PERTURBATION SOLUTION FOR TWO TRAPPED PARTICLES IN AN EFFECTIVE FIELD THEORY FRAMEWORK

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Dana Rynja
Preface

I would like to thank Professor van Kolck for providing such an interesting and fulfilling project for this honors thesis. I thank him, along with Dr. Jimmy Rotureau, for providing me with guidance and insight along the way. I could not have made this thesis without their ample support.
Abstract

Particles interacting with sufficiently low energies have dynamics independent of the details of the interaction. This problem is generalized and extended within the context of an effective field theory (EFT). We investigate the case of two such particles in an harmonic trap and construct the inter-particle potential using an EFT expansion. In position space the effective interaction consists of a series of delta-functions and their derivatives. We approximate the energy spectrum in perturbation theory, compare to the results of analytical solutions and discuss the ordering of terms from the potential within the perturbation expansion.
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Chapter 1

Introduction

The dynamics of particles at low energies is an important case in modern physics as many distinctly quantum mechanical effects are made manifest in these systems. When the relative energies of the interacting particles are small in comparison to the internal excitation energies of the individual particles they demonstrate behavior that is independent of the details of the inter-particle potential. Systems in which the approximation of zero interaction range holds have dynamics governed solely by the two-body scattering length $a_2$. The observable properties of these systems are typically described as being universal because the details of the theory describing their interaction becomes irrelevant [1]. So long as the particles move with sufficiently small momenta, their de Broglie wavelengths are large in comparison to the scale of the details of the interaction and these details can be ignored. These concepts are made more mathematically and physically precise in the context of an effective field theory (EFT), in which the potential can be expanded systematically in a series of contact interactions and their derivatives. The result of this expansion is identical in the two-body system to the effective range expansion of phase shifts in quantum scattering theory [2].

This formalism can be extended to more-body systems, where exact solutions are generally impossible [3]. The EFT serves to delineate the separation of scales between the inter-particle interaction energies and the internal energies of each particle. In the full theory all these dynamics must be accounted for, but in the EFT the internal details are accounted for as effective interactions between the particles.

In the presence of an external trapping potential, the continuum asymptotic scattering states of free particles are replaced by discrete bound states. However, when the interaction range is negligible the system may still exhibit universality. Additionally, a description in terms of the two-body scattering length $a_2$ is still viable as this quantity can be defined based on the asymptotic behavior of the wavefunction. By taking the continuum limit ($\omega \to 0$) one should recover the full description of the asymptotically free particle scattering.

The understanding of the theory behind this problem has largely been motivated by recent advances in atom and molecule trapping experiments [4]. By trapping atoms with lasers the model system we discuss can be reproduced experimentally. The interaction can be tuned using external magnetic fields to create a Feshbach resonance; a near-zero energy bound state between the atoms. These dimers can then be dissociated with radiofrequency fields and their binding energies measured [5]. Experiments in reduced dimension, such as atoms trapped in a waveguide, are able to create bound states of these molecules even in
the limit of weak interaction (negative scattering length) [6]. This is related to the different behavior of singular potentials in lower dimensions. The 1-dimensional delta function, for instance, admits valid bound state solutions without the regularization and renormalization that must be performed in 2 or more dimensions.

The universality of this model makes it widely applicable. The two-nucleon system (the deuteron) has nucleon momenta small compared to the confined quark momenta inside the nucleons, and this bound state has a size much larger than the typical range of the nuclear force. Accordingly, the two-body scattering length for nuclear physics is large in comparison to the range of the strong interaction.

The No Core Shell Model (NCSM) is a numerical method for solving the Schrödinger equation in a truncated harmonic oscillator (HO) basis with oscillator length \( b = 1/\sqrt{\mu \omega} \) (we use units of \( \hbar = 1 \) for the entirety of this discussion) for reduced mass \( \mu \) and frequency \( \omega \) for systems of many particles [7]. In effective field theory the truncation of the model space is responsible for generating effective interactions between the particles. Effective interactions accounting for physics in the ignored parameter space are naturally generated when the EFT is renormalized. This provides a route to calculating observables without ad hoc approximations regarding the form and number of the interaction terms. This method has been applied to low-momentum observables of systems up to nucleon number \( A = 6 \) with reasonable accuracy [8].

