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Density Functional Theory and Phase Shifts

A Thesis Presented for
the Master of Science
Degree
The University of Tennessee, Knoxville

Anthony G. Wald
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Dedication

This thesis is dedicated to my parents Dan and Janet Wald, who persevered through some very difficult times in the past few decades and taught me the true meaning of what it takes to be a family as I observed first-hand how they handled their adversity in their marriage; to my second-oldest brother Rex and his wife Tammy, who showed me just how much generosity two people can inherently possess; to my oldest brother Mark and his wife Anne and son Sean and daughter Sierra, who themselves have had to endure hardships as a family from Mark's two separate deployments to Iraq; and to my sister Debbie, whose religious spirit has inspired me to strengthen my own faith in the Holy Trinity.

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Abstract

This thesis describes how phase shifts of the nucleon-nucleon system may be utilized to determine the nuclear Density Functional (DF). The nucleon-nucleon interaction, hereafter denoted by N-N interaction, is input to quantum many-body calculations. However, this approach complicates the determination of physical quantities such as the calculation of spectroscopic information and of energy levels. A major advantage in employing the approach via Density Functional Theory (DFT) to this system is that the N-N problem can be considered to be a non-interacting, single-particle system.

In order to use DFT one must know the density functional, and this is typically the most difficult aspect of this approach. Usually the DF is parameterized in terms of the density and density gradients, and these parameters are then fit-to-data. In this thesis we consider how the density functional can be related to the phase shifts of the harmonically-trapped two-body system.

Research focusing on a specific density functional within the Local Density Approximation (LDA) was found to produce fair results in reproducing the general N-N interaction ground-state energy. In this methodology, the phase shift formula was approximated to first-order via the effective range expansion, which simplified the problem. This provided a fair description of the ground-state energy for the two-body system, with roughly two-percent error between the theoretical model and the exact energies.

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Chapter 1

Introduction

Before the 1960s, determinations of the ground-state energies of many-body systems were limited in scope and practicality due to computational limitations. It would take theoretical work developed by (among others) Walter Kohn in 1964 to discover a viable density-dependent solution to the problem of ground-state energy calculations involving many-body systems. This novel approach to determining energies, which compared well with experiment, was Kohn's Density Functional Theory (DFT). This method has seen wide applications in chemistry, and as a result Kohn shared the Nobel Prize in Chemistry in 1998 for his work on density functional theory. According to Burke [1], many topics in physics and chemistry, such as atomic gases, solid-state structures, and the magnetic structure of alloys, have benefited greatly from the application of DFT techniques.

Density functional theory differs from the quantum mechanical approach first utilized by Erwin Schrödinger in the Schrödinger equation. The main difference arises in how one treats the wave function Ψ of a system. From Schrödinger's viewpoint, the wave function is the most fundamental piece of information one can have to completely describe a physical system [2]. However, in the DFT methodology Ψ is relegated to secondary importance and is instead largely replaced by a mathematical construct known as a Density Functional (DF). Amazingly, this density functional, whatever *it* is, turns out to have a unique and inherent property that allows it to be considered *universal* in nature [1,3]. That is, once a DF of a system is known, then one can model the fermionic many-body system in the presence of *any* one-body potential. Traditionally, DFT has been successfully applied to electronic systems in chemistry, and physicists in the 1970s began to realize its potential usefulness to the field of nuclear physics [3,4,5].

This thesis considers two principle topics. First, ultra-cold atomic gases are introduced, and the idea of a Local Density Approximation (LDA) is discussed in reference to a dilute atom gas. Second, phase shifts of a harmonically-trapped nucleon-nucleon system are investigated within the density functional theory formalism. In addition, descriptions of future research in the area of DFT applications with respect to this thesis are discussed, along with outlooks for how nuclear physics may benefit from further employments of DFT.

1.1 Eigenvalue Calculation for Many-Body Systems

Upon first consideration, density functional theory does not appear to radically alter the quantum mechanical description of a many-body system; standard techniques such as perturbation theory and Monte Carlo simulations provide the same information as DFT regarding ground-state energies. However, similarities between DFT and other procedures become apparent when one considers large systems of more than a few tens of particles [5,6,7]. This is due to the impracticality of traditional wave function-based quantum mechanics. Solving Schrödinger's equation for a multi-particle system would ideally allow one to find the ground-state wave function, Ψ , and the ground-state energy, E . One can understand this statement by considering first the situation of a one-dimensional single-fermion system in a square well. For example, standard results for this specific case are found in numerous introductory quantum mechanics textbooks, such as Griffiths [2]:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n x}{L}\right), \quad (1.1)$$

$$E_n = \frac{n^2 \hbar^2 \pi^2}{2mL^2}. \quad (1.2)$$

Similarly, a two-dimensional system of a fermion in a square well has the wave function:

$$\psi_n(x, y) = \frac{2}{L} \sin\left(\frac{\pi n_x x}{L}\right) \sin\left(\frac{\pi n_y y}{L}\right). \quad (1.3)$$

One can see that as more dimensions are added to the square well, one finds a product form in each dimension for the wave function. For an N -particle fermionic system, the resulting wave function is quite complicated:

$$\psi(r_1, r_2, \dots, r_N) = \sum c_{i_1 \dots i_N, j_1 \dots j_N, k_1 \dots k_N} \psi_{i_1} \dots \psi_{i_N} \psi_{j_1} \dots \psi_{j_N} \psi_{k_1} \dots \psi_{k_N}. \quad (1.4)$$

Note in this equation that the coefficients guarantee that the resulting wave function is anti-symmetric in nature. If now we consider a one hundred particle fermionic system, instead of two wave functions being multiplied together for two dimensions, one hundred functions are being multiplied together. Thus, the number of interactions within the system is seen to scale

as 10^{3N} , or in this case, 10^{300} possible combinations [6]. This is a problem! Why? At present there is no computer on Earth that has adequate computational power to completely solve this eigenvalue problem [6]. Moreover, even trying to solve this via a computer would be time inefficient. Thus, a dilemma exists: Too many particles effects in an intractable computational task. That is, most physical systems of interest consist of more than just a few particles; due to the number of degrees of freedom involved in these cases, then this is what entails the difficulty of solving these systems numerically. One approach to rectifying this predicament is discussed in the following pages, in which we start with an introduction to density functionals, and continue with some theorems related to the mathematical tool known as density functional theory.

1.2 Density Functionals

A particularly useful approach to the problem of the determination of many-body eigenvalues and energies involves the mathematically rigorous formalism of density functional theory. In order to discuss this in detail some new concepts, including the idea of a *density functional*, need to be introduced. To bridge the gap between standard quantum mechanical methods and this functional theory, and to show the effectiveness of density functionals, in this paragraph we borrow a particularly illustrative comparison in a paper by Capelle [3]. In the introduction it was noted that the wave function of a system contains all the relevant information regarding its observables (or physical properties). To solve for the eigenvalues of a system, one starts with a known external potential, $v(\mathbf{r})$, and inserts this potential into Schrödinger's equation and solves it, thereby determining the wave function for the particular system. From this wave function, one can find physically meaningful observable quantities, such as ground-state energies. Pictorially this may be represented as:

$$v(\mathbf{r}) \Rightarrow \Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) \Rightarrow \rho(\mathbf{r}) \Rightarrow \text{Observables}. \quad (1.5)$$

However, the density functional process is quite different:

$$\rho(\mathbf{r}) \Rightarrow \Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) \Rightarrow v(\mathbf{r}) \Rightarrow \text{Observables}. \quad (1.6)$$

What is the significance of this latter conceptual sequence? To begin with, it implies a powerful assertion that the ground-state particle density $\rho(\mathbf{r})$

directly leads to the external potential $v(\mathbf{r})$. Moreover, every other physical property of the system can then be derived from the density.

