of Eq. (2.7), which is dominant for large \( l \) (i.e., \( V(r) \ll \lim_{l \to \infty} l(l+1)/r^2 \)). This means that scattering is less influential for particles whose total angular momentum is very large.

Regardless of the detailed features of \( V(r) \), scattering can be characterized by the scattering length \( a_{3D} \) and effective range \( r_e \). These scattering parameters indicate how \( u_l(r) \) is affected by the potential at low scattering energies. A simple expression can be derived that relates \( u_l(r) \) to the scattering length \( a_{3D} \). We consider Eq. (2.7)
for only low energy scattering, outside the range of $V(r)$. The $l = 0$, s-wave channel is dominant in this limit and we take $k = 0$ to give:

$$\frac{\partial^2 y_0(r)}{\partial r^2} = 0,$$  \hspace{1cm} (2.10)

where $V(r) = 0$ because we are in the asymptotic regime. The reduced radial wave function $u_0(r)$ has been replaced with $y_0(r)$, which represents the asymptotic form. The solution to this equation is a straight line:

$$y_0(r) = \beta (r - a_{3D}),$$  \hspace{1cm} (2.11)

where $\beta$ is a normalization constant. There is one node, a point where $y_0(r) = 0$, at $r = a_{3D}$. This simple definition of the scattering length is, strictly speaking, no longer valid for any finite scattering energy. In the limit as $k \rightarrow 0$, Eq. (2.10) takes the form of the wave equation:

$$\frac{\partial^2 y_0(r)}{\partial r^2} = -y_0(r)k^2|_{k \rightarrow 0}.$$  \hspace{1cm} (2.12)

The general solution can be written as

$$y_0(r) = a_0 \sin(kr) + b_0 \cos(kr)|_{k \rightarrow 0},$$

$$= \beta \sin(kr + \delta_0)|_{k \rightarrow 0},$$  \hspace{1cm} (2.13)

where $a_0$, $b_0$ and $\beta$ are constants and the $l = 0$ phase shift $\delta_0$ has been explicitly included. As will be seen, the choice for $\beta$ in Eq. (2.13) will impact the definition of the effective range. Following convention [45], we define $\beta = 1/\sin \delta_0$ such that
\( y_0(0) = 1 \) and Eq. (2.13) becomes

\[
y_0(r) = \frac{\sin(kr + \delta_0)}{\sin(\delta_0)} \bigg|_{k \to 0}.
\]  

(2.14)

To determine an expression relating the scattering length to \( \delta_0 \), we expand Eq. (2.14) for small values of \( k \):

\[
y_0(r) = \frac{\sin kr \cos \delta_0 + \cos kr \sin \delta_0}{\sin \delta_0} \bigg|_{k \to 0}
\]

\[
= \left[ \frac{\sin kr}{\tan \delta_0} + \cos kr \right]_{k \to 0}
\]

\[
\approx \left[ \frac{kr}{\tan \delta_0} + \left(1 - \frac{(kr)^2}{2}\right)\right]_{k \to 0}
\]

\[
\approx \frac{k}{\tan \delta_0} \left[ r + \tan \delta_0 \frac{k}{r} \right]_{k \to 0}.
\]  

(2.15)

Using the condition \( y_0(a_{3D}) = 0 \), it follows that the \( l = 0 \) phase shift is given by \( k \cot \delta_0 |_{k \to 0} = -1/a_{3D} \). This is the first order \textit{shape-independent} approximation. Including a higher order term, we have [45]:

\[
k \cot \delta_0 |_{k \to 0} = -\frac{1}{a_{3D}} + \frac{r_e k^2}{2},
\]  

(2.16)

where the effective range is defined as:

\[
r_e = 2 \int_0^\infty \left[ y_0^2(r) - u_0^2(r) \right]_{k \to 0} dr.
\]  

(2.17)

Eq. (2.16), which is often called the effective range expansion, shows how low energy scattering can be described by a broad range of potentials. This is because any well selected function can be tuned to reproduce the desired \( a_{3D} \) and \( r_e \). To calculate the
effective range using Eq. (2.17), $u_0(r)$ is re-scaled to match $y_0(r)$ in the asymptotic regime. This is why, as mentioned earlier, the normalization of $y_0(r)$ will impact $r_e$.

### 2.2 2D Scattering Theory

Now that we have discussed scattering physics in 3D, we turn to the 2D case. Equations can still be written in a center of mass reference frame and we use a cylindrically symmetric potential that depends on the particle separation distance $r$. The time-independent Schrödinger equation for such a system is

\[- \frac{\hbar^2}{2m_r} \nabla^2 \psi(r, \theta) + V(r) \psi(r, \theta) = E \psi(r, \theta) \, . \tag{2.18}\]

The azimuthal angle $\phi$, which ranges from 0 to $\pi$ in 3D, has no meaning in 2D. Inserting the Laplacian for 2D polar coordinates, we can rewrite Eq. (2.18) as

\[\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \psi(r, \theta)}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 \psi(r, \theta)}{\partial \theta^2} + k^2 \psi(r, \theta) - \frac{2m_r}{\hbar^2} V(r) \psi(r, \theta) = 0 \, , \tag{2.19}\]

where $k^2 = 2m_r E/\hbar^2$. Now we perform a partial wave expansion, separating the wave function into a sum over the total angular momentum $l$ of radial and angular products:

\[\psi(r, \theta) = \sum_{l=0}^{\infty} a_l R_l(r) T_l(\theta) \, . \tag{2.20}\]

After this substitution and some simple rearranging, we find that the following equation must be satisfied for all $l$:

\[- \left[ k^2 - \frac{2m_r}{\hbar^2} V(r) \right] = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial R_l(r)}{\partial r} \right) + \frac{1}{r^2} \left( \frac{1}{T_l(\theta)} \right) \frac{\partial^2 T_l(\theta)}{\partial \theta^2} \, , \tag{2.21}\]
where we have removed the summation over partial waves, as was done in 3D. This can be rewritten as

\[ f(r) + g(\theta) = 0, \quad (2.22) \]

where \( f \) depends only on \( r \) and \( g \) includes all the angular dependence. If we imagine keeping \( r \) fixed, then \( g(\theta) = (1/T_l(\theta)) \partial^2 T_l(\theta)/\partial \theta^2 \) must be the same for all values of \( \theta \) if Eq. (2.22) is to be consistent. The angular functions \( T_l(\theta) \), therefore, must satisfy the wave equation:

\[ \frac{\partial^2 T_l(\theta)}{\partial \theta^2} = -c_l T_l(\theta), \quad (2.23) \]

where \( c_l \) is some constant depending on \( l \). The general solution can be written as

\[ T_l(\theta) = a_l \sin(\sqrt{c_l} \theta) + b_l \cos(\sqrt{c_l} \theta). \quad (2.24) \]

Considering, for example, an incident beam at \( \theta = 0 \), we assume symmetric scattering and can thereby eliminate the odd \( \sin \) function dependence. Then, with the simple periodic condition \( T_l(0) = T_l(2\pi) \), we can determine that \( \sqrt{c_l} \) must be an integer \( l \) and Eq. (2.23) can be rewritten as [46]:

\[ \frac{\partial^2 T_l(\theta)}{\partial \theta^2} = -l^2 T_l(\theta), \quad (2.25) \]

with the normalized solution

\[ T_l(\theta) = \frac{1}{\sqrt{\pi}} \cos(l\theta). \quad (2.26) \]

Like the Legendre polynomials used for the 3D wave function, these functions are linearly independent and therefore we were justified in removing the summation for
Eq. (2.21). Using Eq. (2.25) to simplify the angular term and making the substitution
\( R_l(r) \rightarrow u_l(r)/\sqrt{r} \) to simplify the radial term, Eq. (2.21) becomes

\[
- \left[ k^2 - \frac{2m_r V(r)}{\hbar^2} - \frac{l^2}{r^2} \right] = \left( \frac{1}{u_l(r)\sqrt{r}} \right) \frac{\partial}{\partial r} \left[ u_l(r) \sqrt{r} \left( \frac{\partial u_l(r)}{\partial r} - \frac{u_l(r)}{2r} \right) \right] 
\]

(2.27)

Rearranging, we find the Schrödinger equation for the 2D reduced radial wave function

\[ u_l(r) : \]

\[
- \frac{\partial^2 u_l(r)}{\partial r^2} = u_l(r) \left[ k^2 - \frac{2m_r V(r)}{\hbar^2} - \frac{l^2 - 1/4}{r^2} \right], \tag{2.28}
\]

which can be compared to Eq. (2.7) for 3D scattering. Differing from the 3D case, the solution to the 2D equation is related to the radial wave function by \( u_l(r) = \sqrt{r} R_l(r) \) instead of \( u_l(r) = r R_l(r) \).

For purely s-wave scattering we consider only the \( l = 0 \) partial wave:

\[
- \frac{\partial^2 u_0(r)}{\partial r^2} = u_0(r) \left[ k^2 - \frac{2m_r V(r)}{\hbar^2} + \frac{1}{4r^2} \right]. \tag{2.29}
\]

The wave function \( u_0(r) \) can be solved for numerically, although analytic solutions exist for simple potentials such as the square well. The singularity at \( r = 0 \) in Eq. (2.29) means that boundary conditions must be carefully selected, as discussed in detail in Section 2.7. In the asymptotic region, when the radial separation is larger than the range of the potential, Eq. (2.29) simplifies to

\[
\frac{\partial^2 u_0(r)}{\partial r^2} + u_0(r) \left[ k^2 + \frac{1}{4r^2} \right] = 0. \tag{2.30}
\]
A solution for $u_0(r)$ can be written in terms of Bessel functions of the first ($J_n$) and second ($N_n$) kind [47]:

$$u_0(r) \propto \sqrt{r} [J_0(kr) \cos \delta_0 - N_0(kr) \sin \delta_0], \quad (2.31)$$

which can be compared to Eq. (2.8) where spherical Bessel functions are used. By calculating $u_0(r)$ at two radial separations $r_1$ and $r_2$ beyond the range of the potential, the s-wave phase shifts $\delta_0$ can be calculated with the relation

$$\cot \delta_0 = \frac{\tilde{K} N_0(kr_1) - N_0(kr_2)}{\tilde{K} J_0(kr_1) - J_0(kr_2)}, \quad (2.32)$$

where $\tilde{K} = u_0(r_2)\sqrt{r_1}/u_0(r_1)\sqrt{r_2}$.

Now we consider Eq. (2.29) when $k = 0$:

$$\frac{\partial^2 y_0(r)}{\partial r^2} = -\frac{1}{4r^2} y_0(r), \quad (2.33)$$

where $y_0(r)$ represents the asymptotic form of $u_0(r)$. This is the zero-energy Schrödinger equation in the asymptotic region. In general, we can write the solution $y_0(r) = \sqrt{r} (\alpha + \beta \log(r))$ [47]. In this and all other instances we take log to represent the natural logarithm. The 2D scattering length $a_{2D}$, in analogy to the 3D interpretation, is defined as the $r$-intercept of $y_0(r)$. For sufficiently short range potentials, such as those used in Section 2.6, $a_{2D}$ can also be given by the $r$-intercept of $u_0(r)$ for even strongly bound states. Using the condition $y_0(a_{2D}) = 0$, where $a_{2D}$ is the 2D scattering length, we set $\alpha = -\beta \log(a_{2D})$ and the solution becomes $y_0(r) = \beta \sqrt{r} \log(r/a_{2D})$. 

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The choice for $\beta$ will influence the effective range; we set $\beta = -1$ and use the solution
\[
y_0(r) = -\sqrt{r} \log(r/a_{2D}). \tag{2.34}
\]

The $\beta$ parameter was also encountered for the 3D case, seen in Eq. (2.13), where it was determined by setting $y_0(0) = 1$. Ideally, we would use this condition for 2D scattering as well, however $y_0(r)$ in 2D does not extrapolate to $r < 0$ and always approaches 0 at the origin. This is related to the fact that $a_{2D}$, unlike the 3D scattering length, can never be negative. In other words, a 2-particle bound state exists for even arbitrarily weak attraction. Our choice of $\beta = -1$ for the 2D case is consistent with work done in Ref. [48]. Specifically, we have solved the scattering problem for a square well, using Eq. (2.34) to re-scale our numerical solution for $u_0(r)$, and found scattering parameter results that agree with the analytical expressions (which are shown later in this chapter, Eq. (2.50) and Eq. (2.51)).

As previously discussed, the effective range is related to the area between $u_0(r)$ and $y_0(r)$. In 2D this is defined by the integral [48]:
\[
r_e^2 = 4 \int_0^\infty \left[ y_0^2(r) - u_0^2(r) \right]_{k \to 0} dr, \tag{2.35}
\]
and is the second-order term in the effective-range expansion relating low-energy phase shifts $\delta_0$ to the scattering parameters $a_{2D}$ and $r_e$. In 2D for small values of $k$ [47]:
\[
\cot \delta_0 |_{k \to 0} \approx \frac{2}{\pi} \left[ \gamma + \log \left( \frac{ka_{2D}}{2} \right) \right] + \frac{k^2 r_e^2}{4}, \tag{2.36}
\]
where $\gamma \approx 0.577215$ is Euler’s constant. Although differing from the 3D result,
Eq. (2.16), this relationship has the same implication; low energy scattering is independent of the details of the potential. The logarithmic scattering-length dependence in Eq. (2.36) is characteristic of 2D interactions and also appears in the asymptotic solution $y_0(r)$, Eq. (2.34), which describes the kinetic energy alone.

2.3 Runge-Kutta: numerical solutions for $u(r)$

The 3D and 2D wave functions can be determined numerically by solving their respective differential equations, Eq. (2.7) and Eq. (2.28). In this work, we use the Runge-Kutta method which can evaluate differential equations of the form:

$$u''(r) = b(r)u(r),$$

(2.37)

where $u''(r) \equiv \partial^2 u(r)/\partial r^2$ and $b(r)$ can take many forms. For our case, in three dimensions we have:

$$b(r) = -\left[k^2 - \frac{2m_r V(r)}{\hbar^2} - \frac{l(l + 1)}{r^2}\right],$$

(2.38)

and in two dimensions:

$$b(r) = -\left[k^2 - \frac{2m_r V(r)}{\hbar^2} - \frac{l^2 - 1/4}{r^2}\right].$$

(2.39)

Building up to this problem, we first describe the Runge-Kutta method for the first order initial value problem:

$$\frac{\partial f}{\partial r} = F(r, f), \quad f(r_0) = f_0.$$
where \( f(r) \) is a continuous function. It is determined in discrete steps of size \( \delta r \) by computing weighted averages of \( F(r, f) \) at different points along the intervals \( r_n \leq r \leq r_{n+1} \). For example, the first step would have \( r_n = r_0 \) and \( r_{n+1} = r_0 + \delta r \).

The method, written below, is accurate up to \( O(\delta r^4) \) when iterating over a finite interval of \( r \) [49]:

\[
\begin{align*}
  f_{n+1} &= f_n + \frac{\delta r}{6}(k_1 + 2k_2 + 2k_3 + k_4), \\
  k_1 &= F(r_n, f_n), \\
  k_2 &= F(r_n + \frac{\delta r}{2}, f_n + \frac{\delta r}{2}k_1), \\
  k_3 &= F(r_n + \frac{\delta r}{2}, f_n + \frac{\delta r}{2}k_2), \\
  k_4 &= F(r_n + \delta r, f_n + \delta rk_3).
\end{align*}
\]

To solve Eq. (2.37), it is necessary to evaluate \( u(r) \) and \( u'(r) \) simultaneously by solving the coupled system of 1st order differential equations given by:

\[
\begin{align*}
  \frac{\partial u'(r)}{\partial r} &= b(r)u(r) \equiv F(r, u), \quad u'(r_0) = u'_0, \\
  \frac{\partial u(r)}{\partial r} &= u'(r) \equiv \tilde{F}(u'), \quad u(r_0) = u_0.
\end{align*}
\]

Notice that when solving for \( u'(r) \), \( F \) is a function of \( u \). Conversely, when solving for \( u(r) \), \( \tilde{F} \) is a function of \( u' \). The solutions are written as:

\[
\begin{align*}
  u'_{n+1} &= u'_n + \frac{\delta r}{6}(k_{1a} + 2k_{2a} + 2k_{3a} + k_{4a}), \\
  u_{n+1} &= u_n + \frac{\delta r}{6}(k_{1b} + 2k_{2b} + 2k_{3b} + k_{4b}).
\end{align*}
\]

Noting that, e.g., \( \tilde{F}(u' + \frac{\delta r}{2}k_{1a}) = u' + \frac{\delta r}{2}k_{1a} \), the \( k \)'s are written explicitly as:

\[
\begin{align*}
  k_{1b} &= u'_n, \\
  k_{2b} &= u'_n + \frac{\delta r}{2}k_{1a}, \\
  k_{3b} &= u'_n + \frac{\delta r}{2}k_{2a}, \\
  k_{4b} &= u'_n + \delta rk_{3a}, \\
  k_{1a} &= F(r_n, u_n) = b(r_n)u_n,
\end{align*}
\]
\[k_{2a} = F(r_n + \frac{\delta r}{2}, u_n + \frac{\delta r}{2}k_1 b) = b(r_n + \frac{\delta r}{2})[u_n + \frac{\delta r}{2}k_1 b],\]
\[k_{3a} = F(r_n + \frac{\delta r}{2}, u_n + \frac{\delta r}{2}k_2 b) = b(r_n + \frac{\delta r}{2})[u_n + \frac{\delta r}{2}k_2 b],\]
\[k_{4a} = F(r_n + \delta r, u_n + \delta r k_3 b) = b(r_n + \delta r)[u_n + \delta r k_3 b].\]

The initial conditions in 3D are:

\[u(0) = 0 \quad \text{and} \quad u'(0) = 1. \quad (2.42)\]

These are justified as follows. The radial wave function \(R(r)\) is generally not zero at the origin, and \(R(r) = u(r)/r\). So, as \(r \to 0\) we expect that \(u(r) \to 0\) as well. For the second term we set \(\partial u(r)/\partial r \bigg|_{r=0} = 1\); the scale of \(u(r)\) will be affected by this choice, however the final wave function solution is independent as our numerical result is re-scaled to match the asymptotic form.