In the theory for cold atom trapping the presence of the harmonic trap provides a natural basis to work in and the system in discussion is a natural model for cold atoms trapped in a laser trap with length \( b \). The system with infinite scattering length has been solved exactly for the \( A = 2 \) case [9] and for \( A = 3 \) in the unitary limit [10]. For more than 3 particles approximation techniques, such as NCSM, must be used. The EFT expansion as a method for generating interactions within the NCSM provides a generalized and extendable means with which to predict spectra of systems of trapped particles to arbitrary accuracy determined by the number of orders used in the EFT expansion. Increasing the number of orders both speeds the convergence of energies and provides a natural extension to the case of non-zero effective range [11]. Convergence as a function of the size of the model space may also be improved through the use of an alternative regularization scheme [12].

In this work, we present calculations of the energy spectrum for the system of two trapped particles in the regime of trap length to scattering length large and negative. This represents the case of weak coupling in which the scattering of the particles can be treated as a perturbation to the effects of the HO. Based on the results of Busch et al. [9] (also derived in Ref. [11] in the EFT framework), the spectrum of zero effective range is given by solutions of the transcendental equation

\[
\frac{\Gamma(3/4 - E/2\omega)}{\Gamma(1/4 - E/2\omega)} = \frac{b}{2a_2}.
\]

Perturbation theory is applicable in the limit \( b/a_2 \ll 0 \), when the interaction is weak compared to the presence of the trap. The unitary limit \( (b/a_2 = 0) \) is strongly non-perturbative as it represents the case in which the trap’s contribution to the dynamics of one particle is of the order of the effects due to the presence of the other particle. When \( b/a_2 \gg 0 \) the particle interaction is most significant. These latter two cases must be solved with the two potentials treated equally. Later terms in the inter-particle potential can, however, be treated as
perturbations to earlier terms, so long as each higher order term in the potential expansion is weaker than the previous. In the following chapter we introduce some of the necessary background to understanding the problem of two trapped particles in the EFT framework. This is followed by a calculation of the spectrum for two particles in the perturbative regime at leading order and next to leading order and a discussion of the results in first and second order perturbation theory.
Chapter 2

Background: Scattering Concepts, Effective Field Theories and Singular Potentials

The description of the trapped cold particle system as described above involves several concepts beyond the fundamentals of non-relativistic quantum mechanics. Specifically, quantum mechanical scattering processes are covered in shallow detail or not at all. The concepts of EFT are most readily applicable to, and were first utilized in quantum field theory and are foreign to the traditional sequence of undergraduate physics. We will see that the Schrödinger equation with a delta-function potential does not explicitly admit solutions. The delta function is an example of a singular potential; a potential that diverges too sharply near the origin to overcome the centrifugal forces and allow bound state solutions of arbitrarily small size. The process of regularization and renormalization can be applied to these potentials along with the ideas of EFT to show that finite size bound states do exist for this potential and to find the binding energies. These concepts are explored in greater detail in the following sections, as they are readily applicable to the discussion throughout this thesis.

2.1 Scattering

Scattering of asymptotically free particles at low energy is described by the relative phase shift $\delta$ between the incoming and outgoing states in the center of mass frame. For small momenta the phase shifts can be expanded through use of the effective range expansion in the S-wave (see, for example [13])

$$k \cot(\delta_0) = -\frac{1}{a_2} + \frac{1}{2} r_0 k^2 + ...$$ (2.1)

in which $k$ is the relative momentum, $a_2$ is the scattering length and $r_0$ is the effective range of the interaction. This relates the asymptotic (observable) incoming and outgoing states of the particles to the details of the potential. However, for small $k$ all terms beyond $1/a_2$ are suppressed in the proceeding terms, and the system is described entirely in terms of the scattering length to a good approximation.
2.2 Effective Field Theory

Effective field theories have proven useful in the formulation of approximate solutions in situations exhibiting a wide range of clearly separated energy scales. The principle is that the restriction of a system described by an underlying “exact” theory to a certain finite energy scale generates all the possible dynamics by freezing out degrees of freedom that are available at energies higher than some energy. The effects of higher energy phenomena are then mimicked by renormalizing the effective theory. The physics at high energy does not directly affect the dynamics of the system, but there are induced interactions that represent the neglected phase space. Ensuring that these induced interactions do not depend on the specific point at which the energy scale is separated then reproduces the interactions that would be present in the exact solution of the underlying theory. Through this process one can determine some of the nature of the interaction without actually knowing anything of the physical theory governing it. In essence, all theories are effective field theories because there are always greater energies that are not included in the experimental evidence on which a theory can be based.