What exactly *is* a density functional or, for that matter, a functional? Concisely, a functional assigns a function to real numbers, as defined in numerous references; see for example Refs. [1,3]. In contrast, a function assigns real numbers to real numbers. Functionals and functions are distinguished notationally as follows: Functions are written as $f(x)$, where functionals are denoted as $F[f]$.

One of the most basic examples of a functional is the familiar particle number of basic quantum mechanics [3], which is given by:

$$N = \int d^3 \mathbf{r} \cdot n(\mathbf{r}) = N[n], \quad (1.7)$$

where $n(\mathbf{r})$ is the *number* density, or a number per unit volume, and N is a number. Burke [1] provides several examples of functionals based upon angular arguments, and these are reproduced here for clarification. Burke considers periodic angular functions $r(\theta) = r(\theta + 2\pi)$, with the domain $0 \leq \theta \leq 2\pi$. Functions of this nature form closed loops that do not intersect themselves except at the endpoints of the lines, and are restricted to two-dimensional space. The functionals $A[r]$ and $P[r]$, which represent the area and perimeter functionals of a generic $r(\theta)$, given by:

$$P[r] = \int_0^{2\pi} d\theta r(\theta), \quad (1.8)$$

$$A[r] = \frac{1}{2} \int_0^{2\pi} d\theta r^2(\theta). \quad (1.9)$$

On examining these two functionals, one can see that by evaluating the integrand, the functional itself is then known *completely*. This defines a class of functionals known as *local* functionals, and leads to the local density approximation. Simply put, this approximation allows the energy density functional to be written in integral form, with the integrand depending only upon *local* coordinates [5]:

$$E[\rho(\mathbf{r})] \approx \int d^3 \mathbf{r} \left(\varepsilon(\rho(\mathbf{r})) \right), \quad (1.10)$$

Density functionals are another type of functional; these play a crucial role in the determination of the energy of fermionic systems [8]. As an example, in the Thomas-Fermi model the total kinetic energy density functional is [9]:

$$T_{\text{TF}}[\rho] = \frac{3\hbar^2}{10m} \left(3\pi^2\right)^{\frac{2}{3}} \int \rho^{\frac{5}{3}}(\mathbf{r}) d\mathbf{r}. \quad (1.11)$$

The local density approximation can be applied to density functionals. For example, the local approximation of the kinetic energy density functional for a system of spinless fermions in one dimension is [1]:

$$T_s^{\text{loc}}[\rho] = \frac{(\hbar\pi)^2}{6m} \int_{-\infty}^{\infty} dx \rho^3(x). \quad (1.12)$$

1.3 Functional Derivatives

As the previous section has shown, functionals are distinct from functions. Therefore, one needs to understand how to modify various calculus-based concepts in treating functionals. Mathematically, taking a functional derivative for a generic energy density functional $E[\rho]$ is denoted by [5]:

$$\frac{\delta E[\rho(r)]}{\delta \rho(x)} = \lim_{\varepsilon \rightarrow 0} \frac{E[\rho(r) + \varepsilon \delta(r-x)] - E[\rho(r)]}{\varepsilon}. \quad (1.13)$$

Furthermore, taking functional derivatives in the local density approximation is relatively straightforward, and is denoted as follows:

$$E[\rho] = \int dx \varepsilon(\rho(x)), \quad (1.14)$$

$$\frac{\delta E[\rho]}{\delta \rho(x)} = \varepsilon(\rho(x)). \quad (1.15)$$

Suppose one considered a generic functional derivative involving a potential $V_{\text{ext}}(r)$. In the next section we will show how to minimize an energy density functional, but for the purpose of brevity, only the potential term is considered here:

$$\frac{\delta}{\delta\varphi_k^*(\mathbf{x})} \left[\int d^3\mathbf{r} V_{ext}(\mathbf{r})\rho(\mathbf{r}) \right] = \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} \int d^3\mathbf{r} V_{ext}(\mathbf{r})\rho(\mathbf{r}) \left\{ \sum_{j=1}^A \left(\left(\varphi_j^*(\mathbf{r}) + \varepsilon \delta_j^k \delta(\mathbf{x} - \mathbf{r}) \right) \cdot \varphi_j(\mathbf{r}) - \varphi_j^*(\mathbf{r})\varphi_j(\mathbf{r}) \right) \right\}, \quad (1.16)$$

$$\frac{\delta}{\delta\varphi_k^*(\mathbf{x})} \left[\int d^3\mathbf{r} V_{ext}(\mathbf{r})\rho(\mathbf{r}) \right] = \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} \int d^3\mathbf{r} V_{ext}(\mathbf{r}) \left\{ \varepsilon \delta(\mathbf{x} - \mathbf{r})\varphi_j(\mathbf{r}) \right\}, \quad (1.17)$$

$$\frac{\delta}{\delta\varphi_k^*(\mathbf{x})} \left[\int d^3\mathbf{r} V_{ext}(\mathbf{r})\rho(\mathbf{r}) \right] = V_{ext}(\mathbf{x})\varphi_k(\mathbf{x}), \quad (1.18)$$

Another example of how to take a functional derivative can be seen by considering equation (1.9) from the previous section [1]. Recall that this equation describes the area functional $A[r]$. Taking the functional derivative yields:

$$\begin{aligned} A' &= \frac{\delta A[r]}{\delta r(\theta)} = \lim_{\varepsilon \rightarrow 0} \frac{A[r + \delta r] - A[r]}{\varepsilon} \\ &= \lim_{\varepsilon \rightarrow 0} \frac{1}{2} \frac{\int_0^{2\pi} \left(\left\{ r(\theta) + \varepsilon \delta(\theta - \theta_0) \right\}^2 - r(\theta)^2 \right) d\theta}{\varepsilon} \end{aligned} \quad (1.19)$$

$$\frac{\delta A[r]}{\delta r(\theta)} = \frac{\varepsilon r(\theta)}{\varepsilon} = r(\theta), \text{ using } \int_{-\infty}^{\infty} f(k) \delta(k - k') dk = f(k'). \quad (1.20)$$

1.4 Hohenberg-Kohn Theorems and Kohn-Sham Equation

The two Hohenberg-Kohn (HK) theorems are the central pillars of density functional theory [1,9]. First developed by Pierre Hohenberg and Walter Kohn in 1964 [10], these theorems facilitated the discussion of the electron gas in the context of ground-state energies. The Hohenberg-Kohn theorems are powerful statements regarding both the universality of the density functional, and the importance of the density functional itself as key components to DFT and its usage in many-body calculations.