The 2D function for \(b(r)\), Eq. (2.39), is singular at \(r = 0\). This causes problems when identifying the correct initial conditions in Eq. (2.40) because \(r_0\) cannot be set equal to zero. We select points close to the origin, but at sufficiently large \(r\) (as quantified in Section 2.7), and use the initial conditions

\[u_0(r_0) = \sqrt{r_0} \quad \text{and} \quad u'_0(r_0) = 1/(2\sqrt{r_0}), \quad (2.43)\]

which are modeled after the small \(r\) behaviour of \(y_0(r)\) in Eq. (2.34) and \(\partial y_0(r)/\partial r\).

The logarithm term \(\log(r/a_{2D})\) is not included because it causes solutions to be ill-behaved. Instead, we retain only the square root dependence and remove the negative sign because the logarithm term is less than 0 for sufficiently small \(r_0\).
2.3.1 Scattering parameter \((a_{2D} \text{ and } r_e)\) determination

After we solve for \(u_0(r)\) numerically, we determine the asymptotic form, \(y_0(r)\), by extrapolating from two points, \(r_1\) and \(r_2\), outside the range of the potential. We consider two generalizations of Eq. (2.34), and use the fact that \(u_0(r) = y_0(r)\) for both \(r_1\) and \(r_2\) to write

\[
    u_0(r_1) = \xi \sqrt{r_1} \log(r_1 / a_{2D}) \quad \text{and} \quad u_0(r_2) = \xi \sqrt{r_2} \log(r_2 / a_{2D}),
\]

where \(\xi\) has been introduced (in place of \(\beta\)) for the purposes of determining \(a_{2D}\) by extrapolation. This is done using the following equations, which we find by working from Eq. (2.44):

\[
    a_{2D} = r_1 \exp \left[ \frac{u_0(r_1)}{\xi \sqrt{r_1}} \right] , \quad \text{where} \quad \xi = \frac{\sqrt{r_1} u_0(r_2) - \sqrt{r_2} u_0(r_1)}{\sqrt{r_1 r_2} \log(r_2 / r_1)}. \quad (2.45)
\]

This scattering length is then used to determine \(y_0(r)\) as given in Eq. (2.34), which is then in turn used to scale \(u_0(r)\) such that \(u_0(r) = y_0(r)\) at \(r_1\) and \(r_2\). Examples of the wave functions can be seen in Figs. 2.3, 2.4, and 2.5. These figures will be discussed in detail in Section 2.5. The effective range \(r_e\) can then be determined by solving Eq. (2.35), which depends on the difference between \(y_0^2(r)\) and \(u_0^2(r)\).

In order to find the correct asymptotic form \(y_0(r)\), it’s important to solve \(u_0(r)\) up to sufficiently large \(r\), outside the range of the potential. Another technical detail has to do with the scattering energy \(E = \hbar^2 k^2 / 2m_r\). The parameters \(a_{2D}\) and \(r_e\) are defined in the limit of \(E \to 0\). To make sure that finite-energy scattering effects are not influencing our determination of the parameters, we reduce \(E\) until the results for \(a_{2D}\) and \(r_e\) have converged.
2.4 Modified Pöschl-Teller potential

The shape-independent approximations, Eq. (2.16) and Eq. (2.36), tell us that many different looking potentials are capable of describing the same scattering event equivalently. A simple square well potential is often used because it is easy to work with and allows for analytical solutions to the Schrödinger equation. In this work, for QMC calculations and the examples in this chapter, we use the modified Pöschl-Teller potential:

\[
V(r) = -v_0 \frac{\hbar^2 \mu^2}{m_r \cosh^2(\mu r)},
\]

which is purely attractive and continuous. The parameters \(v_0\) and \(\mu\) roughly correspond to the depth and inverse width respectively and are tuned such that \(V(r)\) reproduces the desired scattering parameters \(a_{2D}\) and \(r_e\). We are only interested in scattering between equal mass particles \((m_1 = m_2 = m)\), therefore the reduced mass for a scattering event is given by \(m_r = \frac{1}{m_1} + \frac{1}{m_2} = m/2\).

Both the modified Pöschl-Teller potential and square well are interpretations of a realistic s-wave interaction (which would require a repulsive core), and provide a similar and accurate description of the many body system. Although we only study the 2-body interaction in this chapter, we have tested this claim using quantum Monte Carlo as introduced in Section 3.3. Our energy results for the Slater wave function using the modified Pöschl-Teller potential (see Section 3.2.1) matched closely with Ref. [32] where a square-well potential was used. We tested the square-well potential and found a large decrease in statistical accuracy compared to the equivalent calculation using the modified Pöschl-Teller form, Eq. (2.46).

The scattering parameters are generally a complicated function of \(v_0\) and \(\mu\). In the 3D unitary regime for the strongly interacting Fermi gas, \(v_0\) is set equal to 1 such that
$$a_{3D} = \pm \infty.$$ In this case, we have a simple relationship between $\mu$ and the effective range: $\mu = 2/r_e$. In 2D, there is no unitary regime where scattering length diverges to $\pm \infty$, therefore no such relationship for $\mu$ exists. We tune $v_0$ and $\mu$ manually until $V(r)$ reproduces the desired $a_{2D}$ and $r_e$.

As an example, we have calculated phase shifts for 3D neutron-neutron scattering at low energies by tuning our fully attractive potential to reproduce the scattering length and effective range of the interaction:

$$a_{3D} \approx -18.5 \text{ fm}, \quad r_e \approx 2.7 \text{ fm}. \quad (2.47)$$

We plot the $l = 0$, $l = 1$, and $l = 2$ phase shifts for small scattering energy $E$ in Fig. 2.1. To produce this figure, we determine the phase shifts using Eq. (2.9). This requires numerical solutions for the reduced radial wave functions $u_l(r)$, as described in Section 2.3. As $E \to 0$ we expect s-wave interactions where the total angular momentum is 0 to be dominant. In this limit, as can be seen, phase shifts for channels with $l > 0$ are highly suppressed. This serves to show that low energy interactions can be well described by considering only the s-wave scattering problem.

### 2.5 Bound states in 2D

By plotting the scattering length as a function of the potential depth, we can visualize the formation of bound states. In this respect, a difference exists between the 2D and 3D scattering theories. As the depth of $V(r)$ is increased, the scattering length $a_{2D}$ approaches 0 then diverges to $+\infty$ when a new bound state is created; whereas $a_{3D}$ changes from $-\infty$ to $+\infty$ when a new bound state is formed. In both cases, scattering length of $+\infty$ corresponds to a weakly bound state that becomes
Figure 2.1: The phase shifts for low energy neutron-neutron scattering in 3D, as determined by solving Eq. (2.9). We use the modified Pöschl-Teller potential and tune its parameters $v_0$ and $\mu$ to model the interaction. As can be seen, the p-wave and d-wave channels are highly suppressed at low energies.
tighter as scattering length decreases. The particle pair in 2D has binding energy given by

\[ \epsilon_b = -\frac{4\hbar^2}{ma_{2D}^2e^{2\gamma}}. \]  

This compares to the 3D case where, for equal mass particles, the binding energy of the two particle state is \( \epsilon_{b,3D} = -\hbar^2/(ma_{3D}^2) \). We note that an alternate definition of \( a_{2D} \) is sometimes used in other work: \( a'_{2D} = a_{2D}e^{\gamma}/2 \), such that \( \epsilon_b = -\hbar^2/(ma'_{2D}^2) \).

For fixed values of \( \mu \), the scattering length and effective range are periodic in \( v_0 \). This is illustrated in Fig. 2.2, where we have set \( \mu/k_F = 100 \). Here we have introduced the Fermi wave vector \( k_F \) that has units of inverse length (as does \( \mu \)) and is related to the 2D number density \( n \) by \( k_F = \sqrt{2\pi n} \). When \( a_{2D} \) diverges to \( +\infty \), a new (and initially, arbitrarily weak) bound state is created. In other words, at these values of \( v_0 \), the potential becomes deep enough to support an additional bound state. Near these locations, in this example, we see the effective range become very large. The \( v_0 \) values where \( a_{2D} \to \infty \) depend on the specific \( \mu \) value selected. In the case of an attractive square well potential, the effective range integral in Eq. (2.35) will give a negative number for very strongly bound states, causing the effective range to be imaginary. If plotting scattering parameters for the square well in the same style as Fig. (2.2), we would see a very similar plot. A major distinction is that \( r_e \) would continue decreasing to zero and then become imaginary as \( v_0 \) is increased. Instead of gradually increasing as we approach a new bound state, \( r_e^2 \) becomes increasingly large and negative before diverging to a large positive value after the bound state threshold is surpassed.

Starting in the region where only one bound state can exist (plotted in the inset of Fig. 2.2), we will look at the wave function evolution as the depth of \( V(r) \) is increased. In the top panel of Fig. 2.3, we show the reduced radial wave function...
$u_0(r)$ (solid line) and the asymptotic form $y_0(r)$ (dashed line), as defined by Eq. (2.30) in the limit as $k \to 0$ and Eq. (2.33) respectively. These wave functions are plotted for $v_0 = 0.1, 0.2,$ and $0.4$, with the corresponding potentials shown in the bottom panel. We have expressed $V(r)$ in units of the Fermi energy $\epsilon_F = \hbar^2 k_F^2 / 2m$ and set $\mu/k_F = 100$. The 3 states in this figure are weakly bound and have large scattering lengths which are identified as the points where $y_0(r)$ would become zero. These values are determined by extrapolating $u_0(r)$ as described in Section 2.3.1. In this example, the asymptotic zone is reached far before the wave functions cross the $r$-axis and therefore $u_0(a_{2D}) = y_0(a_{2D}) = 0$.

As $v_0$ is increased further, the non-zero node of $y_0(r)$ becomes increasingly central (i.e., $a_{2D} \to 0$). As depicted in Fig. 2.4, we find that $y_0(r)$ and $u_0(r)$ cross the $r$-axis at dramatically different locations for very strongly bound states and look far more distinct than at smaller $v_0$. In the bottom panel, we plot the effective range integrand in Eq. (2.35). Here the dotted line simply marks the $r$-axis. Curves correspond to wave functions plotted in the top panel, which can be distinguished by line thickness. For $v_0 = 1.2$, the integrand is almost completely positive and peaks where the difference between $u_0(r)$ and $v_0(r)$ is maximum. As $v_0$ is increased, the features become more pronounced and we find large negative contributions to the effective range integral. For this example we find the positive contributions are dominant for any $v_0$. As discussed above, this is not generally true (e.g., for the square well potential where $r_e$ becomes imaginary).

When a new bound state is formed, the scattering length diverges discontinuously to $+\infty$ and an extra node exists. In Fig. 2.5, we show the wave function behaviour past this threshold, where the potential supports two bound states. We plot $V(r)/\epsilon_F$ in the bottom panel as was done in Fig. 2.3. In this figure, however, the scale has
Figure 2.2: The 2D scattering length plotted as a function of the depth parameter for the potential, \( v_0 \). We use the modified Pöschl-Teller potential, Eq. (2.46), and set \( \mu/k_F = 100 \). New bound states are formed when the scattering length diverges to \( +\infty \) at specific values of \( v_0 \). The effective range is shown with a dotted line (red), and becomes large near the locations of new bound states. In the inset we show (in more detail) the regime where only one bound state is supported, which is \( 0 \leq v_0 \lesssim 3.6 \) for this choice of \( \mu \).
Figure 2.3: Reduced radial wave functions $u_0(r)$ and corresponding asymptotic solutions $y_0(r)$ are plotted with solid (black) and dashed (red) lines, respectively. The line thickness indicates which $v_0$ value is used in the potential, Eq. (2.46), and we set $\mu/k_F = 100$. 
Figure 2.4: Reduced radial wave functions $u_0(r)$ and $v_0(r)$ are plotted in the top panel with solid (black) and dotted (red) lines. As the depth of the potential becomes larger, approaching the regime of a second bound state, the scattering length tends towards zero and increasingly significant differences between corresponding wave functions are seen. In the bottom panel we plot the integrand in Eq. (2.35), where the effective range is proportional to the square root of the area under each curve. The width parameter is fixed at $\mu/k_F = 100$. 

\begin{align*}
v_0 &= 1.20 \\
v_0 &= 2.45 \\
v_0 &= 3.00
\end{align*}
Figure 2.5: Reduced radial wave functions are plotted in the region where two bound states can exist. Following the style of Fig. 2.3, $u_0(r)$ is plotted with a solid line (black) and $y_0(r)$ is plotted with dashed line (red). Line thickness represents the value of $v_0$ for the modified Pöschl-Teller potential (plotted in the bottom panel) and the width parameter is fixed at $\mu/k_F = 100$. The extra node at $k_F r \sim 0.01$ indicates the existence of an additional bound state and is unrelated to the scattering length.
increased by an order of magnitude. The scattering length of each state is roughly the same as $a_{2D}$ for the equivalent state in Fig. 2.3.

Unlike the 3D case, as illustrated in this section, purely attractive potentials in 2D support bound states for any strength. Qualitatively, by confining particles to scatter in a plane, it becomes impossible for bodies with pairwise attractive interactions to escape each other. This is related to the $1/r^2$ dependence in Eq. (2.28) that persists even for purely s-wave scattering, as seen by Eq. (2.29) where there is no $-l^2/r^2$ centrifugal barrier. At small $r$ this term becomes large and dramatically affects wave function solutions, despite having an increasingly small contribution as $r \to \infty$. On the other hand, in 3D the reduced radial wave function is defined as $u_0(r) = rR_0(r)$ and the Schrödinger equation has no $1/r^2$ dependence for s-wave scattering. As an aside, the fact that in 2D a bound state always forms regardless of the strength of the attractive interaction brings to mind the Cooper-pair problem, though the latter is a many-body (i.e., beyond two-body) effect.

2.6 The BEC-BCS crossover in 2D

We study Fermi gases in the strongly interacting crossover, where the coupling of opposite spin particles is intermediate; in between the limits of a tightly paired BEC and weakly paired BCS gas. Calculations are done for a range of interaction strengths, defined as

$$\eta = \log(k_F a_{2D}),$$ \hspace{1cm} (2.49)

in order to determine the gas properties for a large fraction of the crossover. The number density of the many-body system is fixed such that $k_F$ is constant, and we vary $a_{2D}$ instead. The diluteness requirement is satisfied by taking $r_e \ll r_0$ where
$r_0 = 1/\sqrt{\pi n}$ is the mean interparticle spacing and we maintain a constant effective range of $k_F r_e = 0.006$ \[50\] by adjusting $\mu$ as $v_0$ is varied. The resulting dependence of interaction strength on $v_0$ is shown in the top panel of Fig. 2.6. We are interested in values of $v_0$ where only one bound state is supported. Corresponding binding energies are plotted in the bottom panel for a fixed value of $\mu/k_F \approx 900$. As $|\epsilon_b|$ becomes increasingly small (on the left side of this figure), the BCS limit is approached; the large $|\epsilon_b|$ limit corresponds to a BEC gas of composite fermion pairs.

Figure 2.7 displays the wave function $u_0(r)$ plotted for various interaction strengths; the logarithmic behaviour of the asymptotic form, Eq. (2.34), is illustrated. Differences near the origin between $u_0(r)$ and $y_0(r)$ are indistinguishable on the main plot because we tune $V(r)$ to be extremely short range. These differences are shown in the inset where the integrand in Eq. (2.35) is plotted for a couple interactions strengths. We are maintaining constant $r_e$, therefore the areas under each curve are equal.

Finally, we note the general differences between the BEC-BCS crossover in 2D and 3D. The scattering length is positive in 2D for any interaction strength $\eta$. Because of this, the identification of the crossover point is more \textit{ad hoc}. It’s been suggested that a natural choice is at the interaction strength where chemical potential changes sign (see the dotted line in Fig. 4.7). On either side we approach different limiting behaviours. The BCS limit corresponds to $k_F a_{2D} \gg 1$ and the BEC limit to $k_F a_{2D} \ll 1$. In 3D, a bound state does not exist for arbitrarily weak interaction, so the scattering length can be negative. For the strongly interacting 3D gas, where the interaction strength is $\eta_{3D} = k_F a_{3D}$, the crossover occurs at the unitary point when $\eta_{3D} \to \pm \infty$. If plotted in the same style as the top panel of Fig. 2.6, this would correspond to a divergence of the interaction strength at some potential depth $v_0$. To the left, on the BCS side of the crossover, the scattering length would be negative and, in the weakly paired
Figure 2.6: The relationship between interaction strength $\eta = \log(k_F a_{2D})$ and $v_0$ of the modified Pöschl-Teller potential $V(r)$ is shown in the top panel. The solid line marks the result where the effective range is maintained constant at $k_F r_e = 0.006$. This is achieved by tuning $\mu$ and $v_0$ in unison. For illustration purposes, we include dashed lines to mark a couple results at fixed values of $\mu$. These are shown for $\mu/k_F = 1075.1$ (turquoise) and $\mu/k_F = 760.5$ (red), which cross the solid line at $\eta = 4$ and $\eta = -1$ respectively. The absolute value of the corresponding binding energy per particle $\epsilon_b/2$ is plotted in the bottom panel. A dramatic increase in $|\epsilon_b|$ is seen as paired particles form increasingly stronger bound states.
Figure 2.7: Wave function solutions to Eq. (2.29) in the limit of zero scattering energy ($k^2 \rightarrow 0$) for the modified Pöschl-Teller potential. Parameters $\mu$ and $v_0$ in $V(r)$ are varied to describe a range of interaction strengths $\eta = \log(k_F a_{2D})$, labeled by line thickness. The scattering length is defined as the point where the wave function crosses the $r$-axis, which is marked with a dashed line. The inset shows the effective range integrand in Eq. (2.35) for two interaction strengths, $\eta = -1$ (thick line) and $\eta = 3$ (thin line).
limit, $n_{3D} \to 0$ from below. On the BEC side of the crossover, a bound state exists and scattering length is positive. This regime would exist to the right of the unitary point and, in the strongly paired limit, $n_{3D} \to 0$ from above.