2.3 Singular Potentials and Renormalization

The effective theory for short range interactions derived in Ref. [2] is represented in the Schrödinger picture as an expansion of the potential as a power series in momentum space. In position space this potential consists of a series of delta functions and their derivatives. The relative strengths of terms are ordered according to the number of derivatives they contain. However, the delta function is an example of a singular potential. In order to find solutions for scattering or bound states from such a potential it must first be regularized. This process is intimately related to the ideas of EFT. An arbitrary division is made between low and high energies, and the system is truncated so that energies above this division are ignored. The coupling constants in the EFT expansion, which account for the strength and shape of the underlying potential, are then chosen in order to reproduce a finite number of observables for any value of the cutoff parameter. Any observables not used in defining the strength of the coupling constants can then be calculated within the theory.

2.3.1 Delta Function in $N$ Dimensions

In order to better understand the character of singular potentials and the renormalization thereof we analyze the problem of 2 particles with reduced mass $\mu$ interacting in free space through a delta function in $N$-dimensions. This same interaction can be used for trapped particles, with the addition of an harmonic oscillator component. We seek to solve the time independent Schrödinger equation in the center of mass frame with relative coordinate $r$

$$-\frac{1}{2\mu}\nabla^2_N\psi(r) + C\delta^{(N)}(r)\psi(r) = E\psi(r),$$

for the allowed energy spectrum, assuming this potential admits bound states (we use units in which $\hbar = 1$ throughout the remainder of this thesis). In momentum space the Schrödinger
equation becomes, in terms of the binding energy \( B = -E \),

\[
\frac{p^2}{2\mu} \phi(p) + \frac{C\psi(0)}{\sqrt{2\pi}} = E\psi(p)
\]

(2.3)

where the derivative term has been integrated by parts under the condition that \( \psi \to 0 \) as \( r \to \infty \) and the other terms follow by definition. Further manipulation brings the Schrödinger equation to the form

\[
\phi(p) = \frac{2\mu C\psi(0)}{(2\pi)^{N/2}} \frac{1}{p^2 + 2\mu B}.
\]

(2.4)

Writing \( \psi(0) \) in terms of a Fourier transform of \( \phi(p) \) we have

\[
\psi(0) = \frac{1}{(2\pi)^{N/2}} \int \phi(p) e^{ipN} d^N p = -\frac{2\mu}{(2\pi)^N} \int \frac{C\psi(0)}{p^2 + 2\mu B} d^N p
\]

(2.5)

which simplifies to

\[
1 = -\frac{2\mu C}{(2\pi)^N} \int \frac{d^N p}{p^2 + 2\mu B}.
\]

(2.6)

The solution of this equation for \( B \) will naively reveal the binding energy for the system in a particular number of dimensions. We will see, however, that in the case of more than 2 dimensions the situation is not so simple.

### 2.3.2 Delta Function in 2 Dimensions

As a demonstration of the peculiarities of the singular delta function potential we attempt to solve the momentum space Schrödinger equation for the binding energy \( B \) in two dimensions. In polar coordinates eq. 2.6 becomes

\[
1 = -\frac{\mu C}{(2\pi)^2} \int_0^{2\pi} \int_0^\infty p dp \frac{p}{p^2 + 2\mu B}.
\]

(2.7)

Upon integration over \( p \) it is found that the integral diverges; no finite-energy bound state seems to exist for the delta function in 2 dimensions. In order to ensure that a valid solution is admitted one must introduce an ultraviolet cutoff \( \Lambda \) in momentum above which there is no contribution to the integral in eq. 2.7. This process is called regularization and \( \Lambda \) plays the role of a regulator in the system. In general the exclusion of higher momenta will make the binding energy \( B \) a function of the cutoff \( \Lambda \). In order to remove this fictitious dependence of binding energy on an arbitrary separation between low momentum and high momentum we vary the parameter \( C \) as a function of \( \Lambda \) in such a way that

\[
\frac{\partial B}{\partial \Lambda} = 0.
\]

(2.8)

This process is called renormalization and equation 2.8 is called a renormalization group equation (RGE). Introducing this regulator and integrating over the angular variable we obtain the definite integral over momentum

\[
1 = -\frac{\mu C}{\pi} \int_0^\Lambda \frac{p dp}{p^2 + 2\mu B}.
\]

(2.9)
Integration over $p$ reveals that

$$-\frac{2\pi}{\mu C} = \ln \left| \frac{\Lambda^2 + 2\mu B}{2\mu B} \right|,$$

(2.10)

or that

$$f(\Lambda, C) = \mu B = \frac{|\Lambda^2|}{2(e^{-2\pi/\mu C} - 1)}.$$  

(2.11)

Eq. 2.8 then constitutes the RGE for this situation, from which the running of $C$ with $\Lambda$ can be obtained that ensures $B$ is independent of the ultraviolet regulator.