Normally (in standard quantum mechanics) one begins with a specified potential $v(\mathbf{r})$ and employs the Schrödinger equation to determine desired observables from $\Psi_0(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$, the ground-state wave function. What the first HK theorem states is that the ground-state density $\rho_0(\mathbf{r})$ itself can provide *exactly* the same information as does the potential [3]. That is, the ground-state energy is a functional of the external potential, and that the potential determines uniquely the density. More importantly, this fact indicates that the ground-state energy is a *functional* of the energy density. This is a statement of the second Hohenberg-Kohn theorem.

Capelle [3] raises an instructive question with respect to the idea that $\rho_0(\mathbf{r})$ gives identical results for observables as does $\Psi_0(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$. How might this be the case? After all, the ground-state wave function Ψ_0 is an N -variable complex-numbered vector-valued function, whereas ρ_0 depends solely upon a single vector variable $\mathbf{r}$. Parr and Yang [9] refer to this predicament as the *v-representable* and *N-representable* conditions, and is discussed in the following paragraph. The *N-representability* clause is a weaker constraint than the *v-representability* case. It is the *v-representability* case that provides a direct relationship between the potential and the density, where the potential determines *uniquely* the ground-state density. Since the ground-state wave function is anti-symmetric, as discussed in section 1.1, then the density is *N-representable*. Therefore, a one-to-one correlation exists between ground-state wave functions and ground-state densities. Another consequence of the HK theorems refers to the minimization of the energy density functional [3]:

$$E_v[\rho_0] \leq E_v[\rho'], \quad (1.21)$$

where $E_v[\rho_0]$ is the true ground-state energy and $E_v[\rho']$ is the calculated energy for any $\rho' \neq \rho_0$.

If one wishes to determine ground-state energies for a system with a Hamiltonian that is not readily solvable by the Schrödinger equation in terms of known functions, a useful method for Schrödinger wave *functions* exists [11], which is the Rayleigh-Ritz Variational Principle. However, the current discussion involves minimization of *functionals*, not functions. As shown in section 1.3, this methodology is different from normal calculus techniques since, for a generic functional $g[\rho]$ in the local density approximation, delta functions complicate the taking of derivatives. Thus one has to perform functional optimization, and therefore uses a slightly modified version of the standard minimization methods of calculus [7]. Procedurally one utilizes the so-called Kohn-Sham equation. In this case, the optimization of the energy density functional takes the following form:

$$E[\rho] = \int d^3\mathbf{r} \left(\tau[\mathbf{r}] + v[\mathbf{r}]\rho[\mathbf{r}] + \varepsilon[\rho] \right), \quad (1.22)$$

$$\frac{\delta E[\rho]}{\delta \rho(\mathbf{r})} = 0, \quad (1.23)$$

where the τ term gives the kinetic energy, the v term corresponds to the potential energy, and the ε term denotes the interaction physics.

1.5 Phase Shifts

Consider a plane wave of the form $\psi = e^{i\mathbf{k}\cdot\mathbf{r}}$. As this incident wave encounters some potential $|V_0|$, the incoming wave scatters from this potential and becomes a reflected outgoing wave. Phase shifts arise from the difference between an incoming and an outgoing wave. A "shift" of the plane wave after reflection is thus observed to have occurred. One may measure phase shifts in radians, with the sign of the phase shift determined by the nature of the potential. For example, an attractive potential will cause the wave function to be "pulled in" towards the potential well, resulting in a positive phase shift. On the other hand, negative phase shifts can occur for repulsive potentials, as the wave function is "pushed out" away from this repulsive well.

An illustrative case of how phase shifts and scattering lengths are connected is reproduced here [12]. In Figures 1-1 to 1-4, Cases (.a) correspond to various potential wells, and Cases (.b) refer to the phase shifts given by the wells. Figure 1-1 Case (i) shows a very shallow attractive potential well having no bound states. The well affects the incoming wave, causing a phase shift of the scattered reflected wave. However, this shift is very small in angle, and is positive. Figure 1-1 Case (ii) shows the resulting phase shift as a scattering state approaches threshold. Figure 1-2 Cases (iii) and (iv) details what occurs when a bound state enters the attractive well. Likewise, Figures 1-3 and 1-4 show for one bound state the changing slopes for phase shifts given various scattering length values. In section 2.1, equation (2.2) we will show a relation between the scattering length and the phase shift. For current purposes, we list mathematically how the phase shift slope corresponds to the scattering length at $k = 0$, which is $-\delta\delta/dk = a$.

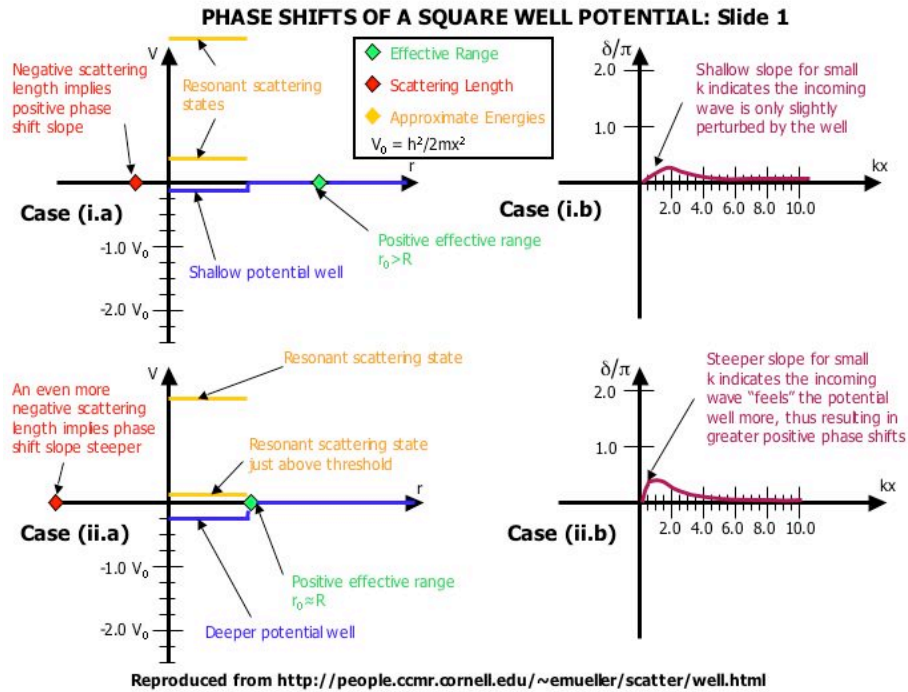


Figure 1-1: The relationship between potentials and phase shifts, I.