2.7 Singularity in the 2D Schrödinger equation

As discussed at the end of Section 2.3, the 2D Schrödinger equation, Eq. (2.28), has a singularity at the origin. Specifically, when $r = 0$ the $(-l^2 + 1/4)/r^2$ term is infinite. This means we cannot use the boundary conditions for the 3D reduced radial wave function, shown in Eq. (2.42). To choose an appropriate boundary condition, a new parameter $r_0$ is introduced. It has units of length and corresponds to the starting value for the numerical solution. As seen in Eq. (2.43), the values of $u_0(r_0)$ and $\partial u_0(r_0)/\partial r$ are approximated using the asymptotic functional form, Eq. (2.34).

The exact choice for $r_0$ is difficult to determine, and depends on the step size of the numerical solution $\delta r$. By increasing $r_0$ from very small values, convergence of $u_0(r)$ can be seen qualitatively by simply plotting the wave functions, but it is difficult to identify the exact value of $r_0$ for which the solution is optimal. An effective method is to increase $r_0$ (starting at $r_0 = \delta r$) until the scattering length and effective range converge. In this section, we illustrate this convergence for various $\delta r$. We use the interaction strength $\eta = 4$ as an example, which corresponds to the scattering length $a_{2D} = e^4/k_F$ and describes interactions on the deep BCS side of the strongly interacting crossover. This scattering length is one of the largest studied in this work and, as such, is relatively difficult to precisely determine using the method in Section 2.3.1.

First we discuss the effective range, plotted in Fig. 2.8 as a function of the starting
point $r_0$ divided by $\delta r$. The range has been tuned to be very small, which is necessary for describing dilute gases. In the top panel we show the results for an attractive square well potential of the form

$$V_{\text{SW}}(r) = \begin{cases} 
-h^2 v_0/m, & r < R; \\
0, & r \geq R,
\end{cases}$$

where $R = 0.0025/k_F$. The depth $v_0$ (which is $> 0$) has been adjusted such that $a_{2D} = e^A/k_F$ by using the analytic formula [48]:

$$a_{2D} = R \exp \left[ \frac{J_0(x)}{xJ_1(x)} \right],$$

(2.50)

where $J_0(x)$ and $J_1(x)$ are Bessel functions and $x = R\sqrt{v_0}$. For the effective range, we have:

$$r_e^2 = R^2 + 2R^2 \left[ \frac{J_0(x)}{xJ_1(x)} \right] - \frac{2}{v_0}.$$  

(2.51)

We find good agreement with the analytic expression, shown with a solid line (blue), when $r_0/\delta r \approx 10$. However, as the starting point is increased the effective range is underestimated. By decreasing the step size to $k_F\delta r = 5 \times 10^{-9}$, we find very good agreement with the analytic effective range expression for $10 \lesssim r_0/\delta r \lesssim 60$.

In the bottom panel, the analogous plot is constructed for the modified Pöschl-Teller potential with $\mu \approx 1075k_F$ and $v_0 \approx 0.068$, where the effective range has been tuned to $k_Fr_e = 0.006$, within acceptable error. There is no analytic expression for the scattering parameters associated with this potential, so we rely on the equivalent scattering problem with a square well potential (i.e., the top panel) to know how $r_0$ should be selected. It should be noted that variations in $r_e$ depicted in this figure are
very small, and more attention is paid to the correct determination of $a_{2D}$.

The scattering length is plotted as a function of $r_0/\delta r$ in Fig. 2.9. Results for our modified Pöschl-Teller potential are shown with solid lines (black) and the equivalent square well behaviour is illustrated using dashed lines (red). We first focus on the square well, where the analytic expression is shown with a solid line (blue). Unlike the effective range case, where we saw increasing overlap between the numerical determination and analytic result when decreasing the step size, the numerical determination of $a_{2D}$ is consistently lower than expected in the same region ($10 \lesssim r_0/\delta r \lesssim 60$). For larger starting values, where the numerical effective range begins to diverge, we find brief overlaps with the analytic and numerical $a_{2D}$ as the scattering length also diverges. We could say, for example, that with $k_F\delta r = 5 \times 10^{-9}$ an appropriate value of the starting point is $r_0/\delta r \approx 400$, however this seems unlikely. We feel that a better reconciliation is to choose a starting value in the range $10 \lesssim r_0/\delta r \lesssim 60$ (for $k_F\delta r \lesssim 5 \times 10^{-9}$), and treat the difference between numerical and analytic scattering length as the error associated with our method.

To ensure the quality of our work, we quantify the error (roughly speaking) of our numerical scattering length calculation based on Fig. 2.9. Assuming that $k_F\delta r \lesssim 5 \times 10^{-9}$, we will estimate an error of $\delta a_{2D} = 0.0003/k_F$ based on the difference in $k_F a_{2D}$ between numerical and analytic expressions for the square well in the converged
Figure 2.8: The dependence of the effective range $r_e$ on $r_0/\delta r$, where $r_0$ determines the boundary condition for the numerical solution in Eq. (2.43) and $\delta r$ is the step size. Imagining $k_F$ to be fixed, the thinner curved lines correspond to smaller integration step size. In the top panel, where numerical square well calculations (red dashed lines) are compared to the analytic result (blue line) for $a_{2D} = e^4/k_F$, we find good agreement over an increasingly broad range of $r_0/\delta r$ values as $\delta r$ is decreased in size. Although we have no analytical expression for $r_e$ of the modified Pöschl-Teller potential, where results are plotted in the bottom panel (black lines), we can imagine it by analogy to the square well relationship seen in the top panel. The effective range is different in each case because we tune our potential, Eq. (2.46), to $k_F r_e \approx 0.006$ and compare to the square well potential used in Ref. [32] where $k_F r_e \approx 0.00819$ for this value of $a_{2D}$. 


Figure 2.9: In a similar style as Fig. 2.8, we plot the 2D scattering length $a_{2D}$ as a function of $r_0/\delta r$, where $r_0$ determines the boundary condition for numerical solution, Eq. (2.43), and $\delta r$ is the step size. Imagining $k_F$ to be fixed, the line thickness is proportional to the integration step size. The square well analytic result $a_{2D} = e^4/k_F$ is plotted (blue solid line) which should first be compared to our square well numerical results (red dashed lines). It’s not surprising that our $a_{2D}$ determination becomes increasingly less sensitive to $r_0/\delta r$ as we decrease $\delta r$, as this was also the case for our effective range. We tune the modified Pöschl-Teller potential such that $a_{2D} = e^4/k_F$ at $r_0/\delta r = 10$ and plot results (black solid lines) for various $\delta r$ corresponding to those used for the square well.
region. The interaction strength, \( \eta = \log(k_Fa_{2D}) \), will then have an error of:

\[
\delta \eta = \frac{\partial \eta}{\partial a_{2D}} \delta a_{2D} = (\partial \log(k_Fa_{2D})/\partial a_{2D}) \delta a_{2D} = \delta a_{2D}/a_{2D} = (0.0003/k_F)/(e^4/k_F) \approx 5.5 \times 10^{-6}. \tag{2.52}
\]

In Chapter 4, we show results for the ground state energy of the gas as a function of \( \eta \). Our statistical uncertainties for the energy calculation are on the order of \( 10^{-3} - 10^{-4} \) in units of \( \epsilon_F/2 \). Because the values for energy and \( \eta \) are on the same order of magnitude, we can compare these errors directly. Therefore the error associated with the determination of \( a_{2D} \) is negligible compared to the statistical uncertainty of the energy (from which all other results follow). If this were not the case, we would need to include x-axis error bars for \( \eta \) in our figures in Chapter 4.

Now we turn our attention to the modified Pöschl-Teller \( a_{2D} \) behaviour in Fig. 2.9, which is similar to that discussed for the square well. We tune \( v_0 \) and \( \mu \) to reproduce the desired scattering length (i.e., \( k_Fa_{2D} = e^4 \approx 54.5981 \)). Based on the convergence of the effective range in Fig. 2.8, we set \( r_0/\delta r = 10 \) and tune \( V(r) \) accordingly. This is why each solid line intersects the analytic result for the square well at \( r_0/\delta r = 10 \).

Generally speaking, the purpose of showing this figure is to motivate the importance of using a small step size for the numerical solution. For relatively large step sizes (e.g., \( k_F\delta r = 2.5 \times 10^{-8} \)), the accuracy of the solution is highly dependent on the value selected for \( r_0 \), in units of \( \delta r \). On the other hand, for relatively small step sizes the solution is dramatically less sensitive to \( r_0/\delta r \). We found it convenient to scale
$r_0$ in sizes of $\delta r$, however this is not a requirement and the sensitivity relationship directly above is indeed a result of this scaling choice.
Chapter 3

2D Many-body system

We will now extend our discussion to many-particle (i.e., $N \geq 3$) systems. The natural starting point is to consider the non-interacting gas, which has a non-trivial description due to the Pauli exclusion principle. Next we look at the full problem and consider two-body interactions between opposite-spin particles. Looking to solve the Schrödinger equation, we introduce the Slater and BCS many-body trial wave functions that include Jastrow correlations. Finally, we discuss quantum Monte Carlo, a numerical technique for determining the ground state energy of quantum gases. In particular we consider the statistical framework, variational Monte Carlo (VMC), and dynamic Monte Carlo (DMC) with importance sampling. In practice, these variational methods are applied using our trial wave functions.

3.1 Non-interacting Fermi gas

A distinguishing feature of the zero-temperature Fermi gas is the occupation of finite-momentum levels due to the Pauli exclusion principle. This has important consequences for the many-body system. Take $N$ particles in a uniform box of length
$L$ with periodic boundary conditions. The thermodynamic-limit (TL) gas is a limiting case of this system where particle number $N \to \infty$ and simulation area $A \to \infty$, while $N/A \to$ constant. Single particle states are written as plane waves: $\psi_k(\mathbf{r}) = e^{i\mathbf{k}_n \cdot \mathbf{r}}/L$, where momentum levels are identified by the wave vector:

$$\mathbf{k}_n = \frac{2\pi}{L} (n_x \hat{x} + n_y \hat{y}).$$  \hfill (3.1)

Each particle has energy $E_n = \hbar^2 \mathbf{k}_n^2 / 2m$, where $m$ is the mass and the energy level is identified by $\mathbf{n} = (n_x, n_y)$. Identical half-odd spin particles must be in distinct states and, at $T = 0$, will occupy all available levels up to the Fermi surface. Particles on the Fermi surface have energy $\epsilon_F = \hbar^2 k_F^2 / 2m$, where $k_F$ is the Fermi wave vector.

In the TL, the energy per particle of the free gas $E_{FG}$ can be derived, as well as a relation between $k_F$ and density. Consider the number of particles $N$ as defined by a summation over momentum states $\mathbf{k}$. In the first line below, the spacing between adjacent momentum states $\delta k_i = 2\pi/L$ is introduced; this can be considered infinitesimally small in the TL.

$$N = 2 \sum_k 1 = 2 \sum_k \frac{\delta k_x \delta k_y}{\delta k_x \delta k_y} = \frac{2L^2}{(2\pi)^2} \sum_k \delta k_x \delta k_y$$

$$= \frac{2L^2}{(2\pi)^2} \int d^2 k \quad \text{as } L \to \infty$$

$$= \frac{2A}{(2\pi)^2} \int_0^{k_F} \int_0^{2\pi} k \, dk \, d\theta$$

$$= \frac{Ak_F^2}{2\pi}.$$  \hfill (3.2)

In the first line, the factor of two exists because we have assumed a two-component gas. The result can be rewritten as $k_F = \sqrt{2\pi n}$, where $n = N/A$ is the 2D number
density. For the energy in this limit, the derivation is similar; we start with the energy per particle
\[
E_{FG}(N) = \frac{2}{N} \sum_k \frac{\hbar^2 k^2}{2m},
\] (3.3)
and can show that in the TL
\[
E_{FG}(N \to \infty) \equiv E_{FG} = \epsilon_F/2.
\] (3.4)

The corresponding expressions in 3D are \(E_{FG} = (3/5)\epsilon_F\) and \(k_F = (3\pi^2 n_{3D})^{1/3}\).

The energy per particle for finite-size systems, \(E_{FG}(N)\), has the largest differences from \(E_{FG}\) for small \(N\). This relative error is shown in Fig. 3.1 and gradually tends towards zero as \(N\) increases. When \(N\) is even, the system has an equal number of spin-up and spin-down particles. Points with odd \(N\) are determined by placing either a spin-up or spin-down particle into the next available momentum state. The inset shows how \(E_{FG}(N)\) fluctuates above and below the TL result at small \(N\).

Different combinations of \(n_x\) and \(n_y\) in Eq. (3.1) can result in the same \(|k_n|\), meaning particles in different states may have the same energy. Closed-shell configurations exist at specific values of \(N\) for finite-sized systems where the population in each energy-level is maximal. By considering equal numbers of spin-up and spin-down particles for even \(N\), the population allowed in each energy level doubles compared to a gas of only indistinguishable particles. In 2D, closed shells occur at total particle number \(N=\{2, 10, 18, 26, 42, 50, 58\ldots\}\), which roughly correspond to the local minima in the inset of Fig. 3.1. For comparison, we note that in 3D the corresponding closed shells occur at total particle number \(N=\{2, 14, 38, 54, 66, 114, 162\ldots\}\).
Figure 3.1: Error associated with finite-size periodic systems, defined in units of $E_{FG}$ as the absolute value of the energy difference between $N$ particles in a finite size box and the TL system where $N \to \infty$ and $V \to \infty$. Largest error is seen for small $N$ where dotted lines are drawn to guide the eye. The inset displays this range on a linear scale. For large values of $N$ the error approaches zero as marked by the dashed line.
3.2 Many-body wave functions for interacting gases

In this Section we show the Hamiltonian and discuss our trial wave functions used to solve the Schrödinger equation. We begin by introducing general features of the many-body wave function $\Psi(R)$, where $R = r_1, r_2, \ldots, r_N$ is the $N$-particle configuration vector. If the particles are indistinguishable (i.e., identical) then the probability density should remain unchanged if two particles are exchanged for one another:

$$|\Psi(r_1, r_2, \cdots)|^2 = |\Psi(r_2, r_1, \cdots)|^2.$$  \hfill (3.5)

This leads to the requirement that $\Psi(R)$ is either symmetric under particle exchange:

$$\Psi(r_1, r_2, \cdots) = \Psi(r_2, r_1, \cdots),$$  \hfill (3.6)

or anti-symmetric:

$$\Psi(r_1, r_2, \cdots) = -\Psi(r_2, r_1, \cdots).$$  \hfill (3.7)

A system of bosons turns out to be symmetric and a system of fermions must be anti-symmetric to satisfy the Pauli exclusion principle. With this in mind, we take care to select appropriate wave functions to describe the Fermi gas. Momentum information of each particle need be encoded into the wave function for an accurate description. When $T = 0$, in the non-interacting case discussed in Section 3.1, these momenta are known exactly.

We consider a two-component Fermi gas described by the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m} \left[ \sum_{i=1}^{N_i} \nabla_i^2 + \sum_{j'=1}^{N_{j'}} \nabla_{j'}^2 \right] + \sum_{i<j'} V(r_{ij'}),$$  \hfill (3.8)
where \( m_\uparrow = m_\downarrow = m \) is the particle mass and total particle number is given by \( N_\uparrow + N_\downarrow = N \). As described in Section 2.6, we take \( V(r_{ij'}) \) to be of the modified Pöschl-Teller form, Eq. (2.46), and consider s-wave interactions between opposite-spin particles. We wish to solve the many-body Schrödinger equation:

\[
\hat{H} \Phi_0(R) = E \Phi_0(R),
\]

(3.9)

where \( \Phi_0(R) \) is an ansatz of the ground state wave function. To do this we project \( \Phi_0(R) \) from a trial wave function \( \Psi_T(R) \) using diffusion Monte Carlo (as will be seen in Section 3.3.2). In this work, \( \Psi_T(R) \) is described as a product of Jastrow functions that depend only on \( R \) and a component \( \Phi(R) \) that depends on the momentum as well as the configuration. The nodes of the many-body wave function (i.e., when \( \Psi_T(R) = 0 \)), which are important for an accurate solution of Eq. (3.9), are decided by the anti-symmetric part of the wave function: \( \Phi(R) \). We study two forms, the Slater wave function \( \Phi_S(R) \) using plane waves and the BCS pairing wave function \( \Phi_{BCS}(R) \). We do not concern ourselves with normalization factors because, as will be seen in Section 3.3, these cancel out in calculations.

