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Two interacting electrons in a harmonic trap

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Abstract

We theoretically study a system consisting of two interacting electrons trapped in a harmonic oscillator of frequency $\omega$. We reduce the six-dimensional problem to a one-dimensional Schrödinger equation. Solutions proposed in a past publication are reviewed and studied thoroughly. These solutions are only found for certain frequencies of the harmonic oscillator. The solutions show a strongly interacting regime for low densities and a weakly interacting regime for high densities. With a number of techniques we tried to find the eigenenergies at any frequency. With a harmonic approximation of the potential we find universal asymptotic $\omega^{2/3}$-behaviour in the strongly interacting limit. We show that in the weakly interacting limit the problem reduces to a normal three-dimensional harmonic oscillator. We also find that when the contribution of the harmonic oscillator to the potential is negligible, the system still can be described by a harmonic oscillator. Using the Hellmann-Feynman theorem we find analytical expressions for the eigenenergies that are valid for every frequency. We also describe a number of methods for finding the wave functions. Finally, we shortly review a many-particle system and show that in the strongly interacting limit the electrons, which are fermions, have a boson-like behaviour.
1. Introduction

A quantum degenerate electron gas is a matter state that has some interesting properties for researchers. For example, it has a relatively high electron density and is relatively cold. As a result the degenerate electron gas can be used for example for electron microscopy, where a high density causes a high resolution, and collision processes, where a high density causes a high collision cross section. Also, a degenerate gas harbours interesting fundamental physics and therefore is fundamentally interesting.

Because of these applications, one wants to realise such a quantum degenerate gas. Contrary to a quantum degenerate gas, a classical electron gas can be relatively easily produced. For example, the conduction electrons in a metal crystal are described by the “free electron model”. Ideally, when trying to make a quantum degenerate electron gas we do not want to use the metal. Without the metal there would be no force that keeps the electrons together so that we need an external trap to keep the electrons together. An example of such an external trap is a harmonic oscillator. Normally, when we consider electrons in a harmonic oscillator we ignore particle interactions. This way, the electrons fill the equidistant energy levels up to the Fermi level.

However, the interaction between the trapped particles cannot be ignored. For trapped atoms in a harmonic oscillator, the interaction between atoms is often modeled by a contact potential. The resulting problem is relatively well known and is also exactly solvable, see [1]. Also, anharmonic contributions to the potential can be regarded as perturbation so that perturbation theory can be applied [2]. For plasmas we can distinguish two different regimes regarding the interactions. One regime is when the interaction is strong and the other when the interaction is weak. The strength of the interaction is indicated by a coupling constant $\Gamma$, defined as the ratio of the potential energy and the kinetic energy. Evidently, a strongly interacting plasma has $\Gamma > 1$ and a weakly interacting plasma has $\Gamma < 1$. We see in figure 1.1 that in general high densities lead to a strong interaction and low densities to a weak interaction.

Figure 1.1: Interaction strength for several plasmas.
CHAPTER 1. INTRODUCTION

For interacting electrons the problem is not easily solved. They interact via the Coulomb potential and the corresponding problem is a fundamental quantum mechanical problem. It is a so-called quasi-exactly-solvable problem and has a connection to $sl_2$-algebra [3]. We will not dive into all of the mathematical background of this problem, but this shows that this is an interesting problem. Since we cannot solve this problem exactly and also can no longer successfully use perturbation theory we will need to find other methods that do give an adequate description of the solutions of the problem. This will be the main focus of this report. However, we do not need to start “from scratch”. An example of a relevant past study about the same problem is the work by Taut [4]. We will use his work as basis and develop new insights into the problem.
2. Standard potentials

In this chapter we will recapitulate some simple potentials that can be solved analytically. Additionally we shall look into the ladder operators for these potentials. We do this since the powerful mechanism of ladder operators can be used to find all eigenstates at once.

2.1 Harmonic oscillator

The first potential is the (one-dimensional) harmonic oscillator:

\[ V(x) = \frac{1}{2} m\omega^2 x^2, \quad (2.1) \]

where \( x \) is the displacement from the equilibrium position. The Schrödinger-equation for one particle in this potential can be solved analytically and is treated in almost every introductory book about quantum mechanics.\(^1\) The eigenenergies are

\[ E_n = \left( n + \frac{1}{2} \right) \hbar \omega, \quad (2.2) \]

where \( n = 0, 1, 2, 3, \ldots \) is the quantum number for this problem. The corresponding wave functions are

\[ \psi_n(x) = \left( \frac{m\omega}{\pi \hbar} \right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n \left( \sqrt{\frac{m\omega}{\hbar}} x \right) \exp \left( -\frac{m\omega x^2}{2\hbar} \right), \quad (2.3) \]

where \( H_n(x) \) are Hermite polynomials in \( x \) of order \( n \).