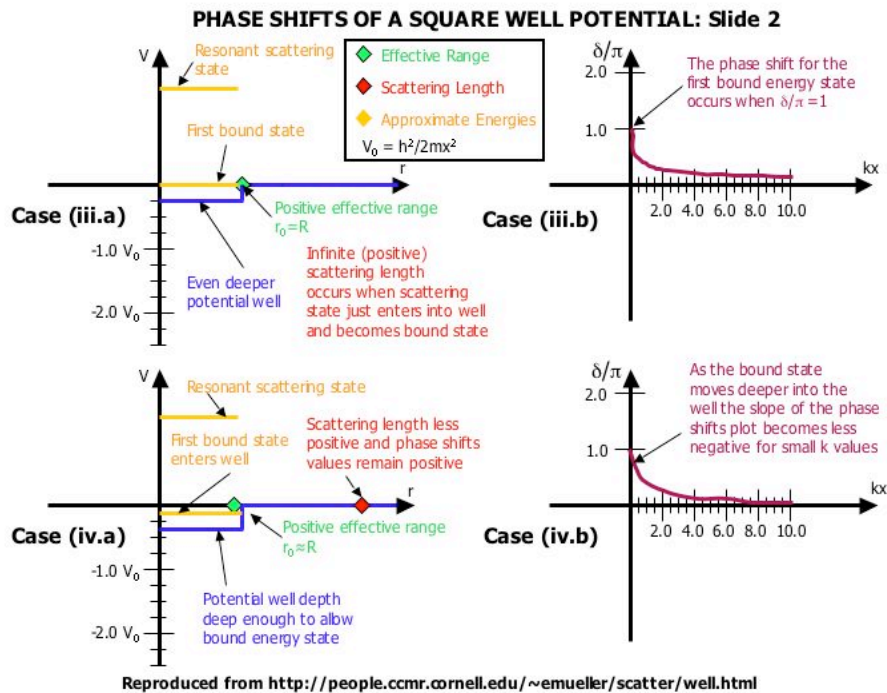


Figure 1-2: The relationship between potentials and phase shifts, II.

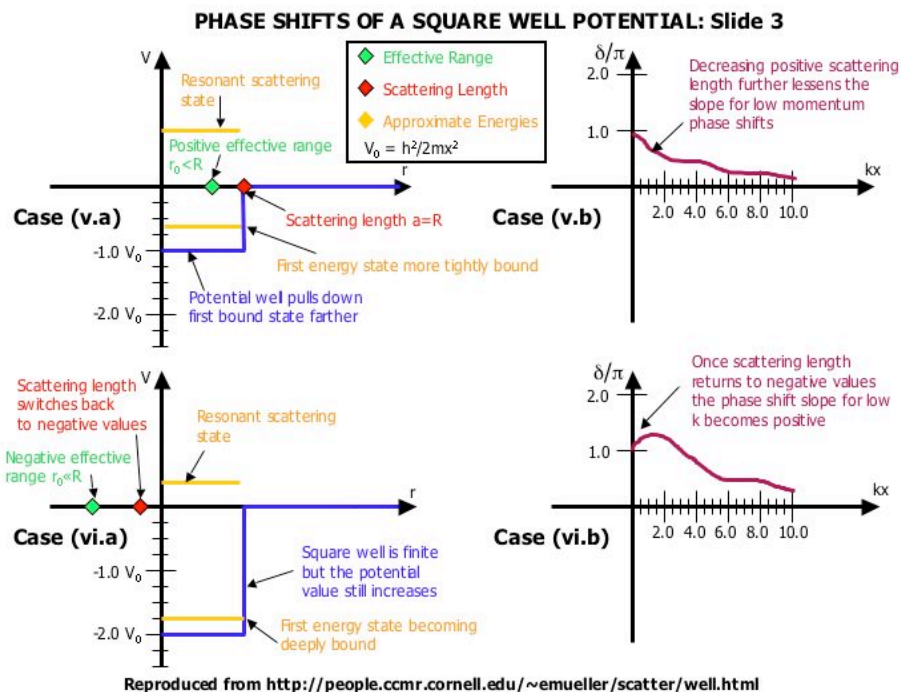


Figure 1-3: The relationship between potentials and phase shifts, III.

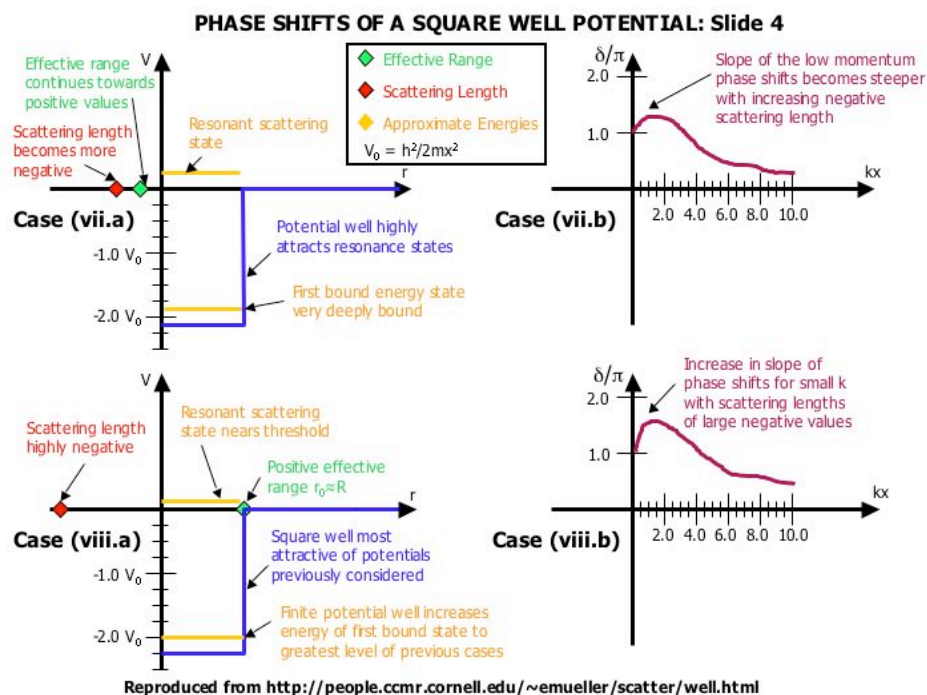


Figure 1-4: The relationship between potentials and phase shifts, IV.

Since the principle goal of this research is to determine how phase shifts can be related to an energy density functional, we present in this section the related results of Kaplan et al. [13]. In this reference, scattering amplitudes for the N-N interaction are investigated via effective field theory and dimensional regularization. Then these theoretical results are compared to fit-to-data theoretical calculations provided by Nijmegen partial-wave analysis.

We will consider the next-to-leading-order approximation for this singlet $^1S_0$ channel, and Figure 1-5 shows this result from [13]. Here this phase shift *does* become negative for large values of momentum (though this is not shown in the plot), and the nearly linear downward slope for large p -values evidences this. Physically this region is where the characteristics of the interaction change from attractive to repulsive. This negative slope suggests the repulsive system can be represented by a (finite) hard-core nucleon-nucleon potential well [5]. Recall that a hard-core potential well of radius R must satisfy the condition $\sin(pR + \delta) = 0$, and therefore the phase shift δ has the value $-pR$.