### 3.2.1 Slater wave function \( \Phi_S(R) \)

We have already discussed the plane wave eigenstates for non-interacting particles in a periodic box: \( \psi_\kappa(r) = e^{i\kappa n \cdot r}/L \) (see Section 3.1). An \( N \)-body wave function can be constructed by multiplying the single-particle plane waves together:

\[
\Psi(R) = \prod_{i=1}^{N} \psi_\kappa(r_i),
\]

however this is not anti-symmetric and therefore cannot describe
fermions in accordance with Eq. (3.7). For our two-component system, we write:

$$\Phi_S(R) = \mathcal{A} \prod_{i=1}^{N_t} \psi_{ki}(r_i) \cdot \mathcal{A} \prod_{j'=1}^{N_t} \psi_{kj'}(r_j'), \tag{3.10}$$

where $\mathcal{A}$ is the anti-symmetrizing operator. This standard fermionic Slater wave function can be expressed in terms of determinants, which makes it appealing for computational methods. It is effective at describing the normal state of Fermi liquids where pairing is weak and can be sufficiently accounted for with the introduction of Jastrow correlations (as will be discussed in Section 3.2.4). The Jastrow-Slater many-body trial wave function is given by

$$\Psi_T(R) = \prod_{ij'} f_{ij}(r_{ij'}) \Phi_S(R), \tag{3.11}$$

where the Jastrow terms, $f_{ij}(r_{ij'})$, include correlations between interacting particles.

### 3.2.2 BCS wave function $\Phi_{BCS}(R)$

Unlike the Slater form which uses non-interacting eigenfunctions, $\Phi_{BCS}(R)$ explicitly accounts for pairing. In some of the Fermi gases we study, pairing is strong enough that $\Phi_S(R)$, as seen in Eq. (3.11), is inadequate. To describe the strongly interacting Fermi gas for any attraction strength, we use the Jastrow-BCS many-body trial wave function:

$$\Phi_{BCS}(R) = \mathcal{A} \left[ \phi(r_{11'}) \phi(r_{22'}) \cdots \phi(r_{N_tN_t'}) \right],$$

$$\Psi_T(R) = \prod_{ij'} f_{ij}(r_{ij'}) \Phi_{BCS}(R). \tag{3.12}$$
As in the Slater case, the anti-symmetry requirement of $\Psi_T(R)$ for the Fermi gas is enforced by the operator $\mathcal{A}$. Evaluating this operation for $N_\uparrow + N'_\downarrow = N$ particles in a fully paired-up system results in a determinant of pairing functions for all interacting particles:

$$
\Phi_{\text{BCS}}(R) \propto \begin{vmatrix}
\phi(r_{1\downarrow'}) & \phi(r_{1\downarrow'}) & \cdots & \phi(r_{1N'_\downarrow}) \\
\phi(r_{2\downarrow'}) & \phi(r_{2\downarrow'}) & \cdots & \phi(r_{2N'_\downarrow}) \\
\vdots & \vdots & \ddots & \vdots \\
\phi(r_{N\downarrow'}) & \phi(r_{N\downarrow'}) & \cdots & \phi(r_{NN'_\downarrow})
\end{vmatrix}.
$$

(3.13)

This ansatz has been used before in 3D Fermi gas systems [19, 20, 51, 52, 53]. The pairing functions are expressed as

$$
\phi(r) = \sum_n \alpha_n e^{i k_n \cdot r} + \tilde{\beta}(r),
$$

(3.14)

which contains variational parameters $\alpha_n$ for each momentum state up to some level $n$. When setting $\alpha_n = 0$ for $|k_n| > k_F$ and $\tilde{\beta}(r) = 0$ in Eq. (3.14), $\Phi_{\text{BCS}}(R)$ becomes equivalent to $\Phi_S(R)$.

Higher momentum contributions are accounted for by the spherically symmetric beta function:

$$
\tilde{\beta}(r) = \beta(r) + \beta(L - r) - 2\beta(L/2) \quad \text{for} \quad r \leq L/2,
$$

$$
= 0 \quad \text{for} \quad r > L/2,
$$

$$
\beta(r) = [1 + cbr] [1 - e^{-dbr}] e^{-br}.
$$

(3.15)

which contains variational parameters $b$, $c$ and $d$. This form of the beta function has been used for 3D calculations, and we have explicitly checked its behaviour in 2D.
Specifically, when calculating the local energy given by $\Psi_T^{-1}(\mathbf{R}) \hat{H} \Psi_T(\mathbf{R})$, we need to evaluate terms of the form $\partial \tilde{\beta}(r)/\partial \alpha_i$, where $\alpha_i$ is the coordinate of a specific particle (e.g., $x_2$, $y_3$...) and $r = \sqrt{\Delta x^2_{ij} + \Delta y^2_{ij}}$ is the radial separation between two particles. Defining $\Delta \alpha_{ij}$ as the projection of $r$ along a coordinate (e.g., $\Delta x_{ij}$ or $\Delta y_{ij}$) we can write:

$$
\frac{\partial \tilde{\beta}(r)}{\partial \alpha_i} = \frac{\partial \tilde{\beta}(r)}{\partial r} \frac{\partial r}{\partial \alpha_i} = \frac{\partial \tilde{\beta}(r)}{\partial r} \frac{1}{2} \sqrt{\Delta x^2_{ij} + \Delta y^2_{ij}} \frac{\partial \Delta \alpha_{ij}}{\partial \alpha_i}
$$

$$
= \frac{\partial \tilde{\beta}(r)}{\partial r} \frac{\Delta \alpha_{ij}}{r} \frac{\partial \Delta \alpha_{ij}}{\partial \alpha_i}
$$

$$
= \pm \frac{\partial \tilde{\beta}(r)}{\partial r} \frac{\Delta \alpha_{ij}}{r},
$$

where $\partial \Delta \alpha_{ij}/\partial \alpha_i$ can be positive or negative 1. For example, $\partial(x_2 - x_5)/\partial x_2 = 1$ and $\partial(x_2 - x_5)/\partial x_5 = -1$.

The result in Eq. (3.16) has a singularity at $r = 0$ due to the $1/r$ term. This can cause large fluctuations in the local energy for small $r$, therefore we define the variational parameter $c$ in Eq. (3.15) such that

$$
\left. \frac{\partial \tilde{\beta}(r)}{\partial r} \right|_{r=0} = \left[ \frac{\partial \beta(r)}{\partial r} + \frac{\partial \beta(L - r)}{\partial r} - 2 \frac{\partial \beta(L/2)}{\partial r} \right]_{r=0} = 0.
$$

(3.17)

Making use of L’Hôpital’s rule, it is mostly straightforward to show that

$$
c = \frac{2 + 2dbL + (dbL)^2 e^{bL(1+d)} + 2db^2 L^2 e^{bL(1+d)} + 2bL - 2e^{dbL}bL - 2e^{dbL}}{2b^2 L^2 (e^{dbL} - 1 - d + de^{bL(1+d)})},
$$

(3.18)

as derived in Appendix A. In this work, we set $b = 0.5k_F$ and $d = 5$, as done in Ref. [20] for the 3D unitary Fermi gas. With these values of $b$ and $d$, we find $c \simeq 3.5$. 

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3.2.3 Pairing function $\phi(r)$ results

Parameters in Eq. (3.14) are optimized using variational Monte Carlo (VMC) energy minimization for the BCS wave function, Eq. (3.12). Unique sets of $\alpha_n$ were determined for each interaction strength using automated optimization techniques [54]. A selection of optimized pairing functions are plotted in Fig. 3.2. These two-body pairing orbitals contain information about the many-body system via the values arrived at for our $\alpha_n$ parameters. They become increasingly localized about the origin as $\eta$, defined in Eq. (2.49), is reduced and pairs become more tightly bound. The domain of $\phi(r)$ in each panel is equal to the maximum distance along the respective path between particles. These paths are discussed in the caption. Nodes exist where $\phi(r)$ crosses the r-axis (marked with a dashed line). These occur in the top panel for $\eta = 0$ and $-1$, where stronger attractions result in more central nodes. For the longer path, shown in the bottom panel, a similar trend is seen. Here we find a similar node across interaction strengths, near the Jastrow-Slater node location. For $\eta = 6$ (not shown in Fig. 3.2), we find the node slightly shifted to the left, closer to the Slater node location.

3.2.4 Jastrow functions $\prod_{ij'} f_J(r_{ij'})$

Jastrow correlation functions $f_J(r)$ are introduced for each pair of interacting particles. These terms have no effect on the nodal structure and, collectively, reduce the overall variance of the calculation. As an example, a system with $N_\uparrow = 3$ and $N_\downarrow = 2$ has $3 \times 2 = 6$ Jastrow terms resulting from the product over $i, j'$ in Eq. (3.11) or Eq. (3.12). By definition, $f_J(r)$ is always positive and tends to 1 for large $r$. When $f_J(r) = 1$, there is no correlation between the particles, and the wave function $\Psi_T(R)$ remains the same as $\Phi(R)$. For small interaction distances, the Jastrow term is either
Figure 3.2: Variationally optimized pairing functions for various interaction strengths. The top panel plots $\phi(r)$ through a path parallel to the box sides, corresponding to the $(1,0)$ or equivalently the $(0,1)$ direction. A path along the $(1,1)$ direction is taken for $\phi(r)$ in the bottom panel plot. The dashed lines are included to show node locations, where $\phi(r) = 0$. 
larger than 1 if the interaction is purely attractive or less than 1 if the opposite.

The function \( f_J(r) \) is determined as a nodeless solution to the radial Schrödinger equation for \( R_0(r) \), which is equivalent to \( u_0(r)/\sqrt{r} \) following from a solution to Eq. (2.29). More explicitly, the differential equation for the Jastrow function is given by [55]:

\[
-\frac{\hbar^2}{m} \nabla^2 f_J(r) + V_J(r)f_J(r) = \lambda f_J(r),
\]

where \( \lambda \) is selected such that \( \partial f_J(r)/\partial r = 0 \) at the healing length \( r = d \) and the solution has no nodes. In this work, we take the potential \( V_J(r) \) to be the same as that in the Hamiltonian, Eq. (2.46). After solving Eq. (3.19), the Jastrow function is re-scaled such that \( f_J(r > d) = 1 \). In practice, we chose \( d \sim L/12 \), where \( L \) is the box length. As the potential depth is increased (see Fig. 2.6) to describe tightly bound pairs in the deep BEC regime, we found it necessary to reduce \( d \) in order to determine a nodeless Jastrow function solution.

Eq. (3.19) can be solved numerically using the Runge-Kutta method described in Section 2.3. Since \( \partial f_J(r)/\partial \theta \) and, in 3D, \( \partial f_J(r)/\partial \phi \) are zero, we are only interested in the radial partial derivative term in the Laplacian. Substitutions are made for \( f_J(r) \) that depend of the dimensionality of the system. In 2D, we make the substitution \( f_J(r) \to u_J(r)/\sqrt{r} \) as done in Section 2.2 for the radial wave function \( R_l(r) \). This results in the simplification of Eq. (3.19):

\[
\frac{\partial^2 u_J(r)}{\partial r^2} = b(r)u_J(r),
\]

\[
b(r) = -\frac{m}{\hbar^2}\left(\lambda - V(r) + \frac{\hbar^2}{4mr^2}\right).
\]

This differential equation is solved for different \( \lambda \) until a satisfactory solution is achieved. Once we have \( u_J(r) \) and \( \partial u_J(r)/\partial r \), the Jastrow function and its first
derivative (which is required to compute the local energy) are determined using:

\[ f_J(r) = \frac{u_J(r)}{\sqrt{r}} \quad \text{and} \quad \frac{\partial f_J(r)}{\partial r} = \frac{\partial}{\partial r} \left( \frac{u_J(r)}{\sqrt{r}} \right) = \frac{1}{\sqrt{r}} \left[ \frac{\partial u_J(r)}{\partial r} - \frac{u_J(r)}{2r} \right]. \tag{3.21} \]

As an aside, we note that \( \frac{\partial^2 f_J(r)}{\partial r^2} \) generally has positive and negative values, thus allowing for the calculated kinetic contribution to be below zero. This was not the case for our work, but can in principle occur for extremely influential Jastrow correlations (e.g., by choosing the depth of \( V_J(r) \) to be large).

### 3.3 Quantum Monte Carlo

Up to this point, we have been interested in setting up the Schrödinger equation, Eq. (3.9), which involved the determination of parameters for our potential and two trial many-body wave functions. Now, we will describe our numerical techniques for determining the ground state energy. Quantum Monte Carlo (QMC) methods allow for an accurate ground-state description of many-body systems from first principles, and are important for constraining theoretical models and guiding experiment [56].

Our QMC techniques are variational in nature, which means that calculations give exact or upper bound estimates of energy expectation values. The statistical basis for these calculations is first outlined, and we introduce variational Monte Carlo (VMC) in tandem. Then we discuss the diffusion Monte Carlo (DMC) framework. One major complication of QMC for Fermi gases is the fermion-sign problem. We use the fixed-node DMC approach, which circumvents the sign problem by restricting transitions across nodal surfaces.
3.3.1 Statistical foundations and VMC

The central limit theorem tells us that an infinite number of random samples from a probability distribution will be normally distributed about the mean value. We discuss this in the context of $dN$-dimensional quantum systems, where $d$ is the dimensionality and $N$ is the number of particles associated with each sampling point. The configuration vector $\mathbf{R} = r_1, \ldots, r_N$ has already been introduced. This is a set of position values within a simulation area (or, in the 3D case, a volume), and may be referred to as a walker.

Consider a probability distribution

$$P(\mathbf{R}) = \frac{\Psi^*(\mathbf{R})\Psi(\mathbf{R})}{\int d\mathbf{R}|\Psi(\mathbf{R})|^2} ,$$

(3.22)

where $|\Psi(\mathbf{R})|^2 = \Psi^*(\mathbf{R})\Psi(\mathbf{R})$ and $\int d\mathbf{R}P(\mathbf{R}) = 1$. The state $\Psi^*(\mathbf{R})$ is the complex conjugate of $\Psi(\mathbf{R})$. Now let’s imagine we know some function $f(\mathbf{R})$ associated with state $\Psi(\mathbf{R})$, and want to calculate the mean:

$$\bar{f} = \frac{\int d\mathbf{R}\Psi^*(\mathbf{R})f(\mathbf{R})\Psi(\mathbf{R})}{\int d\mathbf{R}|\Psi(\mathbf{R})|^2} = \frac{\int dr_1 \int dr_2 \ldots \Psi^*(\mathbf{R})f(\mathbf{R})\Psi(\mathbf{R})}{\int dr_1 \int dr_2 \ldots |\Psi(\mathbf{R})|^2}$$

(3.23)

$$= \int d\mathbf{R}f(\mathbf{R})P(\mathbf{R}) ,$$

where we remind the reader that for $N$ particles: $\int d\mathbf{R} = \int dr_1 \int dr_2 \ldots \int r_N$, and we integrate over the domain of $P(\mathbf{R})$. The standard deviation $\delta$ is defined in terms of the variance $\sigma$:

$$\delta = \frac{\sigma}{\sqrt{M}} = \frac{1}{\sqrt{M}} \left[ \int d\mathbf{R}(f(\mathbf{R}) - \bar{f})^2 P(\mathbf{R}) \right]^{1/2} ,$$

(3.24)

where $M$ is the number of sampling configurations in a random distribution $\mathbf{X}$ defined
by

\[ X = \{ f(R_1), f(R_2), \ldots, f(R_M) \}, \quad (3.25) \]

where \( R_{i \leq M} \) are vectors within the domain of and distributed according to \( P(R) \).

For large enough \( M \), the central limit theorem tells us that \( X \) is normally distributed about the mean value

\[ \bar{f} \approx \frac{f(R_1) + f(R_2) + \ldots + f(R_M)}{M}, \quad (3.26) \]

with standard deviation \( \delta \). As seen in Eq. (3.24), the uncertainty decreases as \( \sqrt{M} \) regardless of dimensionality.

We can use this theorem to calculate energy expectation values in quantum mechanics by determining the weighted average over a probability distribution. For VMC, we calculate the variational estimate:

\[ E_V = \frac{\int dR \Psi_T^*(R) \hat{H} \Psi_T(R) \int dR |\Psi_T(R)|^2}{\int dR |\Psi_T(R)|^2}, \quad (3.27) \]

where \( \Psi_T(R) \) is the trial wave function as seen in Section 3.2 and our Hamiltonian is given in Eq. (3.8). We can rewrite this in the form of Eq. (3.23):

\[ E_V = \frac{\int dR \left[ \Psi_T^{-1}(R) \hat{H} \Psi_T(R) \right] |\Psi_T(R)|^2}{\int dR |\Psi_T(R)|^2} = \int dR E_L(R) P_T(R), \quad (3.28) \]

where \( E_L(R) = \Psi_T^{-1}(R) \hat{H} \Psi_T(R) \) is the local energy of a configuration and \( P_T(R) = |\Psi_T(R)|^2 / \int |\Psi_T(R)|^2 dR \) is the trial probability density. By analogy to Eq. (3.26),
the average energy can be evaluated as

\[ E_V \approx \frac{1}{M} \sum_{i=1}^{M} E_L(R_i), \quad (3.29) \]

given there exists a large number of sampling configurations \( R_{i \leq M} \).