2.1.1 Ladder operators

We can also write the Hamiltonian for this problem in terms of the ladder operators using the factorization method [6] [7] (amongst others). With these ladder operators one is also able to reconstruct all solutions as given above. For this problem, the ladder operators are

\[ \hat{a}_+ = \frac{1}{\sqrt{2\hbar m\omega}} \left( -\hbar \frac{d}{dx} + m\omega x \right), \]
\[ \hat{a}_- = \frac{1}{\sqrt{2\hbar m\omega}} \left( \hbar \frac{d}{dx} + m\omega x \right) = \hat{a}_+^\dagger, \quad (2.4) \]

\(^1\)See for example pages 40-59 of [5].
which are the raising respectively lowering operator, and the Hamiltonian for the harmonic oscillator then can be written in terms of these operators:

\[ \hat{H} = \hbar \omega \left( \hat{a}_- \hat{a}_+ - \frac{1}{2} \right) = \hbar \omega \left( \hat{a}_+ \hat{a}_- + \frac{1}{2} \right), \quad (2.5) \]

where we see that the commutator satisfies

\[ [\hat{a}_-, \hat{a}_+] = 1. \quad (2.6) \]

Using these operators the ground state can be found by solving the differential equation

\[ \hat{a}_- \psi_0 = 0 \quad (2.7) \]

and using normalization to determine the constant of integration. All excited states can be found by using

\[ \psi_n = \frac{1}{\sqrt{n!}} (\hat{a}_+)^n \psi_0. \quad (2.8) \]

### 2.1.2 Three-dimensional harmonic oscillator

For a three-dimensional harmonic oscillator given by

\[ V(r) = \frac{1}{2} \mu \omega^2 r^2, \quad (2.9) \]

the wave functions can be found by either using Cartesian or spherical coordinates. Here the second option is preferred since then the closed form of the wave function is more insightful. A complete derivation can be found in [8], but the results are that the eigenenergies are

\[ E_{kl} = \left( 2k + l + \frac{3}{2} \right) \hbar \omega \quad (2.10) \]

and the wave functions are

\[ \psi_{klm} = N_{kl} r^l \exp \left( -\frac{\mu \omega r^2}{2\hbar} \right) L_k^{(l+\frac{1}{2})} \left( \frac{\mu \omega r^2}{\hbar} \right) Y_l^m(\theta, \phi), \quad (2.11) \]

where \( N_{kl} \) is a normalization constant, \( L_k^{(l+\frac{1}{2})} \) is the associated Laguerre polynomial, \( Y_l^m \) are the spherical harmonics and \( k, l \) and \( m \) are the principal, azimuthal and magnetic quantum numbers, respectively. These can be renumbered to \( \{n, l, m\} \) where \( n = 2k + l \) so that

\[ E_n = \left( n + \frac{3}{2} \right) \hbar \omega. \quad (2.12) \]

The ladder operators for the principal quantum number \( k \) can be reconstructed by using the obtained wave functions. An example of how this can be done can be found in [9]
2.1. HARMONIC OSCILLATOR

(for another potential), but in general the tactic is to find a recurrence relation for the wave functions. Eventually we find

\[\hat{L}_\pm = \mp \frac{1}{8\nu} \frac{\partial^2}{\partial r^2} + \frac{1}{2} r \frac{\partial}{\partial r} \mp \frac{1}{4\nu r} \frac{\partial}{\partial r} \mp \frac{1}{2} \nu r^2 \pm \frac{l(l+1)}{8\nu r^2} + \frac{3}{4},\]  

(2.13)

where \(\nu = \frac{\omega}{2\hbar}\) and the scaling factors\(^2\)

\[l_+(k) = \sqrt{(k+1)\left(k + 1 + \frac{l}{2}\right)}, \quad l_-(k) = \sqrt{k\left(k + l + \frac{1}{2}\right)}.\]  

(2.14)