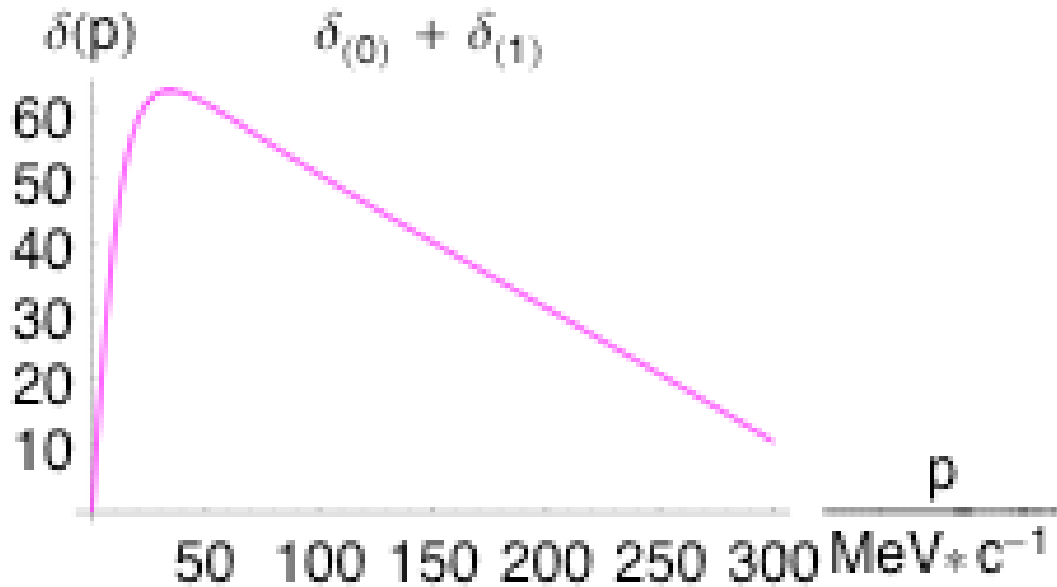


Figure 1-5: Next-to-leading order approximations to N-N phase shifts in the $^1S_0$ channel.

Chapter 2

Ultra-Cold Atom Gases

2.1 Dilute Fermi Gas

Ultra-cold atom gases can be good examples for dilute Fermi gases. In DFT, the energy of a Fermi gas depends only on the density. Of particular note in the following discussion is the situation in which the value of the scattering length a is several orders of magnitude larger than the physical range R of the trapping potential. In this case one can distinguish three distinct density regimes of an atom gas [14]. Specifically, these are dilute, intermediate, and high. We now define these quantities as utilized in this thesis for zero bound potentials, noting that we use the notation for the physical range of the system as R , the average distance between two particles as d_{12} , and the Fermi momentum as k_F . We observe that the Fermi momentum k_F is inversely proportional to the inter-particle distance d_{12} ; that is, $k_F \propto d_{12}^{-1}$. Dilute Fermi gases have the condition that $Rk_F \ll 1$, intermediate-density gases require that $Rk_F \approx 1$, and high-density gases demand that $Rk_F \gg 1$. Thus, in the case of dilute gases the value of the physical range of the system is approximately equal to the inverse of the Fermi momentum. Sometimes this situation is termed a *dilute* degenerate Fermi system. Perhaps a more constructive explanation for a dilute Fermi gas satisfies:

$$\left| a \rho^{\frac{1}{3}} \right| \ll 1, \text{ or } |k_F a| \ll 1. \quad (2.1)$$

Interestingly, once one brings the topic of the scattering length into the mix, then a standard description for just what constitutes a dilute Fermi gas is lacking. The reason for this is that the scattering length approaches infinity when considering the unitary regime (that is, under the conditions of a zero-range interaction and an infinitely negative scattering length). It can be the case that for some physical systems the scattering length a is much greater than the length scale of the physical range R ; that is, for $|a| \gg R$. Then the intermediate-density and the high-density cases are grouped into this

category. This is important since later on in this thesis we discuss situations in which the scattering length can vary without bound.

In this thesis we consider a zero-ranged two-body interaction between harmonically-trapped fermions. The interaction is characterized by its scattering length only, and is given by $V(\mathbf{r}_{12}) = (4\pi a \hbar^2/m)\delta^{(3)}(\mathbf{r}_{12})$. The phase shifts fulfill [15]:

$$-\cot\delta(k_F) \propto \frac{1}{ak_F}. \quad (2.2)$$

As a consequence, the short-range interaction can be modeled as a zero-range interaction.

One example for the leading-order approximation to the N-N phase shifts is shown in Figure 2-1 specifically for the $^1S_0$ channel. Theoretically, this case can be represented as delta function potential [16]. Here the phase shift $\delta(p)$ is in radians and momenta are given in units of MeV/c, and is shown for s-wave scattering only. For low momenta $p \ll 10$ MeV/c, and we are in the regime $|ak_F| \ll 1$. The very steep slope at the origin implies a large, negative scattering length. This is because two neutrons *just barely* fail to bind. On the phase shift plot the graph is seen to asymptotically approach a value of around 1.5 radians after the steep increase observed for low momentum. Physically, this can be understood by considering how an incoming wave "interacts" with a delta function potential. Recall that a delta function is zero everywhere it is defined except for the point where its value is infinite. This mirrors what is shown in Figure 2-1 since for very low momentum the outgoing wave is highly affected by the delta potential, and for high momentum the wave is not perturbed very much due to the scale of the potential. That is, the wavelength of the incoming wave is much larger than that of the length of the contact potential.

For two harmonically-trapped fermions, Busch et al. show how the energy of the relative coordinate is related to the effective range expansion [16], and is outlined in the next few paragraphs. In order to achieve this result, one begins with a two-body system and sets up the Hamiltonian:

$$H_0 = \frac{\mathbf{p}_1^2}{2m} + \frac{\mathbf{p}_2^2}{2m} + \frac{1}{2}m\omega^2(\mathbf{r}_1^2 + \mathbf{r}_2^2) + v(\mathbf{r}_1 - \mathbf{r}_2), \quad (2.3)$$

To simplify the form of the Hamiltonian, the following terms are defined. Let:

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \quad (2.4)$$

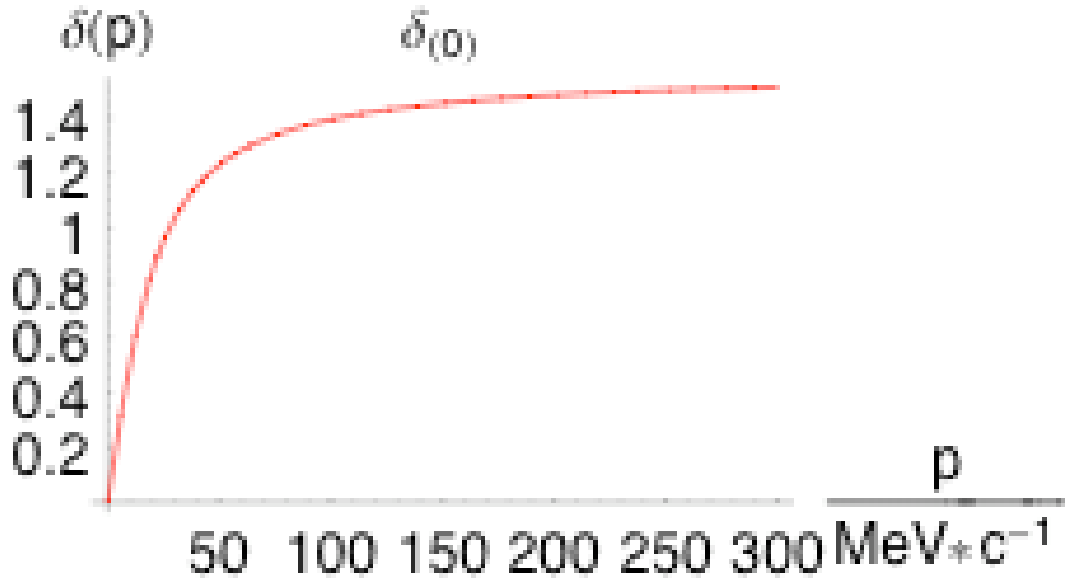


Figure 2-1: Phase shifts modeled by δ - interaction in the $^1S_0$ channel.