In the 3-dimensional case the integral in eq. 2.6 diverges even faster. We would expect this integral to go as $\Lambda$ and so the coupling constant $C$ must go as $1/\Lambda$ in order to account for the divergence of the integral. However, the same sequence of steps can be used in arbitrary numbers of dimensions and only the specifics of the calculations will be changed.
Chapter 3

Two Particles in an Harmonic Trap

Our goal is to solve the Schrödinger equation

\[ \frac{\omega}{2} \left[ -b^2 \nabla^2 + \frac{r^2}{b^2} \right] \psi(r) + (V^{(1)} + V^{(2)} + ...) \psi(r) = E \psi(r), \]  

(3.1)

where the inter-particle potential has been expanded in the low-energy limit as \( V = V^{(1)} + V^{(2)} + ... \) via the methods of EFT. This potential arises as a power series in momentum,

\[ V(p, p') = C_0 + C_2 p^2 + C'_2 p \cdot p' + ... \]  

(3.2)

In position space in terms of the relative coordinate \( r \) we get,

\[ V^{(1)} = C_0 \delta^3(r), \]  

(3.3)

for the leading order (LO) term in the potential and

\[ V^{(2)} = C_0 \delta^3(r) - C_2 \{ \nabla^2 \delta^3(r) + 2[\nabla \delta^3(r)] \cdot \nabla + 2 \delta^3(r) \nabla^2 \} . \]  

(3.4)

for the next to LO (NLO) term [2].

We expand the energies and wavefunctions in terms of the harmonic oscillator basis states \( \psi_{nlm}^{(0)} \) with energies \( E_{nl}^{(0)} \) using the standard methods of perturbation theory. We write a component of the energy expansion at order \( i \) in perturbation theory and with a \( j \)th order term from the potential as \( E_{nl}^{(ij)} \). The energy for a perturbed eigenstate \( \psi_{nlm} \) approximated up to order \( i = N \) in perturbation theory and including \( j = M \) terms from the potential then may be written

\[ E_{nl,NM} = E_{nl}^{(0)} + \sum_{i=1}^{N} \sum_{j=1}^{M} E_{nl}^{(ij)} = E_{nl}^{(11)} + E_{nl}^{(12)} + E_{nl}^{(21)} + ... + E_{nl}^{(MN)} . \]  

(3.5)

Perturbation theory requires computation of the matrix elements involving terms from the \( N \)th order in the potential \( \langle \psi_{nlm} \mid V^{(N)} \mid \psi_{n'l'm'} \rangle \), from which it is simple to see that \( E_{nl}^{(ij)} = 0 \) for \( l \neq 0 \) when the index \( j \leq 2 \) because of the presence of the delta functions at the origin. We therefore restrict the discussion from this point on to s waves so that

\[ E_{nl}^{(ij)} \equiv E_{n}^{(ij)} . \]  

(3.6)
We also therefore write $\psi$ in terms of the zero angular momentum radial harmonic oscillator wavefunctions $\phi_n(r)$,

$$
\phi_n(r) \equiv \psi_{n00}(r) = R_n(r) Y_0^0(\phi, \theta) = \frac{R_n(r)}{4\pi},
$$

(3.7)

$$
\phi_n(r) = \pi^{-3/4} b^{-3/2} [L_n^{(1/2)}(0)]^{-1/2} e^{-r^2/2b^2} L_n^{(1/2)}(r^2/b^2).
$$

(3.8)

The relevant matrix elements for the LO potential reduce to

$$
\langle \phi_n | C_0 \delta^{(3)}(r) | \phi_k \rangle = C_0 \phi_n(0) \phi_k(0) = \frac{\sqrt{L_k^{(1/2)}(0)L_n^{(1/2)}(0)}}{\pi^{3/2} b^3}.
$$

(3.9)

### 3.1 Perturbation Solution with Potential to Leading Order

We begin by calculating the first and second order energy perturbations from the LO potential; $E_n^{(11)}$ and $E_n^{(21)}$. For convenience we additionally expand the coupling constants,

$$
C_0 = \sum_i \sum_j C_0^{(ij)},
$$

(3.10)

and match these with the corresponding terms $E_n^{(ij)} \propto C_0^{(ij)}$. The energy expansion is given by the standard formulas from perturbation theory:

$$
E_n^{(11)} = \langle \phi_n | C_0^{(11)} \delta^{(3)}(r) | \phi_n \rangle,
$$

(3.11)

$$
E_n^{(21)} = \sum_{k=0, k \neq n} \frac{|\langle \phi_k | C_0^{(11)} \delta^{(3)}(r) | \phi_n \rangle|^2}{E_n^{(0)} - E_k^{(0)}} + \langle \phi_n | C_0^{(21)} \delta^{(3)}(r) | \phi_n \rangle.
$$