The complete derivation of these operators can be found in Appendix A.1. Note that the raising and lowering operator are not each others Hermitian conjugate where for the one-dimensional harmonic oscillator this was the case. Consequently, the factorization of the Hamiltonian is also different, here we find

\[\hat{H} = \hbar \omega \left(\hat{L}_+ \hat{L}_- - \hat{L}_- \hat{L}_+\right) = \hbar \omega \left[\hat{L}_+, \hat{L}_-\right]\]  

(2.15)

and since we have the commutators

\[\left[\hat{H}, \hat{L}_+\right] = 2\hbar \omega \hat{L}_+, \quad \left[\hat{H}, \hat{L}_-\right] = -2\hbar \omega \hat{L}_-\]  

(2.16)

these operators are indeed the raising and lowering operators.

\(^2\)The scaling factors are defined by the identity \(\hat{L}_\pm \psi_{k; l; m} = l_\pm(k) \psi_{k; l+1; m}\).
CHAPTER 2. STANDARD POTENTIALS

2.2 Coulomb potential

The potential for two charged particles in one dimension, charges $q_1$ resp. $q_2$, in an otherwise potential-free space is only the interparticle-potential, which is the Coulomb potential:

$$V(r_1, r_2) = \frac{q_1 q_2}{4\pi \varepsilon_0 |r_2 - r_1|} \equiv \frac{k}{|r_2 - r_1|}. \tag{2.17}$$

We transform to center-of-mass and relative coordinates, $R$ and $r$ respectively. The Schrödinger equation for $R$ is one of a free particle and will be disregarded here. The Schrödinger equation for $r$ is

$$-\frac{\hbar^2}{2\mu} \frac{d^2 \psi_r}{dr^2} + \frac{k}{r} \psi_r = E_r \psi_r, \tag{2.18}$$

where we only allow $r > 0$. The eigenenergies are

$$E_r = -\frac{\mu k^2}{2\hbar n^2} \tag{2.19}$$

and the wave functions are

$$\psi_{r,n}(r) = \sqrt{-\frac{4\mu^3 k^3}{\hbar^6 n^5}} (-1)^{n-1} \exp\left(\frac{\mu k r}{\hbar^2 n}\right) L_{n-1}^{(1)} \left( -\frac{2\mu k r}{\hbar^2 n} \right). \tag{2.20}$$

The complete derivation of these wave functions and eigenenergies can be found in Appendix A.2. The ladder operators for the Coulomb problem can again be found using the obtained wave functions. For details about the derivation of these ladder operators, refer to Appendix A.3. The operators are found in the $\rho$-space, where $\rho$ is the transformed $r$-coordinate ($\rho = -\frac{\mu k}{\hbar^2 n} r$), so that they are

$$\hat{\mathcal{L}}_\pm = \frac{1}{2\rho} \frac{d^2}{d\rho^2} \mp \rho \frac{d}{d\rho} + \frac{1}{2}\rho \tag{2.21}$$

with the scaling factors$^3$

$$l_\pm(n) = \sqrt{\frac{(n \pm 1)^3}{n}}. \tag{2.22}$$

Again, the raising and lowering operator are not each others Hermitian conjugate. Curiously, the factorization of the Hamiltonian in $\rho$-space is the same as for the three-dimensional harmonic oscillator, apart from a factor $\hbar \omega$, so

$$\hat{H} = \hat{\mathcal{L}}_+ \hat{\mathcal{L}}_- - \hat{\mathcal{L}}_- \hat{\mathcal{L}}_+ = \left[ \hat{\mathcal{L}}_+, \hat{\mathcal{L}}_- \right]. \tag{2.23}$$

$^3$The scaling factors are defined by the identity $\hat{\mathcal{L}}_\pm \psi_n = l_\pm(n) \psi_{n\pm 1}$. 

2.2. COULOMB POTENTIAL

All eigenfunctions of this Hamiltonian can be found by solving the differential equation\(^4\)

\[ \hat{\mathcal{L}}_+ \psi_1 = 0 \]  

(2.24)

for \(\psi_1(\rho)\) and by using

\[ \psi_n(\rho) = \frac{\left(\hat{\mathcal{L}}_+\right)^n \psi_1(\rho)}{n! \sqrt{n}}. \]  

(2.25)

Note that in fact the one-dimensional Coulomb problem is a lot more complicated than
as it is presented here. For an extensive treatment of the problem, see [10].