$$\mathbf{R} = \frac{\mathbf{r}_1 + \mathbf{r}_2}{2}, \quad (2.5)$$

$$\mathbf{p} = \frac{\mathbf{p}_1 - \mathbf{p}_2}{2}, \quad (2.6)$$

$$\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2, \quad (2.7)$$

Then the potential becomes $v(\mathbf{r})$. Here, $\mathbf{R}$ and $\mathbf{P}$ correspond the center-of-mass coordinates, and $\mathbf{r}$ and $\mathbf{p}$ are the relative coordinates. Utilizing the effective and reduced mass formulas, respectively:

$$M = 2m, \text{ and } \mu = \frac{m}{2}, \quad (2.8)$$

the Hamiltonian can be rewritten to evoke separate parts; a center-of-mass coordinate Hamiltonian, and a relative coordinate Hamiltonian. This is shown below:

$$H_0 = \left(-\frac{\hbar^2}{2M} \nabla_{\mathbf{R}}^2 + \frac{1}{2} M \omega^2 \mathbf{R}^2 \right) + \left(-\frac{\hbar^2}{2\mu} \nabla_{\mathbf{r}}^2 + \frac{1}{2} \mu \omega^2 \mathbf{r}^2 \right) + v(\mathbf{r}), \quad (2.9)$$

For the potential $v(\mathbf{r})$ Busch et al. [16] employs a delta function potential $(4\pi a \hbar^2/m) \delta^{(3)}(\mathbf{r})$. The solution of the Schrödinger equation then gives:

$$\sqrt{2} \frac{\Gamma\left(\frac{3}{4} - \frac{E}{2}\right)}{\Gamma\left(\frac{1}{4} - \frac{E}{2}\right)} = \frac{\lambda}{a}. \quad (2.10)$$

In this formula $\lambda = (\hbar/m\omega)^{1/2}$ is the oscillator length scale (sometimes λ is denoted by l), and in this case λ is set to unity and E is dimensionless in scale and represents the relative energy in terms of $\hbar\omega$. Hence formula (2.10) may be considered to be a relation between the scattering length a and energy E .

2.2 Study of a Two-Fermion System

For the harmonically-trapped two-fermion system, the energy is given by:

$$E[\rho] = \int d^3r \left(\tau + v \cdot \rho + \varepsilon(\rho) \right), \quad (2.11)$$

where the kinetic energy density τ is:

$$\tau = \frac{\hbar^2}{2m} \sum_{j=1}^2 \left(\vec{\nabla} \varphi_j \right)^2, \quad (2.12)$$

and the trapping potential v is:

$$v = \frac{1}{2} m \omega^2 \mathbf{r}^2, \quad (2.13)$$

and the density ρ is:

$$\rho = \sum_{j=1}^2 |\varphi_j(r)|^2. \quad (2.14)$$

The energy density $\varepsilon(\rho)$ is of special importance as it contains all of the interaction physics.

Next we show how one can find an appropriate density functional using the phase shift equation (2.2) and the approximation of a zero effective range. The idea is that once this energy density functional is created, then a comparison can be made between it and the exact ground-state energy found by Busch et. al [16]. As stated in the previous chapter, the use of DFT provides an excellent avenue into the determination of ground-state energies. The difficulty is that an accurate density functional is hard to find. As such, the idea of deriving a density functional rests upon its ability to mimic as closely as possible previously accepted experimental and theoretical results. For the purposes of this discussion, the author considers the following density functional that has been provided by Papenbrock [5]:

$$\varepsilon[\rho] = \frac{\hbar^2}{m} \rho^{\frac{5}{3}} \frac{\pi a \rho^{\frac{1}{3}}}{1 + a d \rho^{\frac{1}{3}}}. \quad (2.15)$$

For this functional, the scattering length is assumed to hold for large values, and d is the only free parameter in the equation. In the unitary regime, this functional had better match up with the results of, for example, Busch et. al [16] for infinite scattering length. Investigating this functional then in the limit as $a \rightarrow -\infty$ gives:

$$\lim_{a \rightarrow -\infty} \varepsilon[\rho] = \lim_{a \rightarrow -\infty} \frac{\hbar^2}{m} \rho^{\frac{5}{3}} \left(\frac{a \rho^{\frac{1}{3}}}{a \rho^{\frac{1}{3}}} \right) \frac{\pi}{\left(a \rho^{\frac{1}{3}} \right)^{-1} + d}, \quad (2.16)$$

$$= \frac{\hbar^2}{m} \rho^{\frac{5}{3}} \cdot \lim_{a \rightarrow -\infty} \frac{\pi}{\left(a \rho^{\frac{1}{3}} \right)^{-1} + d}, \quad (2.17)$$

$$\lim_{a \rightarrow -\infty} \varepsilon[\rho] = \frac{\hbar^2}{m} \rho^{\frac{5}{3}} \frac{\pi}{d}. \quad (2.18)$$

To determine whether this yields the correct slope in this limit, one compares this result with the case given by [16]. For a dilute free Fermi gas, the ground-state energy density of such as gas, as seen in equation (1.11), is:

$$E_{\text{FG}} = \frac{3}{10} \frac{\hbar^2}{m} \left(3\pi^2 \right)^{\frac{2}{3}} \rho^{\frac{5}{3}}. \quad (2.19)$$

However, the energy functional can directly depend upon the density, as shown by Papenbrock [17]:

$$E[\rho] = E_{\text{FG}} + \frac{a\pi \hbar^2}{m} \rho^2. \quad (2.20)$$

Furthermore the ground-state energy *must* be proportional to the free Fermi gas energy:

$$E_{\text{UNITARY}} = \xi E_{\text{FG}} = E_{\text{FG}} + \varepsilon(\rho), \quad (2.21)$$

Therefore, one concludes that $\varepsilon(\rho) = (\xi - 1)E_{\text{FG}}$.

The implication, then, is that equations (2.18) and (2.21) have exactly the same equation form and can then be equated with each other for the purpose of determining the one free parameter, which is d:

$$\lim_{a \rightarrow -\infty} \varepsilon[\rho] = \frac{\hbar^2}{m} \rho^{\frac{5}{3}} \frac{\pi}{d} = (\xi - 1)E_{\text{FG}}. \quad (2.22)$$

Here ξ has a value of 0.44 as shown in reference [18]. Equation (2.22) may now be solved for the unknown parameter d by using equation (2.19):

$$d = \frac{-10\pi}{3 \left(3\pi^2 \right)^{\frac{2}{3}} (1 - \xi)} \approx -2. \quad (2.23)$$

Similarly one can also examine how this energy density functional behaves for zero scattering length. For this situation of a very small scattering length the functional acts as follows [19]:

$$\lim_{\substack{a \rho^{\frac{1}{3}} \ll 1 \\ a \rho^{\frac{1}{3}} \ll 1}} \varepsilon[\rho] = \lim_{\substack{a \rho^{\frac{1}{3}} \ll 1 \\ a \rho^{\frac{1}{3}} \ll 1}} \frac{\hbar^2}{m} \rho^{\frac{5}{3}} \frac{\pi a \rho^{\frac{1}{3}}}{1 + a d \rho^{\frac{1}{3}}} = \frac{a\pi \hbar^2}{m} \rho^2, \quad (2.24)$$

2.3 Comparison between Trial DF and Theory

In the next few paragraphs the author investigates how well the "educated guess" or Ansatz for the density functional of equation (2.15) compares to theoretical results of Busch et al. Due to the complexity of the calculations involved in making this contrast, it was necessary to use numerical methods. Actual coding focused upon the Kohn-Sham (KS) equation for a non-interacting, two-fermion system and was accomplished by employing Fortran90. The algorithm used by the author was adapted from one supplied by T. Papenbrock, which was originally employed for bosons. This computer program solved the KS equation and then numerically determined ground-state energy eigenvalues.