The difficulty in evaluating Eq. (3.29) is acquiring a large set of vectors \( R \) that are distributed according to \( P_T(R) \). We use the Metropolis algorithm to achieve this by sampling the trial wave function. The algorithm, described below, relies on the concept of a Markov chain: a series of states where each is connected, in sequence, according to a specific set of rules. The states must transition randomly according to a transition rule \( T(R' \rightarrow R) \), which gives the probability of going from \( R' \) to \( R \). It is chosen such that each state will depend only on the previous one. As well, the transition rate from \( R' \rightarrow R \) must equal the return rate (a condition called detailed balance):

\[ P(R')T(R' \rightarrow R) = P(R)T(R \rightarrow R'), \quad (3.30) \]

where the weight function \( P(R) \) can be treated as defined in Eq. (3.22). Finally, it must also be ergodic [59]:

- any state can be achieved within a finite number of steps; this ensures that the entire configuration space is traversable
- \( T(R \rightarrow R) > 0 \); there is a chance of staying in the same place when the system steps forward
- the average number of steps required to return to the current state is finite

Such transition probabilities along with the detailed balance condition, Eq. (3.30), guarantee that Markov chains will consist of states which equilibrate according to the
distribution $P(\mathbf{R})$. It was once believed that a probability distribution could only properly be sampled with a completely independent data set. In the early 1900’s, Markov constructed the concept discussed above and thereby showed that dependent data sets can be used [60].

The Metropolis algorithm [57, 58] involves a specific transition rule that satisfies the above conditions. We define a variable $\Lambda(\mathbf{R} \to \mathbf{R}')$ that is determined according to some sampling distribution. It would represent the probability of moving from $\mathbf{R}'$ to $\mathbf{R}$ (and be equivalent to $T(\mathbf{R} \to \mathbf{R}')$) if not for a chance of rejection. Moves are accepted according to:

$$A(\mathbf{R}' \to \mathbf{R}) = \min \left[ 1, \frac{P(\mathbf{R})\Lambda(\mathbf{R} \to \mathbf{R}')}{{P(\mathbf{R}')\Lambda(\mathbf{R}' \to \mathbf{R})}} \right],$$

(3.31)

where

$$T(\mathbf{R}' \to \mathbf{R}) = \Lambda(\mathbf{R} \to \mathbf{R}')A(\mathbf{R} \to \mathbf{R}).$$

(3.32)

Taking the sampling distribution to be symmetric in the sense that $\Lambda(\mathbf{R}' \to \mathbf{R})$ is identical to the opposite transition $\Lambda(\mathbf{R} \to \mathbf{R}')$, we can write the acceptance probability as $A(\mathbf{R}' \to \mathbf{R}) = \min \left[ 1, \frac{P(\mathbf{R})}{P(\mathbf{R}')} \right]$. The details of $\Lambda(\mathbf{R}' \to \mathbf{R})$ depend on the specific QMC method. For VMC we can make randomly selected moves from a uniform distribution, where the distribution size is adjusted such that $A(\mathbf{R}' \to \mathbf{R}) \approx 50\%$. The same result can also be achieved with normally distributed moves, which arise naturally in DMC. To acquire a statistically significant result for Eq. (3.29), we propagate up to 5000 walkers in unison, for thousands of steps each.

We now discuss the usefulness of Eq. (3.27), the variational estimate. This energy expectation value is an upper bound to the true ground state energy of the system: $E_V \geq E_0$. As we will show, this must be the case for any trial wave function $\Psi_T(\mathbf{R})$,
due to the variational principle. In order to find the ground state energy using VMC, we would require the exact ground state wave function. This is not realistic, however the technique is useful for minimization problems where parameters in $\Psi_T(R)$ are varied to find an optimal wave function. The Slater wave function in Eq. (3.11) is a reasonably good estimate of the ground state energy, however it contains no variational parameters. The BCS wave function, Eq. (3.12), has many parameters that can be tuned in order to optimize the nodal structure. We use VMC energy minimization to do this by adjusting the $\alpha$ parameters included in the pairing function, Eq. (3.14).

As will be seen in Section 4.2, it’s also beneficial to vary the momentum state of unpaired particles in the $N_\uparrow \neq N_\downarrow$ system. Aside from wave function optimization, we also use VMC as a tool to acquire a well distributed set of walkers from which to begin DMC.

To conclude this section, we show a proof of the variational principle. We introduce Dirac notation and consider a state $|\Psi_T\rangle = \sum_i c_i |\psi_i\rangle$, where $|\psi_i\rangle$ are the exact eigenstates of the Hamiltonian and $c_i$ are coefficients. Our trial wave functions $\Psi_T(R)$, for example, can be thought of as linear combinations of excited states and the ground state. The general wave function in this proof is normalized in the usual way:

$$\langle \Psi_T | \Psi_T \rangle = \sum_{i,i'} \langle \psi_{i'} | c_{i'}^* c_i | \psi_i \rangle = \sum_i c_i^* c_i = \sum_i |c_i|^2 = 1,$$  

where we use the orthonormality of the basis states $|\psi_i\rangle$ to simplify the second expression. The variational principle can then be seen by writing the energy expectation value in terms of the ground state energy $E_0$:

$$\langle \Psi_T | \hat{H} | \Psi_T \rangle = \left( \sum_{i'} c_{i'}^* \langle \psi_{i'} | \right) \left( \sum_i c_i E_i | \psi_i \rangle \right) = \left( c_0^* \langle \psi_0 | + c_1^* \langle \psi_1 | + c_2^* \langle \psi_2 | + \cdots \right) \left( c_0 E_0 | \psi_0 \rangle + c_1 E_1 | \psi_1 \rangle + c_2 E_2 | \psi_2 \rangle + \cdots \right)$$
\[
= |c_0|^2 E_0 + |c_1|^2 E_1 + |c_2|^2 E_2 + \cdots \\
= |c_0|^2 E_0 + |c_1|^2 (E_0 + \Delta E_1) + |c_2|^2 (E_0 + \Delta E_2) + \cdots \\
= E_0 + (|c_1|^2 \Delta E_1 + |c_2|^2 \Delta E_2 + \cdots ),
\]

where we have used the result in Eq. (3.33) to write the final line. The excitation energies \( \Delta E_i = E_i - E_0 \) must be positive and we also know that \(|c_i|^2 \geq 0\), therefore \( \langle \Psi_T | \hat{H} | \Psi_T \rangle \geq E_0 \). The equality will hold if \(|\Psi_T\rangle\) has 100% overlap with the ground state eigenfunction.

### 3.3.2 Diffusion Monte Carlo

In DMC, we once again take a random walk in configuration space, where now walkers can be terminated in areas of small potential energy and duplicated in areas of large potential energy. As mentioned in the previous section, the configurations from which to begin DMC are acquired using VMC. By propagating this set of walkers in imaginary time \( \tau = it \), we are able to project the ground state \( \Phi_0 \) from the trial wave function. We define

\[
\Psi(\tau) = e^{-(\hat{H} - E_T)\tau} \Psi(0) \\
= e^{-(\hat{H} - E_T)\tau} \Psi_T \\
= c_0 e^{-(E_0 - E_T)\tau} \psi_0 + c_1 e^{-(E_1 - E_T)\tau} \psi_1 + c_2 e^{-(E_2 - E_T)\tau} \psi_2 + \ldots,
\]

where the trial wave function has once again been expressed in terms of the exact eigenstates: \( \Psi_T = \sum_i c_i \psi_i \). The trial energy \( E_T \) is a constant offset applied to the Hamiltonian and is important for controlling simulations. By setting \( E_T \approx E_0 \), we find that as \( \tau \) becomes large the excited-state exponential factors become increasingly

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close to 0 and we are left with

$$\Phi_0 = \Psi(\tau \to \infty) = c_0 \psi_0 \lim_{\tau \to \infty} (e^{-(E_0 - E_T)\tau}),$$

(3.36)

where the ground state exponential remains finite due to competing effects: $\tau \to \infty$ and $E_0 - E_T \approx 0$. In practice, $\tau$ need only be large enough to guarantee that the first excited state term is negligibly small compared to the ground state term. The projected wave function $\psi(R, \tau)$, where we are explicitly labeling the configuration $R$ at time $\tau$, describes a dynamic system that is equilibrating for small $\tau$ and for sufficiently large $\tau$ is the ground state wave function.

The projection is accomplished by iterating over

$$\Psi(R, \tau + \Delta\tau) = \int dRG(R, R'; \Delta\tau)\Psi(R', \tau),$$

(3.37)

where

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

(3.38)

and we have introduced the small time step $\Delta\tau = \tau/n$, where $n$ is the number of steps. This configuration space Green’s function can be evaluated as follows, making use of the Trotter-Suzuki approximation (see Ref. [61]) and expressing the Hamiltonian in terms of kinetic $\hat{T}$ and potential $\hat{V}$ energy operators:

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

$$= \langle R|\left(e^{-\hat{V}\Delta\tau} e^{-\hat{T}\Delta\tau} e^{-\hat{V}\Delta\tau} + O(\Delta\tau^3)\right)|R'\rangle e^{E_T\Delta\tau}$$

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

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

(3.39)
The matrix element can be evaluated (as done in Appendix B) by expanding the $dN$-dimensional configuration vectors: $|\mathbf{R}\rangle = |r_1, r_2, \ldots, r_N\rangle$, and inserting momentum space eigenstates for each dimension. This Green's function is the kinetic energy propagator:

$$\langle \mathbf{R}|e^{-\hat{T}\Delta\tau}|\mathbf{R}'\rangle = \left[\frac{m}{2\pi\hbar^2\Delta\tau}\right]^{\frac{3N}{2}} \exp\left[-\frac{m}{2\hbar^2\Delta\tau}(\mathbf{R} - \mathbf{R}')^2\right]. \quad (3.40)$$

It is a Gaussian distribution generalized to higher dimensions with standard deviation $\sqrt{\hbar^2\Delta\tau/m}$ and centered at $\mathbf{R}'$ (or at zero if we treat $\mathbf{R} - \mathbf{R}'$ as a single vector representing the change in position). The full short time Green's function is given by:

$$G(\mathbf{R}, \mathbf{R}') = \left[\frac{m}{2\pi\hbar^2\Delta\tau}\right]^{\frac{3N}{2}} \exp\left[-\frac{m}{2\hbar^2\Delta\tau}(\mathbf{R} - \mathbf{R}')^2\right]$$

$$\times \exp\left[-\frac{\Delta\tau}{2}(V(\mathbf{R}) + V(\mathbf{R}') - 2E_T)\right], \quad (3.41)$$

reducing to a weight, $P = \exp\left[-\Delta\tau(V(\mathbf{R}) + V(\mathbf{R}') - 2E_T)/2\right]$, associated with some normally distributed value. We interpret $P$ as a probability of branching, where the walker $\mathbf{R}$ in the transition $\mathbf{R}' \rightarrow \mathbf{R}$ may be duplicated several times. This occurs with probability $P - 1$ if $P \geq 1$. The walker can also be removed with probability $1 - P$ if $P < 1$. The number of resulting walkers is given by the integer part of $P + \nu$, where $\nu$ represents a uniformly distributed number in the range from 0 to 1.

DMC expectation values are determined by averaging over a set of equilibrated
configurations. For the energy, we calculate the mixed estimate:

$$
\langle \hat{H} \rangle_M = \frac{\langle \Psi_T | \hat{H} | \Psi(\tau) \rangle}{\langle \Psi_T | \Psi(\tau) \rangle}
$$

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

$$
= \frac{\langle e^{-(\hat{H}-E_T)\tau/2} \Psi_T | \hat{H} | e^{-(\hat{H}-E_T)\tau/2} \Psi_T \rangle}{\langle e^{-(\hat{H}-E_T)\tau/2} \Psi_T | e^{-(\hat{H}-E_T)\tau/2} \Psi_T \rangle}
$$

$$
= \frac{\langle \Psi(\tau/2) | \hat{H} | \Psi(\tau/2) \rangle}{\langle \Psi(\tau/2) | \Psi(\tau/2) \rangle},
$$

where we commute \( \hat{H} \) with itself to go from line 2 to line 3. Using DMC, this is evaluated as a path integral:

$$
\langle \hat{H} \rangle_M = \frac{\int dR_n \Psi_T^*(R_n) \hat{H} \Psi(R_n, \tau)}{\int dR_n \Psi_T^*(R_n) \Psi(R_n, \tau)}
$$

$$
= \frac{\int dR_n dR_{n-1} \ldots dR_0 \Psi_T^*(R_n) \hat{H} G(R_n, R_{n-1}) \ldots G(R_1, R_0) \Psi_T(R_0)}{\int dR_n dR_{n-1} \ldots dR_0 \Psi_T^*(R_n) G(R_n, R_{n-1}) \ldots G(R_1, R_0) \Psi_T(R_0)}.
$$

In the second line, we have removed the explicit \( \tau \) dependence by writing the projected wave function \( \Psi(R_n, \tau) \) in terms of the trial wave function \( \Psi_T(R_0) \). This relationship can be derived as follows:

$$
\Psi(R_n, \tau) = \langle R_n | \Psi(\tau) \rangle
$$

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

$$
= \langle R_n | e^{-(\hat{H}-E_T)\tau} \int dR_{n-1} | R_{n-1} \rangle \langle R_{n-1} | \Psi_T \rangle
$$

$$
= \int dR_{n-1} \langle R_n | e^{-(\hat{H}-E_T)\Delta \tau} | R_{n-1} \rangle \langle R_{n-1} | \prod_{n=1}^{n-1} e^{-(\hat{H}-E_T)\Delta \tau} | \Psi_T \rangle
$$

$$
= \int dR_{n-1} G(R_n, R_{n-1}) \langle R_{n-1} | \prod_{n=1}^{n-1} e^{-(\hat{H}-E_T)\Delta \tau} | \Psi_T \rangle
$$

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\[ \int dR_{n-1}dR_{n-2} \ldots dR_0 G(R_n, R_{n-1})G(R_{n-1}, R_{n-2}) \ldots G(R_1, R_0) \langle R_0 | \Psi_T \rangle, \]

where \( \langle R_0 | \Psi_T \rangle = \Psi_T(R_0) \). Although one integral symbol has been used in the final line, it’s implicit that we integrate over each \( dR_i \).

When using this technique for Fermi gases, we are forced to deal with the fermion sign problem. This is the case because fermions must be described by an antisymmetric wave function, which leads to near equal amounts of positive and negative contribution to the numerator and denominator of Eq. (3.42) and causes the calculation to become dominated by statistical fluctuations. In stochastic integration, the mixed estimate as given by Eq. (3.43) is expressed as a summation over a set of paths \( P_n \). Reading the equation from right to left, we can imagine a path as a walker propagating in imaginary time \( \tau \).

Take a finite number of sampling paths \( N_P \), where the final configurations \( R_n \) are distributed according to \( P(R_n) \), Eq. (3.22); this would require a path distribution of \( P(P_n) \). We rewrite equation Eq. (3.43), treating the numerator and denominator separately and assigning \( P(P_n) \) as a weight factor [62]:

\[
\langle \hat{H} \rangle_M = \frac{\tilde{n}}{\tilde{d}}, \\
\tilde{n} = \sum_{N_P} \frac{\Psi_T(R_n) \hat{H} G(R_n, R_{n-1}) \ldots G(R_1, R_0) \Psi_T(R_0)}{P(P_n)}, \\
\tilde{d} = \sum_{N_P} \frac{\Psi_T(R_n) G(R_n, R_{n-1}) \ldots G(R_1, R_0) \Psi_T(R_0)}{P(P_n)},
\]

(3.45)

where we have assumed \( \Psi_T(R) \) is real. The weight function \( P(P_n) \) will depend on the orientation of each configuration along the particular path. In the above numerator and denominator equations, \( G(R_n, R_{n-1}) \) and \( P(P_n) \) are always positive. Therefore, the sign of each term in the summations will depend on only the signs of
\( \Psi_T(R_n), \Psi_T(R_0), \) and \( \hat{H} \Psi_T(R_n) \) for each path. This last term reduces to a c-number: 
\( E \Psi_T(R_n) \), which can be negative or positive depending on the energy \( E \) and wave function value. If \( \Psi_T(R) \) has positive and negative regions then nodes will be crossed many times for large \( \tau \) (i.e., long paths) and, in the case of an anti-symmetric wave function, both numerator and denominator will approach zero due to near equal amounts of positive and negative contribution. One effective solution is to restrict the ability of \( \Psi_T(R) \) to change sign along any given path. Technically speaking, this \textit{fixed-node} approach involves removing walkers from the calculation when they cross a nodal surface [56]. This method is exact if the nodal structure of \( \Psi_T(R) \) is identical to that of the actual ground state wave function.

The standard DMC technique (e.g., when applied to bosons), is in principle exact. By introducing the fixed-node approximation for fermions, we calculate an upper bound to the true ground state energy as per the variational principle. It’s often not possible to determine the error introduced with the fixed-node approximation. In Chapter 4, however, we quantify the error of our calculations by comparing with other work.