2.2.1 Three-dimensional Coulomb

In three dimensions the Coulomb potential stays the same, but now with position vectors \(r_1\) and \(r_2\). For the relative coordinate this reduces to a Schrödinger equation which is
nothing other than the Schrödinger equation for the hydrogen atom, while the center of
mass still behaves like a free particle. An elaborate treatment of the hydrogen atom can
for example be found in [5]. We are interested in the ladder operators for this problem,
which are

\[ \hat{\mathcal{L}}_{\pm} = \frac{1}{2} \rho \frac{d^2}{d\rho^2} \mp \rho \frac{d}{d\rho} + \frac{1}{2} \rho - \frac{l(l+1)}{2\rho}. \]  

(2.26)

Note that these are operators in \(\rho\)-space and furthermore are the ladder operators for
\(u_n(\rho)\). The wave function \(\psi_{nlm}\) can be found by using

\[ \psi_{nlm} = \frac{u_n(r)}{r} Y_{lm}^{m}(\theta, \phi). \]  

(2.27)

The ladder operators can easily be found by making the Ansatz that the operators for
the three-dimensional case are the same as for the one-dimensional case but with an
extra term that introduces the \(\frac{1}{\rho}\) behavior of the centrifugal term. If this Ansatz seems
too “ad hoc”, one can always apply the same tactic as was done before to find the ladder
operators: rewriting \(\frac{du_n}{d\rho}\) in terms of \(u_n\) and \(u_{n\pm1}\).

---

\(^4\)The observant reader might have seen that this is a second order differential equation and that therefore the solution will contain two integration constants, whereas we can only eliminate one by demanding that the solution is normalized. The second integration constant is eliminated by demanding that the solution is zero at \(r = 0\).
3. Eigenenergies

In this chapter we will manipulate the Schrödinger equation for our problem. Taut [4] has shown that some solutions can be found as a power series. We will walk through that derivation but now including all physical constants. Furthermore we will investigate the eigenenergies using various methods. In the end we will say something about the energy of general states and also about the many-particle problem.

3.1 Formulation of our problem

Two interacting charged particles in a harmonic oscillator are characterized by the potential

$$V(r_1, r_2) = \frac{1}{2} m_1 \omega^2 |r_1|^2 + \frac{1}{2} m_2 \omega^2 |r_2|^2 + \frac{q_1 q_2}{4 \pi \varepsilon_0 |r_2 - r_1|}.$$  

(3.1)

The Schrödinger equation for this potential in the center-of-mass and relative coordinates becomes

$$\begin{align*}
-\frac{\hbar^2}{2M} \nabla^2_R \psi - \frac{\hbar^2}{2\mu} \nabla^2_r \psi + \left( \frac{1}{2} M \omega^2 |R|^2 + \frac{1}{2} \mu \omega^2 |r|^2 + \frac{k}{r} \right) \psi &= E \psi. \\
(3.2)
\end{align*}$$

This can be separated using $\psi(r, R) = \Psi(r) \phi(R)$. The Schrödinger equation for $\phi$ is one of a three dimensional harmonic oscillator which was treated in section 2.1.2 and will be disregarded here. The potential is a central potential in $r$ so we make the Ansatz

$$\Psi(r) = \frac{u(r)}{r} Y_l^m(\theta, \phi).$$  

(3.3)

With this Ansatz the Schrödinger equation reduces to

$$\begin{align*}
-\frac{\hbar^2}{2\mu} \frac{d^2 u}{dr^2} + \left( \frac{1}{2} \mu \omega^2 r^2 + \frac{k}{r} + \frac{\hbar^2 l(l+1)}{2\mu r^2} \right) u &= E' u, \\
(3.4)
\end{align*}$$

where we see the appearance of the centrifugal barrier.\(^5\) Next, we substitute $\rho = \sqrt{\frac{\mu \omega}{\hbar}} r$ to find

$$\begin{align*}
-\frac{d^2 u}{d\rho^2} + \left( \rho^2 + \frac{k}{\rho} + \frac{l(l+1)}{\rho^2} \right) u &= E u, \\
(3.5)
\end{align*}$$

\(^5\)Note that the one-dimensional problem is also described by this differential equation but then with $l = 0$ and where $u$ is replaced by the wave function $\psi$. 