(3.12)

We define

$$
A_0^{(ij)} \equiv \frac{C_0^{(ij)}}{\pi^{3/2} b^3},
$$

(3.13)

so that the energy perturbations becomes

$$
E_n = (3/2 + 2n) \omega + A_0^{(11)} L_n^{(1/2)}(0) + \frac{(A_0^{(11)})^2 L_n^{(1/2)}(0)}{2} \sum_{k=0, k \neq n} \frac{L_k^{(1/2)}(0)}{n-k} L_n^{(1/2)}(0) + A_0^{(21)} L_n^{(1/2)}(0).
$$

(3.14)

Naively at this point one would evaluate the sum for the 2nd order perturbation, use measured observables to fix the constants $A_0^{(ij)}$, and obtain the general formula for the energies up to 2nd order. It turns out, however, that the sum in the 2nd order energy is divergent, and that mathematically no finite energy eigensolutions exist for this potential. Physically, one must consider the consequences of the approximations that have been made. The reduction of the potentially complicated short range potential to the leading order (LO)
effective potential is only possible at low energies where the unknown small-distance structure does not come into play due to the uncertainty principle. Eigenstates of higher and higher energies (and thus momenta) probe smaller and smaller spatial scales and the inclusion of eigenstates all the way up to \( n = \infty \) contradicts the assumptions that allowed the effective potential to be used. We thus introduce a high-energy cutoff \( \Lambda = E_{n_{\text{max}}} \) and it is assumed that there is no contribution from higher energy eigenstates. However, this assumption is also unphysical by itself in that all energies can potentially contribute, and this means that the observable energies would become functions of the number of states included, \( n_{\text{max}} \). We remedy this by allowing the coupling “constants” \( C_0 \) (and thus the “constants” \( A_0^{(ij)} \)) to be functions of \( n_{\text{max}} \), and enforce that they vary in such a way as to make \( E_n \) not sensitively dependent on \( n_{\text{max}} \). This renormalization and regularization is the process through which the dependence of the observable potential on the scattering energy is accounted for. In other words,

\[
A_0^{(ij)} = A_0^{(ij)}(n_{\text{max}}), \quad E_n = E_n(A_0(n_{\text{max}}), n_{\text{max}}), \quad E_n(A_0(n_{\text{max}}), n_{\text{max}}) \approx \text{const.}
\]

To make sense of this physically one can consider that higher energy states probe the potential at a higher resolution than do the low-energy states. We account for this by letting the strength of the effective potential vary with the maximum energy included. In this case the energies can be written

\[
E_n = (2n + 3/2)\omega + A_0^{(11)}(n_{\text{max}})L_{n}^{(1/2)}(0) + \frac{(A_0^{(11)})^2(n_{\text{max}})}{2} L_{n}^{(1/2)}(0) \sum_{k=0, k \neq n}^{n_{\text{max}}} \frac{L_k^{(1/2)}(0)}{n - k} + A_0^{(21)}(n_{\text{max}}) + \ldots
\]  

This constitutes a renormalization of the singular delta function potential. Notice that the \( n_{\text{max}} \) dependence must only appear in \( A_0^{(21)} \) as there is no divergence in first order perturbation theory. The \( A_0^{(21)} \) term is then used to renormalize the infinity that would otherwise appear in the \( (A_0^{(11)})^2 \) term when \( n_{\text{max}} \) increases without bound. We adjust \( A_0^{(11)} \) to fit the ground state perfectly using only first order perturbation theory so that

\[
A_0^{(11)} = E_0 - E_0^{(0)}
\]

where we have used \( L_0^{(1/2)}(0) = 1 \). Since we have let first order perturbation theory determine the ground state the second order terms must cancel zero for \( n = 0 \):

\[
A_0^{(21)} = -\frac{(A_0^{(11)})^2}{2} \sum_{k=1}^{n_{\text{max}}} \frac{L_k^{(1/2)}(0)}{-k}.
\]

Thus

\[
E_n = (2n + 3/2)\omega + A_0^{(11)}L_{n}^{(1/2)}(0) \left( 1 - \frac{A_0^{(11)}}{2} S_0(n_{\text{max}}) + \frac{A_0^{(11)}}{2} S_n(n_{\text{max}}) \right) + \ldots
\]
in which we have defined
\[ S_n \equiv \sum_{k=0, k \neq n}^{n_{max}} \frac{L_k^{(1/2)}(0)}{n-k}. \]  
(3.22)