Of importance in this plot is how well both the curve provided by the exact Hamiltonian [16] and the graph corresponding to the educated guess for the density functional are in agreement. Figure 2-2 shows this plot, and there are several ways to measure accuracy between these two graphs. First, one can consider how well the values of the endpoints match. Second, one can investigate the slopes of each curve at their endpoints. In the limits where the functional has been fit to theory (the limits $a \rightarrow -\infty$ and $a\rho^{1/3} \ll 1$), there is very good agreement by construction of the density functional. For intermediate values of a , the discrepancy between the exact result [16] and the DFT plot is nearly two-percent. For an initial guess at the DF, this achievement is promising; however, finding a more accurate density functional would better test the DFT methodology.

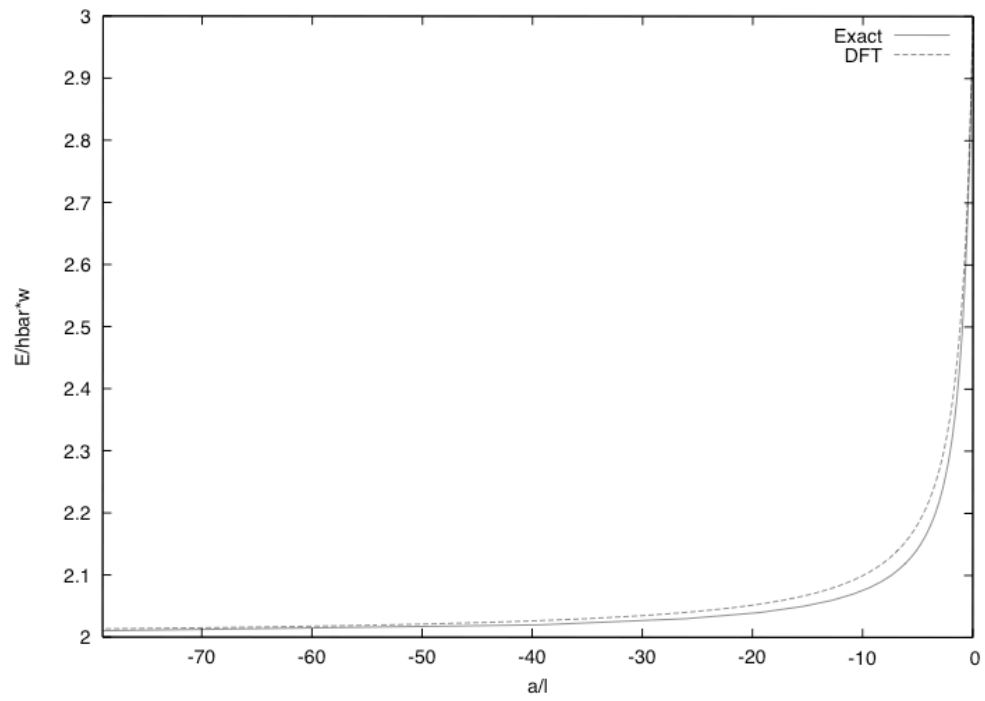


Figure 2-2: Comparison between DFT and exact results for the ground-state energy of a two-fermion system.

Chapter 3

Nucleon-Nucleon Phase Shifts

3.1 Harmonically-Trapped Neutron System

One method to extend density functional theory to the nucleon-nucleon system is to consider how the energy of the ground-state relates to the phase shifts. Beginning with the work done by Busch et. al [16], the formula relating energy values to a specific phase shift was studied:

$$\sqrt{2} \frac{\Gamma\left(-\frac{E}{2} + \frac{3}{4}\right)}{\Gamma\left(-\frac{E}{2} + \frac{1}{4}\right)} = -\cot\delta(k_F). \quad (3.1)$$

Of particular note in this equation is the $\cot\delta(k_F)$ term on the right-hand side. For the purposes of this work, it was required to solve the above equation for the *full* phase shifts δ as a function of the energy E (where E actually is E divided by $\hbar\omega$) [13]. This exercise is necessary since in order to employ DFT one needs to find a suitable energy density. Completion of this task is a fairly simple procedure of just plugging equation (3.1) into a mathematical computer program, plotting the graph of E versus δ , and re-arranging the data set. Generating this table of values creates the desired result shown in Figure 3-1. Several points can be considered in this plot. At very large oscillator lengths the energy approaches a value of $3\hbar\omega/2$ as the system becomes very dilute. In addition, note that $\lambda = 4$ fm corresponds to nuclear saturation. The next step would be to determine an energy density functional that would (ideally) match up very well with this result for harmonically-trapped neutrons.

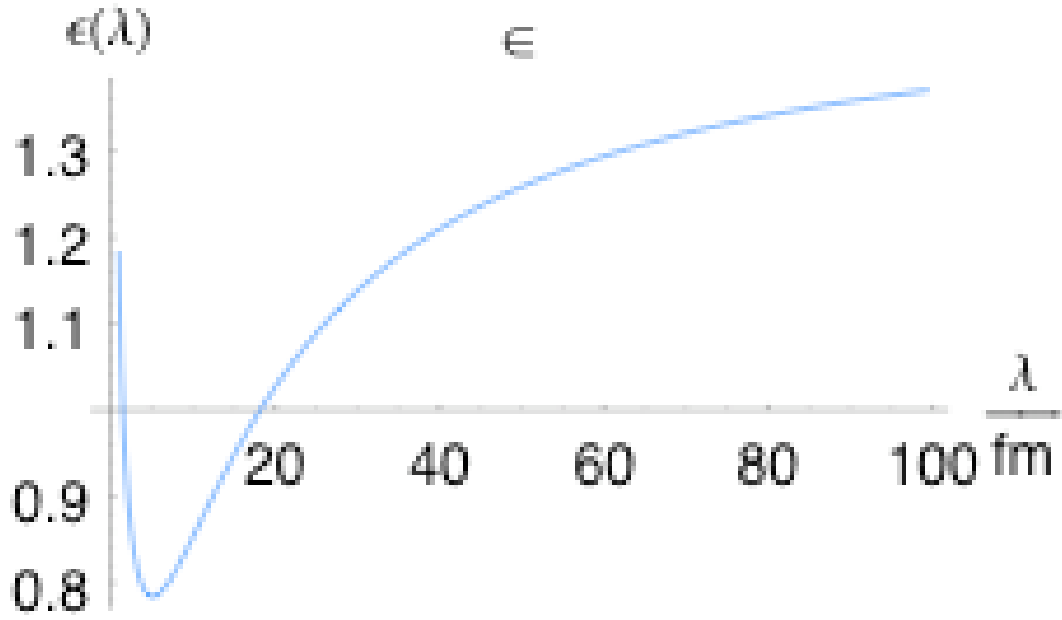


Figure 3-1: Plot of energy density as a function of the oscillator length λ of the harmonic trap.