The GFMC algorithm as described up to this point is sufficient to evaluate Eq. (3.42), however with just this basic design the walker population can undergo large fluctuations which make simulations inefficient. These fluctuations can be reduced by implementing an \textit{importance sampling} procedure in which a guiding function is introduced into the many body Schrödinger equation (see Ref. [63]). For the time evolving state \( \Psi(R, \tau) \) this equation is

\[
-\hbar \frac{\partial}{\partial \tau} \Psi(R, \tau) = (\hat{H} - E_T) \Psi(R, \tau).
\] (3.46)
Multiplying both sides by our guiding function, \( \Psi_T(R) \) (i.e., the trial wave function), we get

\[
-\hbar \Psi_T(R) \frac{\partial}{\partial \tau} \Psi(R, \tau) = \Psi_T(R) \hat{H} \Psi(R, \tau) - \Psi_T(R) E_T \Psi(R, \tau),
\]

\[
-\hbar \frac{\partial}{\partial \tau} [\Psi(R, \tau) \Psi_T(R)] = \Psi_T(R) \left[ - \sum_i \frac{\hbar^2}{2m_i} \nabla_i^2 \Psi(R, \tau) + V(R) \Psi(R, \tau) \right] - E_T \Psi(R, \tau) \Psi_T(R),
\]

(3.47)

where we have used the following identity to make a substitution in the 3rd line:

\[
\nabla^2 (\Psi \Psi_T) = \nabla \cdot (\Psi \nabla \Psi_T) + \nabla \cdot (\Psi_T \nabla \Psi)
\]

(3.48)

and introduced a general Hamiltonian, \( \hat{H} = - \sum_i (\hbar^2 / 2m_i) \nabla_i^2 + \hat{V} \), where we sum over \( i \) particles and define \( \hat{V} \Psi(R, \tau) = V(R) \Psi(R, \tau) \). Given the following expansion:

\[
\nabla \cdot \left[ \Psi \Psi_T \left( \frac{\nabla \Psi_T}{\Psi_T} \right) \right] = \nabla \cdot (\Psi \nabla \Psi_T)
\]

(3.49)

\[
= \Psi \nabla^2 \Psi_T + \nabla \Psi \cdot \nabla \Psi_T,
\]
we make another substitution and find:

\[-\hbar \Psi_T(R) \frac{\partial}{\partial \tau} \Psi(R, \tau) = -\sum_i \frac{\hbar^2}{2m_i} \nabla_i^2 [\Psi(R, \tau) \Psi_T(R)] - \sum_i \frac{\hbar^2}{2m_i} \Psi(R, \tau) \nabla_i^2 \Psi_T(R)\]

\[+ \sum_i \frac{\hbar^2}{m_i} \nabla_i \cdot \left[ \Psi(R, \tau) \Psi_T(R) \left( \frac{\nabla_i \Psi_T(R)}{\Psi_T(R)} \right) \right] + \left[ V(R) - E_T \right] \Psi(R, \tau) \Psi_T(R) \]

\[= -\sum_i \frac{\hbar^2}{2m_i} \nabla_i^2 \left[ \Psi(R, \tau) \Psi_T(R) \right] + \sum_i \frac{\hbar^2}{m_i} \nabla_i \cdot \left[ \Psi(R, \tau) \Psi_T(R) \left( \frac{\nabla_i \Psi_T(R)}{\Psi_T(R)} \right) \right] \]

\[+ \left[ -\sum_i \frac{\hbar^2}{2m_i} \left( \frac{\nabla_i^2 \Psi_T(R)}{\Psi_T(R)} \right) + V(R) - E_T \right] \Psi(R, \tau) \Psi_T(R). \]

(3.50)

Expressing this result in terms of the importance sampled wave function \( f(R, \tau) = \Psi(R, \tau) \Psi_T(R) \) and the local energy \( E_L(R) = \Psi_T^{-1}(R) \hat{H} \Psi_T(R) \), we find the following Schrödinger equation:

\[-\hbar \frac{\partial}{\partial \tau} f(R, \tau) = -\sum_i \frac{\hbar^2}{2m_i} \nabla_i^2 f(R, \tau) + \sum_i \frac{\hbar^2}{m_i} \nabla_i \cdot \left[ \left( \frac{\nabla_i \Psi_T(R)}{\Psi_T(R)} \right) f(R, \tau) \right] \]

\[+ [E_L(R) - E_T] f(R, \tau). \]

(3.51)

We define the *drift velocity* as \( v_{D,i}(R) = 2 \nabla_i \Psi_T(R) / \Psi_T(R) \) and introduce an operator \( \hat{F} \), defined such that

\[ \hat{F} f(R, \tau) = \sum_i \frac{\hbar^2}{m_i} \nabla_i \cdot \left[ \left( \frac{\nabla_i \Psi_T(R)}{\Psi_T(R)} \right) f(R, \tau) \right] \]

\[= \sum_i \frac{\hbar^2}{2m_i} \nabla_i \cdot \left[ v_{D,i}(R) f(R, \tau) \right]. \]

(3.52)

A new Green’s function must be used to propagate \( f(R, \tau) \). Rewriting Eq. (3.38), we
now have (see Refs. [64, 65])

\[ \tilde{G}(\mathbf{R}, \mathbf{R}') = \langle \mathbf{R} | e^{-(\hat{T} + \hat{F} + E_L - E_T) \Delta \tau} | \mathbf{R}' \rangle \]

\[ \approx \langle \mathbf{R} | e^{-(E_L - E_T) \frac{\Delta \tau}{2}} e^{-\hat{T} \Delta \tau} e^{-\hat{F} \Delta \tau} e^{-(E_L - E_T) \frac{\Delta \tau}{2}} | \mathbf{R}' \rangle \]

\[ = e^{-(E_L(\mathbf{R}) - E_T) \frac{\Delta \tau}{2}} \langle \mathbf{R} | e^{-\hat{T} \Delta \tau} e^{-\hat{F} \Delta \tau} | \mathbf{R}' \rangle e^{-(E_L(\mathbf{R}') - E_T) \frac{\Delta \tau}{2}}, \quad (3.53) \]

where

\[ f(\mathbf{R}, \tau + \Delta \tau) = \int d\mathbf{R'} \tilde{G}(\mathbf{R}, \mathbf{R}'; \Delta \tau) f(\mathbf{R}', \tau). \quad (3.54) \]

The kinetic energy propagator previously seen in Eq. (3.40) must be modified to include the drifting factors. This derivation can be seen at the end of Appendix B, where we include the extra drifting term \( \hat{F} \) that depends on the momentum (as opposed to \( \hat{T} \), which depends on the momentum squared). In analogy to Eq. (3.41), the new Green’s function evaluated up to \( O(\Delta \tau^2) \) is

\[ \tilde{G}(\mathbf{R}, \mathbf{R}') = \left[ \frac{m}{2\pi \hbar^2 \Delta \tau} \right]^{\frac{3N}{2}} \exp \left[ -\frac{m}{2} \frac{(\mathbf{R} - \mathbf{R}' - \mathbf{v}_D(\mathbf{R}) \Delta \tau \hbar^2 / m)^2}{\hbar^2 \Delta \tau} \right] \]

\[ \times \exp \left[ -\frac{\Delta \tau}{2} (E_L(\mathbf{R}) + E_L(\mathbf{R}') - 2E_T) \right], \quad (3.55) \]

where \( \mathbf{v}_D(\mathbf{R}) = (\mathbf{v}_{D,1}(\mathbf{R}), \mathbf{v}_{D,2}(\mathbf{R}), \ldots, \mathbf{v}_{D,N}(\mathbf{R})) \). The use of importance sampling will reduce walker population fluctuations because the branching term has been modified such that local energies are being evaluated in place of the (less stable) potential energies. As well, the drift velocity shifts walkers into configurations that correspond to larger \( |\Psi_T(\mathbf{R})| \), which maintains walker density in good areas of phase space. This also helps satisfy the fixed-node condition by drifting walkers away from the nodes of \( \Psi_T(\mathbf{R}) \).
Chapter 4

Strongly interacting 2D Fermi gases in the BEC-BCS crossover

Now that the problem has been set up and our methods seen in detail, we turn our attention once again to the dilute Fermi gas with tunable interactions. We study interaction strengths where the gas is in between a BEC state of tightly bound pairs (dimers) and a weakly paired BCS superfluid. In this regime, the gases are said to be strongly interacting and their properties are not fully understood. As expected we find that the mean-field BCS calculation, which gives the correct energy on each side of the crossover, is unreliable in between.

We present the results of our DMC calculations, first showing the energy per particle. We compare the mixed estimate, Eq. (3.42), as computed for Jastrow-Slater and Jastrow-BCS wave functions. Our variationally-optimal ground-state energy results are parameterized to find an equation of state (EOS) from which we determine Tan’s contact parameter and the chemical potential. Finally we calculate the pairing gap in the single particle excitation spectrum.
4.1 Equation of State

Figure 4.1 shows the ground-state energy per particle in the BEC-BCS crossover. The mean-field calculation [31] gives an energy per particle of

\[ E_{\text{BCS}} = E_{\text{FG}} + \epsilon_b/2, \quad (4.1) \]

where \( \epsilon_b \) is given by Eq. (2.48). Mean-field theory is expected to be accurate for weakly paired systems in the BCS limit (when \( E/N \to E_{\text{FG}} \)). The BEC limit of tightly bound pairs is also expected to be reasonably well described by mean field. On that side of the crossover, the energy scale grows rapidly by many orders of magnitude due to large binding energies. The QMC results become increasingly similar to mean-field predictions in each limit. Differences between our calculations and previous QMC results only become clear when subtracting the two-body binding energy contribution. We will compare to these studies in detail in Section 4.1.1.

The question arises of which wave function to use. We have introduced two many-body wave functions in Chapter 3. We test the Jastrow-Slater wave function \( \Phi_S(R) \), Eq. (3.11), for strongly interacting gases to quantify its shortcomings. This wave function has a long history of describing weak pairing in quantum gases. It can be seen from previous works on the 2D Fermi gases [32, 33] that \( \Phi_S(R) \) describes the weakly paired regime well on the BCS side of the crossover. Because it only accounts for pairing through the Jastrow component, \( \Phi_S(R) \) is not expected to provide reliable ground-state energies when the coupling is sufficiently strong. Also, this form has limited freedom to optimize the many-body wave-function nodes. The Jastrow-BCS wave function \( \Phi_{\text{BCS}}(R) \), Eq (3.12), contains parameters which are variationally optimized for each \( \eta \) independently. It is possible to choose the undetermined \( \alpha \)
Figure 4.1: Total energy per particle of the 2D strongly interacting Fermi gas. Thermodynamic limit extrapolated QMC data is plotted with a solid line (blue). At this energy resolution, all QMC results are in good agreement. The mean-field result is shown as a dashed line (black) for comparison. This is expected to be reasonably accurate for $|\eta| \gg 1$. Half of the binding energy per particle is plotted with a dotted line (orange). There is logarithmically small binding energy in the BCS limit and $|\epsilon_b|$ becomes very large in the BEC limit.
Figure 4.2: Our DMC energy results for the strongly interacting Fermi gas in the BEC-BCS crossover. The binding energy per particle has been subtracted and the units are $E_{FG} = \hbar^2 k_F^2 / 4m$. Our DMC calculations for the Jastrow-BCS and Jastrow-Slater wave functions are shown with circles (blue) and triangles (purple), respectively. With decreasing $\eta$, we see increasingly significant improvements over the Slater energy results by using the optimized BCS wave function.
Table 4.1: Our energy per particle values for 2D strongly interacting Fermi gases in the BEC-BCS crossover. We show results of \( N = 26 \) DMC calculations with variationally optimized Jastrow-BCS wave functions. The interaction strength is given by \( \eta = \log(k_F a_{2D}) \) and energies are expressed in units of the non-interacting gas \( E_{FG} = \epsilon_F/2 \). In Section 4.1.3, we parameterize the right column \( E/N - \epsilon_b/2 \) to determine an EOS.

<table>
<thead>
<tr>
<th>( \eta )</th>
<th>( E/N )</th>
<th>( \epsilon_b/2 )</th>
<th>( E/N - \epsilon_b/2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>-1.00</td>
<td>-18.5251(9)</td>
<td>-18.6344</td>
<td>0.1093(9)</td>
</tr>
<tr>
<td>-0.50</td>
<td>-6.7219(15)</td>
<td>-6.8552</td>
<td>0.1333(15)</td>
</tr>
<tr>
<td>0.00</td>
<td>-2.33831(55)</td>
<td>-2.52189</td>
<td>0.18358(55)</td>
</tr>
<tr>
<td>0.50</td>
<td>-0.66305(45)</td>
<td>-0.92775</td>
<td>0.26470(45)</td>
</tr>
<tr>
<td>0.75</td>
<td>-0.24619(34)</td>
<td>-0.56271</td>
<td>0.31652(34)</td>
</tr>
<tr>
<td>1.00</td>
<td>0.02976(23)</td>
<td>-0.34130</td>
<td>0.37106(23)</td>
</tr>
<tr>
<td>1.44</td>
<td>0.32673(28)</td>
<td>-0.14156</td>
<td>0.46829(28)</td>
</tr>
<tr>
<td>1.50</td>
<td>0.35600(28)</td>
<td>-0.12556</td>
<td>0.48156(28)</td>
</tr>
<tr>
<td>2.00</td>
<td>0.53274(16)</td>
<td>-0.04619</td>
<td>0.57893(16)</td>
</tr>
<tr>
<td>2.15</td>
<td>0.57010(19)</td>
<td>-0.03422</td>
<td>0.60432(19)</td>
</tr>
<tr>
<td>3.00</td>
<td>0.70844(15)</td>
<td>-0.00625</td>
<td>0.71469(15)</td>
</tr>
<tr>
<td>4.00</td>
<td>0.79185(14)</td>
<td>-0.00085</td>
<td>0.79270(14)</td>
</tr>
<tr>
<td>5.00</td>
<td>0.84125(11)</td>
<td>-0.00011</td>
<td>0.84136(11)</td>
</tr>
</tbody>
</table>

parameters in the pairing function, Eq. (3.14), such that \( \Phi_{BCS}(\mathbf{R}) \) has the same nodes as \( \Phi_S(\mathbf{R}) \). This is generally the set of \( \alpha \)'s used as the starting point for optimization.

Our DMC energy results are shown in Tab. 4.1 and plotted in Fig. 4.2 with half of the two-body binding energy \( \epsilon_b \) subtracted. The energy per particle is shown as a function of interaction strength \( \eta = \log(k_F a_{2D}) \) in units of \( E_{FG} \). Error bars represent statistical uncertainty, which is much smaller than the circular symbol used to mark each point. The triangles are calculated using the Jastrow-Slater wave function [50], and we see significant improvements in the crossover and BEC regimes by optimizing the pairing function. In this plot, the mean-field result would correspond to a horizontal line at 1. In the BEC limit of tightly bound pairs, however, it appears that \( E/N \rightarrow \epsilon_b/2 \). Although the QMC results seem to suggest a trend away from the BEC
mean field prediction, the binding energy becomes very large in this limit such that
$|\epsilon_b| \gg E_{FG}$ and $E_{BCS} \approx \epsilon_b/2$.

4.1.1 Comparison to previous ab initio methods

We compare to previous DMC [32] and AFQMC [33] results for the strongly interacting 2D gas in Fig. 4.3. The previous DMC results were calculated using a square well potential to model two-body interactions, and wave functions with only one variational parameter (at most); a Jastrow-Slater wave function was used for $\eta > 1$, and a BCS-pairing wave function was used for $\eta < 1$. In our calculations, we use a continuous potential, Eq. (2.46), that decays smoothly. More importantly, we optimize 10 variational parameters in the pairing function in Eq. (3.12), for each calculation. We see a notable improvement from previous DMC ground-state energy results in the crossover region. The DMC method is variational, so our lower energy results are closer to the true ground-state energy. We directly compare results for $\eta = 0.75$, $\eta = 1.44$, and $\eta = 2.15$ [50], and find improvements of 12%, 12%, and 6%, respectively, on the scale of Fig. 4.3.

The AFQMC method used by Shi et al is in principle exact, in the sense that it does not suffer from the sign problem for $N_\uparrow = N_\downarrow$ configurations. Therefore, limitations of the fixed-node approximation can be seen by comparing our DMC results with AFQMC. The error introduced by this approximation is quite small: differences are 0.014 $E_{FG}$ at most. For comparison, in 3D the AFQMC energy per particle for the unitary Fermi gas is 0.372(5) $E_{FG}$ [66]; this can be compared to a detailed DMC study which finds an energy of $\sim 0.3897(4) E_{FG}$ [53]. While this result was for one interaction strength in the middle of the 3D crossover, we find a similar difference for a range of $\eta$ on the BCS side of the 2D crossover. For $\eta < 1$, we find increasingly
Figure 4.3: The energy per-particle results for various \textit{ab initio} QMC methods are compared. Our optimized Jastrow-BCS wave function results are shown with circles (blue). These closely follow the AFQMC energy results of Shi \textit{et al} [33], plotted as diamonds (green). Previous DMC energy results of Bertaina & Giorgini [32] are plotted as squares (red); since DMC is variational, the new results show a notable improvement. Note that the error bars, which are provided for all data, are comparable to the symbol size (or larger) only for previous DMC results.
smaller differences between DMC and AFQMC as we approach the BEC limit.

### 4.1.2 Finite size corrections

All energy results seen up to this point are for $N = 26$; such a system size is well suited to simulate the $N \to \infty$ 2D system in the region studied here. Specifically, after finite-size corrections are applied, the $N = 26$ AFQMC energies calculated by Shi et al differ from their $N \to \infty$ energies by $0.003 \, E_{\text{FG}}$ or less for interaction strengths $\eta < 1$. For $\eta > 1$ the maximum difference from the AFQMC TL value is $0.01 \, E_{\text{FG}}$ at $\eta \approx 2$. Finite-size effects (first touched upon in Section 3.1) are addressed by applying a TL correction to QMC energy calculations. Specifically, the finite-size effects for the Slater wave function are illustrated as a function of $N$ in Fig. 3.1. Here we see reasonably small variation from the TL for $N = 26$: for very large $\eta$ (say $\eta > 4$) such a correction would essentially all come from the kinetic energy and would be $\sim 0.041 \, E_{\text{FG}}$; this matches the correction used by Bertaina & Giorgini [32] (from Fermi liquid theory) at $\eta \gtrsim 1$. As alluded to but not explicitly written, this specific correction arises by considering the difference in kinetic energy between $N = 26$ and $N \to \infty$ systems.