We can combine the sums \( S_n \) and \( S_0 \),
\[ S_n - S_0 = \sum_{k=0, k \neq n}^{n_{max}} \frac{\Gamma(k+3/2)}{k!(n-k)\Gamma(3/2)} - \sum_{k=1}^{n_{max}} \frac{\Gamma(k+3/2)}{k!(0-k)\Gamma(3/2)}, \]  
(3.23)
to make
\[ S_n - S_0 = \frac{1}{n} + \frac{\Gamma(n+3/2)}{n\cdot n!\Gamma(3/2)} - \frac{n}{\Gamma(3/2)} \sum_{k=1}^{n_{max}} \frac{\Gamma(k+3/2)}{k!\cdot k(k-n)}, \quad n \neq 0, \]  
(3.24)
which more explicitly shows how the introduction of an \( n_{max} \) dependence in \( A_0^{(21)} \) suppresses the divergence the original sum. Inserting this into the 2nd order energy expansion eq. 3.21 we find a somewhat compact expression for the excited state energies up to second order,
\[ E_n = (2n + 3/2)\omega + \left[ \frac{A_0^{(11)}}{n!\Gamma(3/2)} \right] \left[ 1 + \frac{\Gamma(n+3/2)}{n\cdot n!\Gamma(3/2)} - \frac{n}{\Gamma(3/2)} \sum_{k=1}^{n_{max}} \frac{\Gamma(k+3/2)}{k!\cdot k(k-n)} \right] + \ldots, \quad n \neq 0. \]  
(3.25)

It is most convenient to investigate the properties of these energy solutions by comparing the running of their numerical values to those from other techniques. We illustrate the results of LO calculations in figures 3.1 and 3.2. As a measure of the success of the perturbation expansion we compare the results to the exact Busch at al. relation eq. 1.1 derived analytically for the regularized delta-function potential [9]. We are restricted to the case where
\[ \frac{b}{a_2} < 0 \]  
(3.26)
so that the perturbed energies are near to the base harmonic oscillator levels, as can be seen from the solutions of the transcendental eq. 1.1. We refer to accuracy as the percent difference between the results of the perturbation expansion to the predictions of the analytical formula.

The first order results are seen to have an accuracy in the range of 2% in the case where \( b/a_2 = -2 \) and 0.5% for \( b/a_2 = -4 \). Accuracy increases rapidly as \( a_2 \) becomes small and negative, reaching of order 0.1% for \( b/a_2 = -10 \) (fig. 3.2). The second order energies do not appear to be converging to higher accuracy than first order within reasonable values of \( n_{max} \). In fig. 3.1 the second order theory predicts a high accuracy over a range of \( n_{max} \) from 10 to 25 but it is unclear if the solutions are converging at this point or if they will become less accurate at larger \( n_{max} \). In the \( b/a_2 = -10 \) and -20 cases the second order solution clearly does not progress rapidly enough to provide an improvement over first order. We discuss the possible meaning of this in chapter 4.
The inconsistency of the above results with what one would expect from basic perturbation theory (the second order theory is out-performed by first order) suggests that we include the NLO potential in order to try to force a more definite convergence of the perturbation series. The NLO potential, given by equation 3.4, still only perturbs S-waves. We include the NLO potential in first order perturbation theory:

\[ E_{n}^{(12)} = \langle \psi_{n} | V_{n}^{(2)} | \psi_{n} \rangle = \left[ C_{0}^{(12)} + 4 \mu C_{2}^{(12)} E_{n}^{(0)} \right] |\phi_{n}(0)|^{2}. \]  

(3.27)

We can choose to place the first order correction from the NLO potential with any arbitrary order in the perturbation series in the LO potential. Including this NLO term should only have a positive constructive effect when it is placed at an appropriate order in the LO expansion such that \( E_{n}^{(12)} \) is of the order of \( E_{n}^{(1)} \).