where $k = 2k \sqrt{\frac{\mu}{\hbar \omega}}$ and $E = \frac{2E'}{\hbar \omega}$. Now, we separate $u(\rho) = f(\rho) \exp\left(-\frac{1}{2} \rho^2\right)$ so that we find the differential equation for $f$:

$$\frac{d^2 f}{d\rho^2} + 2\rho \frac{df}{d\rho} + \left(1 + \frac{k}{\rho} + \frac{l(l+1)}{\rho^2}\right) f = Ef. \quad (3.6)$$

### 3.2 Taut’s solutions

Taut [4] has shown that some solutions of (3.6) can be found by assuming that $f$ is a power series:

$$f(\rho) = \rho^b \sum_{\nu=0}^{\infty} a_\nu \rho^\nu, \quad (3.7)$$

where $a_0 \neq 0$ and $b$ is a constant that yet has to be determined. Putting this power series into (3.6) and using the fact that the coefficient of each power has to be the same on the left-hand side as on the right-hand side of (3.6) we find for the $\rho^{b-2}$-monomial

$$b(b-1)a_0 - l(l+1)a_0 = 0. \quad (3.8)$$

Since $b > 0$ (otherwise $u(\rho)$ would diverge for $\rho \downarrow 0$) we find that $b = l + 1$. Regarding the $\rho^{b-1}$-monomial we find that

$$(b + 1)b a_1 - ka_0 - l(l+1)a_1 = 0 \Rightarrow a_1 = \frac{k}{2(l+1)}a_0. \quad (3.9)$$

Regarding the $\rho^{b+n}$-monomial with $n \geq 0$ we find a recurrence relation for the coefficients:

$$a_{n+2} = \frac{k}{(n+2)(n+2l+3)} a_{n+1} + \frac{2(l+n) + 3 - E}{(n+2)(n+2l+3)} a_n. \quad (3.10)$$

The discretization of the energy follows from the fact that $u(\rho)$ has to be normalized. However, because this is a relatively complex recurrence relation the normalization does not immediately imply that the power series must terminate, as was the case for the harmonic oscillator. Luckily, conversely, if the series terminate we know for sure that $u(\rho)$ is normalizable. So, let us assume that the series terminates after $j$ terms. We then know that

$$a_{j-2} \neq 0, a_{j-1} \neq 0, a_j = 0, a_{j+1} = 0 \quad (3.11)$$

holds. These conditions are sufficient since the recurrence relation will make sure that every $a_\nu$ with $\nu > j$ will be 0. Using the recurrence relation (3.10) we know that

$$a_{j+1} = \frac{k}{(j+1)(j+2l+2)} a_j + \frac{2(l+j+1) - 1 - E}{(j+1)(j+2l+2)} a_{j-1}$$

$$= \frac{2(l+j+1) - 1 - E}{(j+1)(j+2l+2)} a_{j-1} = 0. \quad (3.12)$$
3.2. TAUT’S SOLUTIONS

For this equation to hold we must have

\[ E = 2(j + l) + 1. \]  

(3.13)

The second equation, \( a_j = 0 \), issues a constraint on \( k \), in fact, it specifies \( k \). In other words, we are only able to find analytical solutions for this problem for certain “special” values of \( k \), \( \mu \) and \( \omega \).

With \( k = \frac{e^2}{4\pi\epsilon_0} \) and \( \mu = \frac{1}{2}m_e \), where \( e \) is the electron charge and \( m_e \) the electron mass, we find a countably infinite number of energies and corresponding frequencies. The energies for the three lowest states with \( l = 0 \) are plotted in figure 3.1. Energies for excited states or states with \( l \neq 0 \) can also be found by using the method described above. In figure 3.1 we used \( k \) as the principle quantum number which is in accordance with the notation for the three dimensional harmonic oscillator. Instead of showing the energy itself we show the energy divided by \( \hbar \omega \), which is the energy quantum for the harmonic oscillator. The dotted lines are the asymptotes of the energy for \( \omega \to \infty \). These follow from the argumentation that in the limit of \( \omega \to \infty \) the Coulomb repulsion in the potential will become negligible with respect to the harmonic oscillator contribution at every \( r \).\(^6\) Therefore, we will end up with a three-dimensional harmonic oscillator which has energies \((2k + l + \frac{3}{2}) \hbar \omega \). These thus are the lines that are shown in the figure. When \( \omega \) is large but not infinite we suspect (and also can see) that the energy is approximately that of a harmonic oscillator.