For $\eta < 4$, using the BCS wave function, the finite-size effects are greatly reduced since pairing is taken into account. One way to estimate their magnitude is to solve the mean-field BCS problem for both infinite and finite-size systems and compare the two, as was done in Ref. [21] for neutrons. We define

$$E_{\text{TL}} \equiv E_{\text{QMC}}(N) + \Delta E_{\text{BCS}}(N) \quad (4.2)$$

where $E_{\text{QMC}}(N)$ is our DMC energy. The correction, $\Delta E_{\text{BCS}}(N) = E_{\text{BCS}} - E_{\text{BCS}}(N)$,
Figure 4.4: The difference in energy between $E_{\text{BCS}} = E_{\text{FG}} + \epsilon_b/2$ and the finite size solution $E_{\text{BCS}}(N = 26)$, plotted for $\eta > 0$. Diamond points (green) were determined by Shi et al [67] and the solid line (black) is our interpolation.
is the difference in energy between the BCS solutions for infinite and finite size systems, where $E_{\text{BCS}}$ is given in Eq. (4.1). Shi et al have solved $\Delta E_{\text{BCS}}(N = 26)$ for the 2D Fermi gas, and indeed find the correction to be quite small in the crossover: 0.001 $E_{\text{FG}}$ at $\eta \approx 1$ and 0.01 $E_{\text{FG}}$ at $\eta \approx 2$ [33, 67]. This is visualized in Fig. 4.4, where we plot their values as well as our interpolation. It is easy to see that no finite-size correction is necessary in the deep BEC regime (or near it). In the BCS limit we find $\Delta E_{\text{BCS}}(N = 26)$ roughly approaches the Slater correction of 0.041 $E_{\text{FG}}$.

### 4.1.3 EOS parameterization

Our TL equation of state is parametrized using similar methods as in Refs. [32, 33]. We fit to a 7th-order polynomial for the crossover region: $f(\eta) = \sum_{i=0}^{7} c_i \eta^i$, a dimer form in the BEC regime (see Ref. [38]), and an expansion of $1/\eta$ in the BCS regime (see Ref. [68]). For $\eta < -0.25$ we fit to:

$$f^{\text{BEC}}(\eta) = \frac{1}{2x} \left[ 1 - \frac{\log(x) + d}{x} + \sum_{i=0}^{2} c_i \left[\log(x)\right]^i \right], \quad (4.3)$$

where $x = \log[4\pi/(k_F a_d)^2] \approx 3.703 - 2\eta$ (for the dimer scattering length $a_d \approx 0.557 a_{2D}$) and $d = \log \pi + 2\gamma + 0.5$. For $\eta > 2.5$ we fit to:

$$f^{\text{BCS}}(\eta) = 1 - \frac{1}{\eta} + \sum_{i=2}^{4} \frac{c_i}{\eta^i}. \quad (4.4)$$

Values of $c_i$ in Eq. (4.3) and Eq. (4.4) are determined using continuity conditions for $f$, $\partial f/\partial \eta$, and $\partial^2 f/\partial \eta^2$ at the matching points. We pick our matching points to optimize the overall fit and include as much of the crossover polynomial function as possible. Also, we ensure that our matching point for Eq. (4.3) is selected on the BEC side of the crossover. In Tab. 4.2 we give the parameters for our TL corrected
EOS. This method is also used to produce the lines of best fit seen in Fig. 4.3 for Bertaina & Giorgini and Shi et al.

Table 4.2: The final parameters for our EOS, where we fit to \((E_{TL}/N - \epsilon_b/2)/E_{FG}\). A 7th-order polynomial \(f(\eta)\) is used in the crossover regime and we fit to \(f^{\text{BEC}}(\eta)\) and \(f^{\text{BCS}}(\eta)\) on either side. Their functional forms, Eq. (4.3) and Eq. (4.4), are based on the limiting behaviour on each side of the crossover and they each contain 3 parameters that are determined by continuity restrictions. In an effort to include as much of the intermediate polynomial as possible and minimize the overall variance of our fit, we select the matching points as \(\eta = -0.25\) and \(\eta = 2.5\).

<table>
<thead>
<tr>
<th>(c_i)</th>
<th>(f^{\text{BEC}}(\eta))</th>
<th>(f(\eta))</th>
<th>(f^{\text{BCS}}(\eta))</th>
</tr>
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<tr>
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</tr>
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</tr>
<tr>
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<td>(c_7)</td>
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</tr>
</tbody>
</table>

### 4.1.4 Contact parameter

The contact parameter is universal for dilute Fermi gases [39, 40], and can be related to thermodynamic quantities including the pressure and chemical potential. It describes the momentum distribution \(n(k)\) behaviour at large \(k\) and therefore encodes information about short-range physics. We derive a relation between the contact and the derivative of our EOS with respect to \(\eta\). This task requires little effort, as our starting point is the 2D contact defined in Ref. [69]:

\[
C'(E) = \frac{2\pi m}{\hbar^2} \left. \frac{dE}{d \log(a_{2D})} \right|_{A,\mu},
\]  

(4.5)
Figure 4.5: The contact parameter as determined by the EOS derivative. The result from our DMC method is plotted as the solid line (blue) and we compare to other QMC results. We show previous DMC [32] with a dotted line (red), and AFQMC [33] with a dashed line (green). Qualitatively, the contact reaches a maximum on the BCS side of the strong coupling regime and decays more rapidly on the BEC side of the crossover.
where $E$ is the total energy and, because the derivative is taken at constant entropy, we have explicitly included the fact that area $A$ and chemical potential $\mu$ are constant (see Ref. [70]). The chain rule can be used to show that $dE/d\log(a_{2D}) = dE/d\log(k_Fa_{2D})$.

In general $E = E(N, A, a_{2D})$, however $N$ and $A$ are treated as constant, allowing us to pass $N$ and $k_F = \sqrt{2\pi N/A}$ into the derivative:

$$C'(E) = N \frac{2\pi m}{\hbar^2} \frac{d(E/N)}{d\eta} = A \frac{k_F^2 m}{\hbar^2} \frac{d(E/N)}{d\eta}$$

$$= A \frac{k_F^2 m \epsilon_F}{\hbar^2} \frac{d[(E/N)(2/\epsilon_F)]}{d\eta}$$

$$= A \frac{k_F^4}{4} \frac{d[(E/N)/E_{FG}]}{d\eta}. \quad (4.6)$$

In line 2 we multiply and divide by the non-interacting Fermi gas energy, $E_{FG} = \epsilon_F/2 = \hbar^2 k_F^2/4m$. As can be seen, the contact $C'(E)$ as defined in Ref. [69] depends on $A$, and is therefore an extensive quantity. We define the contact to be intensive: \( \tilde{C}(E) \equiv C'(E)/A \), such that $\tilde{C}(E)$ remains constant regardless of gas area $A$.

In 3D the contact parameter's magnitude steadily declines as one goes from the BEC to the BCS regime [71]. Qualitatively, something similar happens in 2D. In order to bring out more detailed effects, following from Eq. (4.6) we subtract the two-body binding energy contribution and thereby relate our EOS to the (“many-body”) contact density as follows:

$$\frac{C}{k_F^4} = \frac{1}{k_F^4} \left( \tilde{C}(E_{TL}) - \tilde{C}(N\epsilon_b/2) \right)$$

$$= \frac{1}{4} \frac{d[(E_{TL}/N)/E_{FG}]}{d\eta} - \frac{1}{4} \frac{d[(\epsilon_b/2)/E_{FG}]}{d\eta}, \quad (4.7)$$

where $N\epsilon_b/2$ is the total binding energy and $E_{TL}$ is defined in Eq. (4.2). Our results are shown along with other QMC calculations in Fig. 4.5. We find a maximum value
of $C/k_F^4 \approx 0.054$ at $\eta \approx 1$. Our curve is slightly different than Shi et al who find a maximum of $C/k_F^4 \approx 0.05$ at roughly the same $\eta$. Bertaina & Giorgini find a higher and significantly more narrow peak at $\eta \approx 0.5$.

4.1.5 Chemical potential

We have determined the chemical potential $\mu$ using our EOS. In order to derive a relationship, we define

$$\zeta(\eta) = \frac{E_{\text{TL}}(\eta)}{N} \frac{1}{E_{\text{FG}}} = \frac{2E_{\text{TL}}(\eta)}{N\epsilon_F}, \quad (4.8)$$

where $E_{\text{TL}}(\eta)$ is the total ground state energy. This quantity is related to our parameterized EOS (see Section 4.1.3), where we fit to $f(\eta) = (E_{\text{TL}}/N - \epsilon_b/2)/E_{\text{FG}}$; the new quantity $\zeta(\eta)$ can easily be determined by adding $\epsilon_b/2$ in units of $E_{\text{FG}}$ to $f(\eta)$. Noting that $\epsilon_F = (\pi N \hbar^2)/(m A)$ in 2D (using $k_F^2 = 2\pi N/A$), the chemical potential is related to $\zeta(\eta)$ as follows:

$$\mu = \frac{\partial E_{\text{TL}}}{\partial N} = \frac{\partial}{\partial N} \left[ \frac{\epsilon_F N \zeta(\eta)}{2} \right]$$

$$= \frac{1}{2} \frac{\partial \epsilon_F N}{\partial N} \zeta(\eta) + \frac{\epsilon_F N}{2} \frac{\partial \zeta(\eta)}{\partial \eta} \frac{\partial N}{\partial N}$$

$$= \frac{1}{2} \frac{\partial}{\partial N} \left( \frac{\pi N^2 \hbar^2}{m A} \right) \zeta(\eta) + \frac{\epsilon_F N}{2} \frac{\partial \zeta(\eta)}{\partial \eta} \frac{\partial N}{\partial N}$$

$$= \left( \frac{\pi N \hbar^2}{m A} \right) \zeta(\eta) + \frac{\epsilon_F \partial \zeta(\eta)}{4} \frac{\partial N}{\partial \eta}$$

$$= \epsilon_F \zeta(\eta) + \frac{\epsilon_F \partial \zeta(\eta)}{4} \frac{\partial N}{\partial \eta}. \quad (4.9)$$
Figure 4.6: The chemical potential for strongly interacting 2D Fermi gases in the BEC-BCS crossover. Our result (maroon) is shown along with AFQMC (orange) and Hartree-Fock calculations in each limit (red and green). The blue circles are experimental results [28], for which a trend away from the QMC calculations is seen in the BCS limit. It’s difficult to directly compare our $T = 0$ results with experiment due to finite-temperature and quasi-2D effects. This figure has been provided by Tilman Enss [72] and we note that an alternate definition of $a_{2D}$ has been used (see the beginning of Section 2.5). As such, the x-axis must be shifted by $\log(2/e^\gamma) \approx 0.12$ to the right to match the $\eta$ used for all other plots. Furthermore, the binding energy here is defined to be positive (in contrast to our definition in Eq. (2.48)) and the natural logarithm is written as $\ln$ instead of $\log$. 
In the third line we have evaluated $\partial \eta / \partial N$ using

$$\frac{\partial [\log (k_Fa_{2D})]}{\partial N} = \frac{\partial [\log (\sqrt{2\pi N/A} a_{2D})]}{\partial N} = \frac{1}{2N}.$$ (4.10)

Expressing the chemical potential in units of the non-interacting Fermi gas, we find

$$\frac{\mu_{\text{FG}}}{E_{\text{FG}}} = 2 \left( \zeta(\eta) + \frac{1}{4} \frac{\partial \zeta(\eta)}{\partial \eta} \right).$$ (4.11)

Our result is plotted in Fig. 4.6, which shows the chemical potential with half of the two-body binding energy subtracted. Our DMC determination is the maroon line, which is very similar to the orange line for AFQMC [33]. The blue circles are experimental results [28], which match very nicely with QMC in the deep BEC regime. Differences become more significant in the BCS limit, due to finite-temperature and quasi-2D effects in the experiment. Shown with red and green lines are the Hartree-Fock calculations for Bose and Fermi gases, respectively.

### 4.2 Pairing gap

The single-particle excitation-spectrum pairing gap can be calculated by comparing the total energy of configurations with an unpaired particle to that of fully paired-up systems (i.e., from the odd-even energy staggering) [18]. For the 2D gas, the only previous ab initio calculation of the pairing gap is the one by Bertaina & Giorgini [32]. Because we have variationally improved the EOS, it is justified to re-calculate the pairing gap using our new many-body wave functions. For the case when $N_\uparrow \neq N_\downarrow$, the BCS wave function in Eq. (3.12) is no longer valid. Adding one additional particle to an even system such that we have $M = (N - 1)/2$ pairs, the
wave function can be written as:

$$\Phi_{\text{BCS}}(R) = A[\phi(r_{11'})\phi(r_{22'})...\phi(r_{MM'})\psi_{k_u}(r)], \quad (4.12)$$

where the unpaired particle at position $r$ and momentum $k_u$ is placed into a plane-wave eigenstate. Arbitrarily selecting the particle to be spin-up, the wave function is given by the determinant

$$\Phi_{\text{BCS}}(R) \propto \begin{vmatrix} \phi(r_{11'}) & \phi(r_{12'}) & \cdots & \phi(r_{1M'}) & \psi_{k_u}(r_1) \\ \phi(r_{21'}) & \phi(r_{22'}) & \cdots & \phi(r_{2M'}) & \psi_{k_u}(r_2) \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \phi(r_{M+1,1'}) & \phi(r_{M+1,2'}) & \cdots & \phi(r_{M+1,M'}) & \psi_{k_u}(r_{M+1}) \end{vmatrix}. \quad (4.13)$$

The extra particle’s momentum must be treated as a variational parameter. For $N = 27$ systems (with one unpaired particle), we found the optimal $|k_u|$, in units of $2\pi/L$, to be 0 for $\eta \lesssim -1$ and $\sqrt{5}$ for $\eta \gtrsim 3$. In the crossover region we see a smooth transition as more (or less) momentum levels become available to the extra particle. Note that for our $N = 26$ system, the maximum k-state occupied in the Slater case is $k_{\text{max}} = (2\pi/L)\sqrt{5}$. Our results are consistent with variational calculations for the 3D Fermi gas, which find $|k_u| = 0$ in the BEC limit and $|k_u| = k_{\text{max}}$ in the BCS limit [51].

To determine the pairing gap, we use the odd-even energy staggering:

$$\Delta_{\text{gap}} = E(N + 1) - \frac{1}{2}[E(N) + E(N + 2)], \quad (4.14)$$

where $N$ is an even number. Accurate calculations are possible for cold atomic gases because $\Delta_{\text{gap}}$ is a large fraction of the total energy. Each of our points in Fig. 4.7
Figure 4.7: The pairing gap in the strong coupling crossover. The binding energy per particle has been subtracted and the units are $\epsilon_F = \hbar^2 k_F^2 / 2m = 2 E_{FG}$. Our results are shown with circular symbols (blue) and the mean-field prediction is shown with a solid line (black). Our calculated chemical potential $\mu$ becomes zero for the interaction strength $\eta \approx 0.65$. This location is marked with a dotted line (blue). Mean-field theory predicts that $\mu = 0$ where the curve becomes flat, at $\eta \approx 0.12$. 

\[ \Delta_{\text{gap}} + \epsilon_0 / 2 \left[ \epsilon_F \right] \]

\[ \eta = \log(k_F a_{2D}) \]
is the result of 3 separate DMC simulations. We find a broad peak about \( \eta = 0 \) at \( \Delta_{\text{gap}} + \epsilon_b/2 \approx 0.65 \epsilon_F \). The mean-field description identifies \( \Delta_{\text{gap}} \) as the minimum Bogoliubov quasiparticle energy, giving \( \Delta_{\text{gap}} = \sqrt{2\epsilon_F|\epsilon_b|} \) for positive \( \mu \) when \( \epsilon_F > |\epsilon_b|/2 \) and \( \Delta_{\text{gap}} = \epsilon_F + |\epsilon_b|/2 \) for negative \( \mu \) when \( \epsilon_F < |\epsilon_b|/2 \) [30, 31]. The mean-field chemical potential is given by \( \mu = \epsilon_F + \epsilon_b/2 \), and the transition between gap equations at \( \mu = 0 \) corresponds to \( \eta \approx 0.12 \). Evaluating the derivative \( \partial E_{\text{TL}}/\partial N \) (see Section 4.1.5) we find that for our strongly coupled theory the chemical potential changes sign at \( \eta \approx 0.65 \).