We can calculate the form of \( E_{n}^{(12)} \) in general because we have forced the ground state to be fixed exactly by the leading order potential in first order perturbation theory,

\[ E_{n} = (2n + 3/2)\omega + A_{0}^{(11)} L_{n}^{(1/2)}(0) + A_{0}^{(12)} L_{n}^{(1/2)}(0) + 4 \mu C_{2}^{(12)} E_{n}^{(0)} |\phi_{n}(0)|^{2}. \]  

(3.28)

Inserting \( E_{n}^{(0)} = (3/2 + 2n)\omega \) and forcing the LO term to reproduce the ground state energy just as we did for the case without \( V_{n}^{(2)} \) we see that

\[ C_{0}^{(12)} + 4 \mu C_{2}^{(12)} (3/2)\omega = 0. \]  

(3.29)

The two coupling constants in the NLO theory are therefore related by

\[ C_{0}^{(12)} = -6 \mu \omega C_{2}^{(12)}. \]  

(3.30)
In terms of $C_2^{(12)}$ then the NLO potential introduces a first order perturbation

$$E_n^{(12)} = A_0^{(12)} n L_n^{(1/2)}(0).$$  \hfill (3.31)

where we have defined

$$A_2^{(12)} = \frac{8\mu\omega C_2^{(12)}}{\pi^{3/2} b^3}$$  \hfill (3.32)

For the case where we include $V^{(2)}$ as a first order correction to terms $E_n^{(11)}$ the energies are

$$E_n = (2n + 3/2)\omega + A_0^{(11)} L_n^{(1/2)}(0) + A_0^{(12)} n L_n^{(1/2)}(0).$$  \hfill (3.33)

By letting the $V^{(2)}$ term reproduce the first excited state energy we find that

$$A_2^{(12)} = \frac{E_1 - (E_1^{(0)} + E_1^{(11)})}{L_1^{(1/2)}(0)}$$  \hfill (3.34)

We may alternatively incorporate $E_n^{(12)}$ as a first order perturbation to $E_n^{(21)}$ by letting

$$E_n^{(21)} + E_n^{(12)} = \sum_{k=0,k\neq n}^{\infty} \frac{\langle \phi_k | V^{(0)} | \phi_n \rangle^2}{E_n^{(0)} - E_k^{(0)}} + \langle \phi_n | V^{(1)} | \phi_n \rangle$$  \hfill (3.35)

be the second order term in the perturbation expansion. We let $E_1^{(21)} = 0$ as in eq. 3.20 and separately force $E_1^{(12)} = 0$ as in eq. 3.29 and then fix the coupling constant $A_2^{(12)}$ by again enforcing that the prediction for $E_1$ be exact,

$$A_2^{(12)}(n_{max}) = \frac{E_1 - (E_1^{(0)} + E_1^{(11)} + E_1^{(21)}(n_{max}))}{L_1^{(1/2)}(0)}.$$  \hfill (3.36)
The energy expansion is therefore

\[ E_n = (2n + 3/2)\omega + A_0^{(11)} \frac{\Gamma(n + 3/2)}{n!\Gamma(3/2)} \times \]
\[ \times \left[ 1 + A_0^{(11)} \frac{1}{2} \left( \frac{1}{n} + \frac{\Gamma(n + 3/2)}{n \cdot n!\Gamma(3/2)} - \frac{n}{\Gamma(3/2)} \sum_{k=1, k \neq n}^{n_{\text{max}}} \frac{\Gamma(k + 3/2)}{k! \cdot k(k - n)} \right) \right] \]
\[ + \frac{A_2^{(12)} \Gamma(n + 3/2)}{(n - 1)!\Gamma(3/2)} + \ldots; n \neq 0. \]  

(3.37)

for the case where we let the second order energy be \( E_n^{(12)} + E_n^{(21)} \) and where \( A_0^{(11)} \) and \( A_2^{(12)} \) are evaluated as in eqs. 3.19 and 3.36, respectively. This formula provides the approximate energies in a given model space defined up to a maximum number of oscillator levels \( n_{\text{max}} \).

From inspection of figs. 3.3 and 3.4 it is seen that the inclusion of the NLO term along with the LO potential in first order perturbation theory does not significantly improve upon the case of LO alone, nor does it seem to guarantee an improvement at all. At smaller \(|b/a_2|\) the inclusion of the NLO term somewhat improves accuracy, but we find that at \( b/a_2 \leq -20 \) the trend reverses. It is not clear that introducing the NLO potential in first order perturbation theory is the correct ordering of expansion terms. Results of second order perturbation theory including the potential to NLO are presented in figs. 3.3 and 3.4. Accuracy increases from order 0.05% in for \( b/a_2 = -2 \) to better than 0.01% and then .005% at \( b/a_2 = -10 \) and \( b/2a_2 = -20 \), respectively.