As mentioned in the introduction, for plasmas we can distinguish a strongly interacting and a weakly interacting regime. These are characterized by the coupling constant \( \Gamma \), defined as the ratio of the potential energy and the kinetic energy. We saw that high densities lead to a strong interaction and low densities to a weak interaction. For our problem we can also define a coupling constant but now as the ratio of the contribution of the Coulomb repulsion to the energy and the contribution of the harmonic oscillator. From figure 3.1 we can again distinguish two regimes. The first is the weakly interacting regime where the Coulomb repulsion does only affect the energies (and eigenstates) limitedly and \( \frac{E'}{\hbar \omega} \) is close to the asymptote. This is found for high frequencies as we discussed above. On the other side of the figure we recognize the strongly interacting regime where the energy is much larger than that of a harmonic oscillator. The energy diverges which is caused by the fact that the Coulombic part of the potential becomes larger and larger with respect to the part that describes the harmonic oscillator for decreasing frequencies. The correlation between the interaction regimes and the density is somewhat counter-intuitive. Namely, for a high \( \omega \) the value of \( r \) at which \( V(r) \) is minimal is relatively low. This means that \( \langle r \rangle \) is quite low and thus that the distance between the two electrons is low. This corresponds to a high density. So a high density corresponds to a weakly interacting regime and vice versa, a low density corresponds to a strongly interacting regime. This is actually opposite of the behaviour we saw in

\(^{6}\)This argumentation might be flawed since at \( r = 0 \) the Coulomb part never is negligible. A more correct description would be a harmonic oscillator with a \( \delta \)-function at \( r = 0 \). This problem can be solved exactly, see for example [1] and [2]. Remarkably, the description of a single harmonic oscillator is sufficient here.
The transition between the two regimes is situated around $\omega = 10^{16}$ Hz. This frequency corresponds to a number density of about $10^{29}$ electrons per cubic meter. This density is very high and indicates that for most real-life systems we need to deal with the strongly interacting regime.

Note that with Taut’s method we can only find the shown set of eigenenergies. As we want to know the eigenenergies for any frequency we will try to find (analytical) methods that can predict the eigenenergies or at least approximate them. This is done in the coming sections. In the end we will also investigate the eigenenergies for more general quantum numbers, as we only studied the first three states with $l = 0$ here.

Figure 3.1: Energies of the first three eigenstates for $l = 0$ in terms of $\hbar \omega$ as function of $\omega$ ($\omega_0$ is a reference frequency of 1 Hz). Only for certain frequencies eigenstates and corresponding energies can be found, as was demonstrated by Taut. The expected asymptotes for $\omega \to \infty$ are shown as well. We see a transition around $\omega = 10^{16}$ Hz between a strongly interacting and a weakly interacting regime.
3.3 Perturbation theory

A first candidate to give a description of the eigenenergies as function of $\omega$ is perturbation theory. When $\omega$ is very large in comparison to $k$ we can regard the Coulomb potential as a perturbation. This means that we might be able to predict the eigenenergies in the weakly interacting regime, a regime where Taut’s method can not find any eigenenergies (see figure 3.1). We can now write the following Hamiltonians (in the relative coordinate)

$$
\hat{H}^0 = -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{1}{2} \mu \omega^2 r^2 + \frac{\hbar^2 l(l + 1)}{2\mu r^2},
$$

$$
\hat{H}' = \frac{1}{r},
$$

$$
\hat{H} = \hat{H}^0 + k \hat{H}'.
$$

(3.14)

Even though $k$ itself is not necessarily small, it is small with respect to the eigenvalues of $\hat{H}_0$ which scale as $\hbar \omega$. This way we can still use perturbation theory. The eigenfunctions and eigenenergies of $\hat{H}^0$ are well-known since this is just the Hamiltonian of a three-dimensional harmonic oscillator which was treated in section 2.1.2. For the eigenenergies of $\hat{H}$ we can now write

$$
E_n = E_n^0 + k E_n^1 + k^2 E_n^2 + \ldots.
$$

(3.15)

First we will investigate the ground state energy. The ground state of the unperturbed Hamiltonian $\hat{H}^0$ is $\psi_{000}$ which is given by equation (2.11). It has energy $E_{000}^0 = \frac{3}{2} \hbar \omega$ so that to zeroth order, the ground state energy will be

$$
E^{(0)}_{00} = \frac{3}{2} \hbar \omega.
$$

(3.16)