Considering the energy difference between mean field and QMC in Fig. 4.1, it’s not expected that the mean field will give accurate pairing gaps in the crossover: our gaps in the strongly coupled regime of the crossover are smaller than the mean-field values. This was first found by Bertaina & Giorgini [32], but our detailed values are different due to improved optimization. Our results follow a smoother trend and have significantly smaller error bars. Note that as we go deep into the BCS regime, one expects from the theory of Gorkov and Melik-Barkhudarov that the pairing gap should be suppressed by a factor of \( e \) with respect to the BCS value [37]. (This is to be compared with the factor of \( (4e)^{1/3} \) that appears in the 3D case [73]). Our (finite-size uncorrected) results do not exhibit such a suppression. Of course, it is very difficult to extract a pairing gap from DMC simulations for \( \eta \gg 1 \), where the gap is small.
Chapter 5

Summary and outlook

We have performed \textit{ab initio} calculations of the ground state energy for strongly interacting two-component Fermi gases in 2D. Probing the BEC-BCS crossover, we studied a range of interaction strengths. This was accomplished by varying the potential, Eq. (2.46), in our Hamiltonian, Eq. (3.8). In order to determine a relationship between the potential parameters $v_0$ and $\mu$ and the interaction strength $\eta$ for the many-body problem (see Fig. 2.6), we have solved the two-body problem. Scattering theory for both 2D and 3D collisions was introduced in Chapter 2, where we examined relationships between the radial wave functions $u(r)$ and the scattering parameters $a$ and $r_e$ (as illustrated in Fig. 2.7 for the 2D case). Although the 2D and 3D scattering theories were developed to nearly the same extent, we paid close attention to the 2D problem and our numerical solution techniques. Turning to the many-body context, in Chapter 3 we first determined the energy of a non-interacting, two-component Fermi gas as a function of the particle number $N$. Specifically, in Fig. 3.1, we examined finite-size effects. When including interactions, the many-body wave function is non-trivial to determine. We discussed two trial wave functions, Eq. (3.10) and Eq. (3.12), with focus on their application to QMC. Results were shown in Fig. 3.2 for the pairing...
functions, Eq. (3.14), as determined by variational energy minimization of the BCS wave function. In Section 3.3 of this chapter, the Monte Carlo method was discussed: we introduced foundational concepts, VMC, and studied DMC in detail.

Finally, we showed our results in Chapter 4. We found significant improvements over previous DMC ground-state energy calculations of Fermi gases in the strongly interacting crossover. When comparing to AFQMC calculations, our EOS was found to be very similar as a result of our variational minimization of the effects of the fixed-node approximation. All QMC calculations were found to be in good agreement on the BCS side of the crossover for $\eta \gtrsim 3$. In this regime, the Jastrow-Slater wave function, Eq. (3.11), can provide a good description of the weak many-body pairing. For $\eta \lesssim 3$, we showed the Jastrow-Slater wave function is inadequate (see Fig. 4.2) and the Jastrow-BCS pairing wave function, Eq. (3.12), provides an increasingly better description as we cross over into the BEC regime. Using our EOS, we also determined the contact parameter and chemical potential. These look similar to the AFQMC results and our contact peaks at roughly the same interaction strength $\eta \approx 1$. Our final results are the pairing gaps for various $\eta$, which are currently the most dependable predictions available for the 2D Fermi gas. After subtracting the binding energy per particle, we found the gap to be a significant fraction of the Fermi energy in the strongly coupled crossover regime.

There are many research opportunities that naturally follow from the present work. The pairing evolution between dimensions could be studied by probing the transition of the Fermi gas between 2D and 3D. This has already been achieved in experiment [74, 75]. Our study could be extended to the quasi-2D regime by introducing a finite box-length or an external trap in the third dimension. Another possible research avenue involves a two-component Fermi gas in mixed dimensions,
where one species is confined to 2D and the other is free to move in 3D space [76]. Two-dimensional polarized gases would also be amenable to a study along the lines of the present work. Furthermore, the 2D Fermi gas could be studied under the influence of a periodic external potential. This model could describe a two-component gas in an optical lattice [77, 78], and has recently been applied to the problem of neutron matter interacting with a lattice of ions in a neutron star [79]. Another interesting problem is the two-component Fermi gas with spin-orbit coupled interactions. Experimentalists have been able to induce spin-orbit interactions in the 3D Fermi gas by creating an effective p-wave coupling between opposite spin particles [80]. One of the factors that makes this gas interesting is the prediction that spin-orbit interactions increase the critical temperature [81].
Determination of the $c$ parameter in the beta function $\tilde{\beta}(r)$

As discussed in Section 3.2.2, the beta function defined by

$$
\tilde{\beta}(r) = \beta(r) + \beta(L - r) - 2\beta(L/2) \quad \text{for } r \leq L/2,
$$

$$
= 0 \quad \text{for } r > L/2,
$$

$$
\beta(r) = [1 + cbr] [1 - e^{-dbr}] \frac{e^{-br}}{dbr} ,
$$

(1)

should satisfy the equation

$$
\left. \frac{\partial \tilde{\beta}(r)}{\partial r} \right|_{r=0} = \left[ \frac{\partial \beta(r)}{\partial r} + \frac{\partial \beta(L-r)}{\partial r} - 2 \frac{\partial \beta(L/2)}{\partial r} \right]_{r=0} = 0 .
$$

(2)

The parameters $b$ and $d$ are determined variationally and $c$ is given by Eq. (3.18), which follows from the evaluation of Eq. (2) above. In order to show this, we first evaluate the $\partial \beta(r)/\partial r$ term, which can be arranged as

$$
\frac{\partial \beta(r)}{\partial r} = - \frac{(1 - e^{-dbr}) e^{-br}}{dr} - \frac{(1 - e^{-dbr}) cbe^{-br}}{d} + cbe^{-dbr} e^{-br}
$$

$$
+ \left[ \frac{e^{-dbr} e^{-br}}{r} - \frac{(1 - e^{-dbr}) e^{-br}}{dbr^2} \right] .
$$

(3)
Each term is treated independently in the limit as \( r \to 0 \). The final two (in square brackets) are grouped together before using L'Hôpital's rule to evaluate the limit of the combined function. The rule is applicable when both numerator and denominator approach 0 as \( r \to 0 \), and in the following lines it’s used implicitly.

\[
\frac{\partial \beta(r)}{\partial r} \bigg|_{r=0} = - \left. \frac{d b e^{-d b r} e^{-b r}}{d} \right|_{r=0} + cb + \left[ \left. \frac{d b r e^{-d b r} e^{-b r} - (1 - e^{-d b r}) e^{-b r}}{d b r^2} \right|_{r=0} \right]
\]

\[
= -b + cb + \left[ \left. \frac{d b r e^{-d b r} e^{-b r} - (1 - e^{-d b r}) e^{-b r}}{d b r^2} \right|_{r=0} \right]
\]

\[
= -b + cb - \frac{d b}{2},
\]

where the term in square brackets has been evaluated as follows:

\[
\left[ \frac{d b r e^{-d b r} e^{-b r} - (1 - e^{-d b r}) e^{-b r}}{d b r^2} \right]_{r=0} = \left. \frac{-d b^2 r(1 + d) e^{-d b r} e^{-b r} + b(1 - e^{-d b r}) e^{-b r}}{2 d b r} \right|_{r=0}
\]

\[
= - \left. \frac{b(1 + d)}{2} + \frac{b e^{-b r} e^{-d b r} - b^2 e^{-b r} (1 - e^{-d b r})}{2 d b} \right|_{r=0}
\]

\[
= - \frac{d b}{2}.
\]

(5)

The result in Eq. (5) can also be arrived at by taking the zero-order term of a Taylor expansion about \( r = 0 \). The \( L \) dependence in the expression for \( c \) is introduced by the \( \partial \beta(L - r)/\partial r \) term, which is evaluated in a similar way. We begin by arranging the derivative as

\[
\frac{\partial \beta(L - r)}{\partial r} = \frac{e^{-b L} e^{b r}}{d b (L - r)} \left[ - c b (1 - e^{-d b L} e^{d b r}) - (1 + c b L - c b r)(d b e^{-d b L} e^{d b r}) 
\right.
\]

\[
+ b (1 + c b L - c b r)(1 - e^{-d b L} e^{d b r}) + \frac{(1 + c b L - c b r)(1 - e^{-d b L} e^{d b r})}{L - r} \right].
\]

(6)
At $r = 0$ this becomes

\[
\left. \frac{\partial \beta(L - r)}{\partial r} \right|_{r=0} = \frac{e^{-bL}}{dbL} \left[ -cb(1 - e^{-dbL}) - (1 + cbL)(db e^{-dbL}) \right.
\]
\[
+ b(1 + cbL)(1 - e^{-dbL}) + \frac{(1 + cbL)(1 - e^{-dbL})}{L} \left. \right|_{r=0} \]
\[
= \frac{e^{-bL}}{dbL} \left[ c(-db^2Le^{-dbL} + b^2L - b^2Le^{-dbL}) - db e^{-dbL} + b - be^{-dbL} + \frac{1}{L} - \frac{e^{-dbL}}{L} \right] .
\]

(7)

The $\tilde{\beta}(L/2)$ term has no $r$ dependence so $\partial \beta(L/2)/\partial r = 0$. We are now able to evaluate Eq. (2):

\[
0 = \left[ \frac{\partial \beta(r)}{\partial r} + \frac{\partial \beta(L - r)}{\partial r} - 2 \frac{\partial \beta(L/2)}{\partial r} \right]_{r=0}
\]
\[
= -b + cb - \frac{db}{2} + \frac{e^{-bL}}{dbL} \left[ c(-db^2Le^{-dbL} + b^2L - b^2Le^{-dbL}) \right.
\]
\[
- db e^{-dbL} + b - be^{-dbL} + \frac{1}{L} - \frac{e^{-dbL}}{L} \left. \right]
\]
\[
= c \left[ \frac{e^{-bL}}{dbL} \left( b^2L - b^2Le^{-dbL} - db^2Le^{-dbL} \right) + b \right]
\]
\[
- \frac{e^{-bL}}{dbL} \left[ \frac{e^{-dbL}}{L} + db e^{-dbL} + be^{-dbL} - b - \frac{1}{L} \right] - \frac{db}{2} - b .
\]

(8)

Multiplying each side by $2dbL^2e^{bL}e^{dbL}$ and rearranging, we find the result for $c$:

\[
c = \frac{2 + 2dbL + (dbL)^2e^{bL(1+d)} + 2db^2L^2e^{bL(1+d)} + 2bL - 2e^{dbL}bL - 2e^{dbL}}{2b^2L^2(e^{dbL} - 1 - d + de^{bL(1+d)})} .
\]

(9)
Appendix B

The kinetic energy propagator for N particles in 2D

First we evaluate the spatial expectation value of $e^{-\hat{T}\Delta\tau}$ for 1 particle, and write the kinetic energy operator as $\hat{T} = -\hat{p}^2/2m$, where $\hat{p}$ is the momentum operator. The momentum eigenstates $|p\rangle$ satisfy the relation $\hat{p}|p\rangle = p|p\rangle$, where the c-number $p$ is the momentum of state $|p\rangle$. The expectation value we are interested in is defined as

$$
\langle R|e^{-\hat{T}\Delta\tau}|R'\rangle_{N=1} = \langle r|e^{-\frac{\hat{p}^2\Delta\tau}{2m}}|r'\rangle \tag{10}
$$

There are two independent integrations required, which we evaluate by introducing the momentum-space resolution of the identity operator: $1 = \int_{-\infty}^{\infty} dp|p\rangle\langle p|$. For the x component:

$$
\int_{-\infty}^{\infty} dp_x \langle x|e^{-\frac{\hat{p}^2\Delta\tau}{2m}}|p_x\rangle\langle p_x|x'\rangle
$$

$$
= \int_{-\infty}^{\infty} dp_x \langle x|p_x\rangle e^{-\frac{p_x^2\Delta\tau}{2m}}\langle p_x|x'\rangle
$$

$$
= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dp_x e^{-\frac{p_x^2\Delta\tau}{2m} + p_x \frac{\hbar}{2m}(x-x')} \tag{10}
$$

$$
= \frac{1}{2\pi\hbar} \sqrt{\frac{2m\pi}{\Delta\tau}} e^{-\frac{m(x-x')^2}{2\Delta\tau \hbar^2}}
$$

95
\[ \langle r | e^{-\hat{T}\tau} | r' \rangle = \left[ \frac{m}{2\pi \hbar^2 \Delta \tau} \right]^{2} e^{-\frac{m(x-x')^2}{2\Delta \tau \hbar^2}} e^{-\frac{m(y-y')^2}{2\Delta \tau \hbar^2}}. \]  

In the 3rd line we have substituted plane waves in place of the inner products using 
\[ \langle x | p \rangle = e^{ipx/\hbar}/\sqrt{2\pi \hbar} \text{ and } \langle p | x \rangle = e^{-ipx/\hbar}/\sqrt{2\pi \hbar} \text{ and in the 4th line we have evaluated the Gaussian integral: } \int e^{-ap^2+bp} dp = \sqrt{\pi/a} e^{b^2/4a}. \]  

Now including the y component:

\[ \langle r | e^{-\hat{T}\tau} | r' \rangle = \left[ \frac{m}{2\pi \hbar^2 \Delta \tau} \right]^{2} e^{-\frac{m(x-x')^2}{2\Delta \tau \hbar^2}} e^{-\frac{m(y-y')^2}{2\Delta \tau \hbar^2}}. \]  

Generalizing to \( N \) particles we note that \( \hat{p}^2 = \hat{p}_{1,x}^2 + \hat{p}_{1,y}^2 + \cdots + \hat{p}_{N,x}^2 + \hat{p}_{N,y}^2 \), and solve the full problem:

\[ \langle R | e^{-\hat{T}\tau} | R' \rangle = \langle r_1, r_2, \ldots, r_N | \prod_{i=1}^{N} e^{-\frac{\hat{p}_{i,x}^2}{2m}} | r_1, r_2, \ldots, r_N \rangle \]

\[ = \langle r_1, r_2, \ldots, r_N | \prod_{i=1}^{N} e^{-\frac{\hat{p}_{i,x}^2 + \hat{p}_{i,y}^2}{2m}} | r_1, r_2, \ldots, r_N \rangle \]

\[ = \left[ \frac{m}{2\pi \hbar^2 \Delta \tau} \right]^{3N} \prod_{i=1}^{N} e^{-\frac{m(r_{i,x}-r'_{i,x})^2}{2\Delta \tau \hbar^2}} \]

\[ = \left[ \frac{m}{2\pi \hbar^2 \Delta \tau} \right]^{3N} e^{-\frac{m(R-R')^2}{2\Delta \tau \hbar^2}}. \]  

(13)
The importance sampled propagator

The importance sampled kinetic energy propagator is defined by \( \langle R | e^{-\hat{T} \Delta \tau} e^{-\hat{F} \Delta \tau} | R' \rangle \), where

\[
\hat{F}(R, \tau) = \sum_i \frac{\hbar^2}{2m_i} \nabla_i \cdot \left[ v_{D,i}(R) f(R, \tau) \right]
= \sum_i \frac{\hbar^2}{2m_i} \left[ \nabla_i v_{D,i}(R) + v_{D,i}(R) \nabla_i \right] f(R, \tau)
= \sum_i \frac{i \hbar}{2m_i} \left[ p_i v_{D,i}(R) + v_{D,i}(R) \hat{p}_i \right] f(R, \tau).
\]

(14)

We make a substitution for the momentum operator \( \hat{p}_i = -i \hbar \nabla_i \), where the \( i \) index represents particle number. The first del operator in line 2 is acting on \( v_{D,i} \), so we substitute for the momentum c-value \( p_i \). The propagator can be expanded as

\[
\langle R | e^{-\hat{T} \Delta \tau} e^{-\hat{F} \Delta \tau} | R' \rangle
= \langle r_1, r_2, \ldots, r_N | \prod_i e^{-\frac{\rho^2 \Delta \tau}{2m_i}} e^{-i \hbar \Delta \tau \left[ p_i v_{D,i} + v_{D,i} \hat{p}_i \right]} | r_1, r_2, \ldots, r_N \rangle.
\]

(15)

We first consider the x-component term for one particle; inserting the momentum-space resolution of the identity operator we find

\[
\int_{-\infty}^{\infty} dp_x \langle x | e^{-\frac{\rho^2 \Delta \tau}{2m_i}} e^{-i \hbar \Delta \tau \left[ p_i v_{D,i} + v_{D,i} \hat{p}_i \right]} | p_x \rangle \langle p_x | x' \rangle
= \int_{-\infty}^{\infty} dp_x \langle x | p_x \rangle e^{-\frac{p_x^2 \Delta \tau}{2m_i}} e^{-i \hbar \Delta \tau \left[ p_x v_{D,x} + \hat{p}_x \right]} \langle p_x | x' \rangle.
\]
\[
\frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dp_x e^{-p_x^2 \Delta\tau/2m + p_x \frac{1}{\hbar} (x - x' - \frac{\hbar^2 \Delta\tau}{m} v_{D,x})} = \frac{1}{2\pi\hbar} \sqrt{\frac{2m\pi}{\Delta\tau}} e^{-\frac{m(x - x' - v_{D,x} \Delta\tau \hbar^2 / m)^2}{2\Delta\tau \hbar^2}} = \sqrt{\frac{m}{2\pi\hbar^2 \Delta\tau}} e^{-\frac{m(x - x' - v_{D,x} \Delta\tau \hbar^2 / m)^2}{2\Delta\tau \hbar^2}}. \tag{16}
\]

For \( N \) particles, by analogy to Eq. (13), we have

\[
\langle R | e^{-\hat{T}\Delta\tau} e^{-\hat{F}\Delta\tau} | R' \rangle = \left[ \sqrt{\frac{m}{2\pi\hbar^2 \Delta\tau}} \right]^{3N} e^{-\frac{m(R - R' - v_D(R) \Delta\tau \hbar^2 / m)^2}{2\Delta\tau \hbar^2}}, \tag{17}
\]

where \( v_D(R) = (v_{D,1,x}, v_{D,1,y}, \ldots, v_{D,N,x}, v_{D,N,y}) \).
Bibliography


[50] For the Jastrow-Slater calculations as well as when comparing Jastrow-BCS results to Bertainá & Giorgini we tune $V(r)$, Eq. (2.46), to match their effective range. Explicitly, for $\eta = 0.75, 1.44, \text{ and } 2.15$, the values are $k_{F}r_{e} \approx 0.0068, 0.0071, \text{ and } 0.0075$ respectively. We have checked that there is no noteworthy effect arising from this minor variation.


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