Figure 3.3: Comparison of exact solutions to first and second order approximations at NLO for \( b/a_2 = -2 \) (left) and -4 (right).
Figure 3.4: Comparison of exact solutions to first and second order approximations at NLO for $b/a_2$ -10 (left) and -20 (right).
Chapter 4

Discussion

The behavior of the perturbation series using only the $V^{(1)}$ term in the potential does not seem to be representative of a uniformly converging perturbation expansion. As seen in fig. 4.1 the second order term in the expansion is contributing too much and actually resulting in larger errors than the first order theory. In the case where $b/a_2 = -10$ the perturbed energy of the second excited state differs from the base harmonic oscillator level by $0.2/5.5 = 3.6\%$ so one would expect that the perturbation series would not be facing any serious problems. It appears that the second order term does not converge quickly enough to improve upon the first order within a reasonable limit of $n_{\text{max}}$. Even as the perturbation on the base HO levels reaches the $1\%$ level with $b/a_2 = -20$ the first order outperforms the second order by a small factor. It appears that the relative accuracy of the second order to first order actually decreases as the potential becomes weaker as is apparent in figs. 3.1 and 3.2. In fig. 4.1 we show the behavior of the perturbation solutions for several of the low lying excited states for the case $b/a_2 = -10$. Apparently, the behavior is qualitatively the same for other energy levels.

In order to better understand the perturbation series we introduce the NLO potential as a first order perturbation to the first order term in $V^{(1)}$ and alternatively as a perturbation on the second order term in $V^{(1)}$. In fig. 4.2 we show the behavior of the NLO perturbation solutions for low lying excited states in the case $b/a_2 = -10$. The behavior is qualitatively the same in each case, as it was with only the LO potential included. The energies predicted in figs. 3.3 and 3.4 show a clear improvement over all predictions involving only the $V^{(1)}$ term. Going to third order in this term will be necessary to further explore the dependence on the ordering of the NLO terms.
Figure 4.1: Comparison of exact solutions to first and second order approximations at LO for $b/a_2 = -10$. Upper left: $n=2$, upper right: $n=3$, lower left: $n=4$, lower right: $n=5$. 
Figure 4.2: Comparison of exact solutions to first and second order approximations at NLO for \( b/a_2 = -10 \). Upper left: \( n=2 \), upper right: \( n=3 \), lower left: \( n=4 \), lower right: \( n=5 \).
Chapter 5

Conclusions

We have seen that perturbation theory produces accurate energy predictions for most negative values of $b/a_2$. However, the convergence of second order perturbation theory for the LO effective potential is questionable. Inclusion of the NLO potential as a first order perturbation to the second order LO perturbation increases the accuracy of a factor of 10. The terms including the NLO potential converge quickly in all cases; a model space no larger than $n_{\text{max}} = 25$ generally provides as much accuracy as is possible given the ignored terms from the energy expansion. Introducing a larger model space beyond this point only improves predictions by a factor of less than 1. The exact accuracy of perturbation theory at all orders depends substantially on the energy levels being considered, and can vary by as much as a factor of 5 from state to state. However, there is a uniform trend to higher accuracies as smaller values of $b/a_2$ are considered.

In order to determine if the inclusion of higher order terms in the perturbation expansion at LO provides a definite increase in accuracy, it will be useful to calculate the results from third order perturbation theory with the NLO term excluded entirely. After confirming the convergence of the LO perturbation expansion we will hopefully better understand the placement of the NLO terms in the perturbation expansion of the exact energy (EFT to all orders). Based on the continuum situation, the NLO potential when expanded to first order should not appear until the third order perturbation term in the LO potential [2]. However, the results presented above indicate that the $V^{(2)}$ term works effectively when coupled with the second order $V^{(1)}$ term.

A natural and useful extension of these methods is to systems of more numerous particles. The system of $A$ particles is modeled to leading order, for instance, by the Hamiltonian

$$H = \sum_{i=0}^{A} \left(\frac{p_i^2}{2m} + \frac{1}{2}m\omega^2 r_i^2\right) + C_0 \sum_{[i<j]} \delta^{(3)}(\mathbf{r}_i - \mathbf{r}_j)$$

where $[i < j]$ enforces that only particles of opposite spin interact [14]. Perturbation theory makes for a smaller computational load than exact diagonalization, and prediction of energy spectra of multi-particle systems may possibly be carried out in larger model spaces with no great loss in accuracy so long as the particle interactions are weak. Both the experimental and theoretical study of trapped cold atoms have progressed greatly in the last decade. However, understanding of strongly coupled many particle systems is still incomplete. Effective field
theories are likely to continue to play a role in building upon present understanding of trapped atoms light nuclei.