The first order correction is given by

$$
E_{00}^{(1)} = \langle \psi_{000} | \hat{H}' | \psi_{000} \rangle = \int_0^\infty \int_0^{2\pi} \int_0^{2\pi} \psi_{000}(r, \theta, \phi) \frac{1}{r} \psi_{000}(r, \theta, \phi) r^2 \sin(\theta) d\phi d\theta dr = 2 \sqrt{\frac{\mu \omega}{\pi \hbar}}.
$$

(3.17)

Up to first order we thus find

$$
E_{00}^{(1)} = E_{00}^0 + k E_{00}^1 = \frac{3}{2} \hbar \omega + 2k \sqrt{\frac{\mu \omega}{\pi \hbar}}.
$$

(3.18)

The second order correction can also by calculated but not in closed form and will be omitted here. As we will compare this method with the analytical energies presented in figure 3.1 we will investigate the first order energies for the states with $k = 1$, $l = 0$ and with $k = 2$, $l = 0$ too. The integrals for these states can be evaluated to find

$$
E_{10}^{(1)} = \frac{7}{2} \hbar \omega + \frac{5k}{3} \sqrt{\frac{\mu \omega}{\pi \hbar}},
$$

$$
E_{20}^{(1)} = \frac{11}{2} \hbar \omega + \frac{89k}{60} \sqrt{\frac{\mu \omega}{\pi \hbar}}.
$$

(3.19)
The integrals for other states can also conveniently be calculated to find the first order energies for those states. The first order energies can be seen in figure 3.2. We see that the energies do not go through the analytical points for $\omega < 10^{16}$ Hz and this is of course because of the fact that this is the strongly interacting regime where the Coulomb potential is no longer a small perturbation but rather a large disturbance. We also see that for larger frequencies the perturbation theory approach seems adequate and this has the same explanation. The asymptotes of the energies found by a perturbation approach correspond to the expected asymptotes as shown in figure 3.1. So concluding, we see that the perturbation theory approach works well in the weakly interacting regime, which is what we expected.

![Figure 3.2: Comparison of first order eigenenergies from perturbation theory (lines) and the analytically found eigenenergies for certain $\omega$ (dots). $\omega_0$ is a reference frequency of 1 Hz. We see that perturbation theory works well in the weakly interacting regime which is what one expects from perturbation theory.](image-url)
3.4 Harmonic approximation

Another approach that can be used to find the eigenenergies is that instead of using the effective potential as in equation (3.4),

\[ V_{\text{eff}}(r) = \frac{1}{2} \mu \omega^2 r^2 + \frac{k}{r} + \frac{\hbar^2 l(l+1)}{2\mu r^2}, \] (3.20)

we can approximate this potential with another potential that has the form of a harmonic oscillator:

\[ \tilde{V}(r) = V_0 + \frac{1}{2} \mu \tilde{\omega}^2 (r - r_0)^2, \] (3.21)

where \( r_0 \) is the \( r \) at which \( V_{\text{eff}}(r) \) is minimal, \( V_0 \) is the corresponding value of \( V_{\text{eff}} \) and \( \tilde{\omega} \) is determined by the second derivative of \( V_{\text{eff}}(r) \) at \( r = r_0 \). Using these definitions we find that \( r_0 \) is the solution of

\[ \frac{dV_{\text{eff}}}{dr}(r = r_0) = 0 \Rightarrow r_0^4 \mu \omega^2 - r_0 k - \frac{\hbar^2 l(l+1)}{\mu} = 0 \] (3.22)

and we find that

\[ \tilde{\omega} = \sqrt{\omega^2 + \frac{2k}{\mu r_0^4} + \frac{3\hbar^2 l(l+1)}{\mu^2 r_0^4}}. \] (3.23)

With this approximate potential we can solve the Schrödinger equation exactly\(^7\) and find that the eigenenergies are given by

\[ E'_n = V_0 + \left(n + \frac{1}{2}\right) \hbar \tilde{\omega}, \] (3.24)

whereas the corresponding wave functions are given by

\[ u_n(r) = A_n H_n \left( \sqrt{\frac{\mu \tilde{\omega}}{\hbar}} (r - r_0) \right) \exp \left( -\frac{\mu \tilde{\omega}}{2\hbar} (r - r_0)^2 \right), \] (3.25)

where \( A_n \) is a normalization constant and \( n = 0, 1, 2, 3, \ldots \). For \( l = 0 \) we find the energies

\[ E'_n = \frac{3}{2} \left( \mu k^2 \omega^2 \right)^{1/3} + \left(n + \frac{1}{2}\right) \sqrt{3} \hbar \omega. \] (3.26)