3.2 Future Research and Outlook

DFT has been shown in this thesis to be a promising alternative in the determination of ground-state energies for harmonically-trapped systems. However, given the nearly two-percent error between the exact ground-state energy values and the ground-state energy values calculated via DFT for the dilute atom gas, we ask whether this is an acceptable discrepancy. Since modern nuclear theory models typically provide a less than one-tenth of one percent error in ground-state energies, our two-percent difference between ground-state energy levels seems high [5]. As a way to reduce this error, research could be extended to focus on modifying the energy density functional such that, in the comparison plot between exact and DFT ground-state energies, the slopes in the unitary regime would agree. Recall that the single unknown parameter d allowed only a determination of the slopes at or near zero scattering length; then in order to match the slopes at infinity we need a second parameter (call it g). The new energy density functional could then take the form [5]:

$$\varepsilon_{\text{NEW}}[\rho] = \frac{\hbar^2}{m} \rho^{\frac{5}{3}} \frac{\pi}{g} \tan^{-1} \left(g a \rho^{\frac{1}{3}} \right), \quad (3.2)$$

$$\text{where } g = \frac{5\pi^2}{3(3\pi^2)^{\frac{2}{3}}(\xi - 1)} \approx -3. \quad (3.3)$$

If this new functional reduced the two-percent error, then further adjustments of the density functionals could be made. This could consist of taking a linear combination of the two energy density functionals under the influence of a weighting scale variable (call it α). The hope is that this constraint could be tuned to allow additional lessening in the discrepancy between the exact and theoretical cases for ground-state energy values. This combination of density functionals may be given by [5]:

$$\varepsilon_{\text{Combination}}[\rho] = \left(\alpha \right) \left(\frac{\hbar^2}{m} \rho^{\frac{5}{3}} \frac{\pi a}{1 + a \rho^{\frac{1}{3}}} \right) + (1 - \alpha) \left(\frac{\hbar^2}{m} \rho^{\frac{5}{3}} \frac{\pi}{g} \tan^{-1} \left(g a \rho^{\frac{1}{3}} \right) \right), \quad (3.4)$$

with α having the range as follows: $\{\alpha \in \Re : 0 \leq \alpha \leq 1\}$.

Another option for continued research would deal with developing an energy density functional for the harmonically-trapped nucleon-nucleon system. In this case ρ is proportional to λ^{-3} in the local density approximation and $\varepsilon(\lambda)$ then transforms into $\varepsilon(\rho^{-1/3})$. Thus one effectively has an idea of how to proceed in determining a rudimentary form for an energy density functional for the more complicated case of nucleon-nucleon systems. A natural question arises, however, as to whether we have any hope that the DFT method works for the N -body case. The answer is given in the coefficient of π in both the energy density functional for the ultra-cold atom gas case and the energy density functional for the nucleon-nucleon case [5]. Because each case gives *exactly* π as the coefficient, then this suggests that the N -body situation and the two-body system can both be effectively analyzed using the DFT methodology.

Conclusions

This thesis attempts to relate nuclear density functionals to nucleon-nucleon phase shifts. For the harmonically-trapped two-fermion system with a zero-range interaction, a relation given by Busch et al. [16] connects the ground-state energy to the phase shifts of the two-body interaction. Since there are difficulties in using traditional quantum methods to finding exact solutions of many-body quantum systems, we introduced a simple Ansatz for a density functional in the local density approximation to address this issue. Our Ansatz for the density functional was motivated by known correct limits (within LDA) as the value of the scattering length approached both zero and negative infinity. Next the Hohenberg-Kohn theorems were employed, along with the Euler-Lagrange equation in DFT, leading to a Kohn-Sham eigenvalue relationship, which was then solved numerically. Once the computed energy and density values converged, the results were plotted and compared with previous analytic exact results. Deviation of approximately two-percent was seen in the comparison between the two theories. Thus density functional theory provided fair results, indicating a positive outlook for continued utilization of DFT as it applies to harmonically-trapped two-fermion systems.

Future research in this area would focus upon two topics. First, it would be nice to enhance the density functional in equation (2.15) so that the two-percent error could be reduced further and give a good match to the exact results of Busch et al. One possibility discussed was to insert a second parameter numerically ranging between zero and one into the density functional in the hopes of accomplishing a more accurate comparison of the energy versus scattering length data plot of Figure 2-2. Second, more research could be performed on the nucleon-nucleon trapped system by attempting to guess a suitable energy density functional for that situation. In conclusion, further research can be expected to produce accurate enough results to warrant comparisons between DFT and more complicated particle systems such as the harmonically-trapped N-N system.

Bibliography

Bibliography

- [1] K. Burke *et al.*, *The ABC of DFT*, <http://dft.rutgers.edu/kieron/beta/>.
- [2] D. J. Griffiths, *Introduction to Quantum Mechanics*, 1st ed. (Prentice Hall, Inc., New Jersey, 1995).
- [3] K. Capelle, e-print cond-mat/0211443.
- [4] E. K. U. Gross and R. M. Dreizler, *Density Functional Theory, NATO ASI Series B: Physics Vol. 337*, (Plenum Press, New York and London, 1995).
- [5] T. Papenbrock, *personal communication*.
- [6] W. Kohn, Rev. Mod. Phys. **71**, 1253 (1999).
- [7] W. Kohn and L. J. Sham, Phys. Rev. **140**, A1133 (1965).
- [8] T. A. Arias, *Notes on the "ab initio" theory of molecules and solids: Density Functional Theory (DFT)*, people.ccmr.cornell.edu/~muchomas/P480/Notes/dft/dft.html.
- [9] R. C. Parr and W. Yang, *Density Functional Theory of Atoms and Molecules*, 1st ed. (Oxford University Press, Inc., New York, 1989).
- [10] P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964).
- [11] E. Merzbacher, *Quantum Mechanics*, 3rd ed. (John Wiley & Sons, Inc., New York, 1998).
- [12] E. Mueller, *Theory of Quantum Degenerate Gases*, <http://www.physics.ohio-state.edu/~emueller/thesis/>.
- [13] D. B. Kaplan *et al.*, Phys. Lett. B424, 390 (1998).
- [14] H. Heiselberg, Phys. Rev. A63, 043606 (2002).
- [15] H. Bethe, Phys. Rev. **76**, 38 (1949).
- [16] T. Busch *et al.*, Found. of Phys., **28**, No. 4 (1998).
- [17] T. Papenbrock, Phys. Rev. A, **72**, 041603(R) (2005).
- [18] J. Carlson, *et al.*, Phys. Rev. Lett., **91**, 050401 (2003).
- [19] W. Lenz, Z. Phys. **56**, 778 (1929).

Vita

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