We can again compare these energies to the known eigenenergies as found in section 3.2. This is shown in figure 3.3. We see that this is already in general a better approximation of the eigenenergies than with the perturbation theory. However we also see that these

\(^7\)The potential in equation (3.21) is just a shifted harmonic oscillator. With an adequate transformation of coordinates we return to the Schrödinger equation for a simple one-dimensional harmonic oscillator, which was treated in section 2.1.
energies are not correct everywhere. For example, the energies show incorrect asymptotic behaviour: \( \frac{E'_n(\omega)}{\hbar \omega} \to \sqrt{3} \left( n + \frac{1}{2} \right) \hbar \omega \) for \( \omega \to \infty \) where the factor \( \sqrt{3} \) is incorrect. For low \( \omega \) however we see that the energies are almost perfect. This means that we have now, in addition to the limit of \( \omega \to \infty \), also found another asymptote:

\[
\frac{E'_n}{\hbar \omega} \sim C \omega^{-\frac{1}{3}},
\]

(3.27)

for \( \omega \downarrow 0 \), where the constant \( C \) is given by

\[
C = \lim_{\omega \downarrow 0} \left( \frac{E'_n}{\hbar \omega} \right) \omega^\frac{1}{3} = \frac{3}{2} \left( \frac{\mu k^2}{\hbar^3} \right)^{1/3} \approx 411,664 \ s^{-\frac{1}{3}}.
\]

(3.28)

For \( l \neq 0 \) the energies can also be determined exactly, however this becomes a very large expression which we will not show here. It is interesting to investigate the limit of \( \omega \downarrow 0 \) for these states and we find that the same energies are obtained as for \( l = 0 \). This means that this is universal asymptotic behaviour, for every set of quantum numbers \( k, l \) and \( m \) the energy will show the asymptotic behaviour given by equation (3.27). The harmonic approximation works so well for small \( \omega \) since then the absolute energies \( E'_n \) are low and therefore, these energies are close to the minimum of the potential. This is exactly where a Taylor approximation works best. So for low \( \omega \), in the strongly interacting regime, one is able to make a Taylor expansion of the potential and use that approximation instead. Even though we can explain why the harmonic approximation works so well it still is counter-intuitive: if we turn off the harmonic potential (which is essentially what we do when \( \omega \) goes to 0) we can still describe our system with a harmonic oscillator.

From figure 3.3 we see that not only the asymptotic behaviour of the ground state is correct for \( \omega \downarrow 0 \) but also for excited states with \( k \neq 0 \), meaning that the energies in (3.26) are a complete description of the energies of all states with \( l = 0 \) (at least in the limit of \( \omega \downarrow 0 \)). We thus find that the spacing between energy levels with different principal quantum numbers \( k \) is exactly \( \sqrt{3} \hbar \omega \). All in all this means that, together with the energies from the previous section, we have the eigenenergies in the two limits. We could put these together to find the energy at any \( \omega \) but these energies would behave badly for \( \omega \) that are in neither limit. Therefore we will use some other approaches in the next sections.
Figure 3.3: Eigenenergies as found by making a Taylor approximation of the potential around its minimum and solving the corresponding Schrödinger equation exactly. The dots correspond to the exact eigenenergies as found in section 3.2. \( \omega_0 \) is a reference frequency of 1 Hz. We see that the harmonic approximation works very well for small \( \omega \), i.e. in the weakly interacting regime.
3.5 Hellmann-Feynman theorem

In the previous sections we were able to predict the behaviour of the eigenenergies in two limiting cases of $\omega$ but as was mentioned we are also interested in transient behaviour between these two limits. In this section we want to replicate this transient behaviour. If we go back to section 3.2 we saw that we were able to analytically calculate the eigenenergies for certain $\omega$’s. But we can do more, using the Hellmann-Feynman theorem [11] we are also able to calculate $\frac{dE'}{d\omega}$ at those frequencies:

$$\frac{dE'}{d\omega} = \mu \omega \int_0^\infty r^2 |u(r)|^2 dr = \mu \omega \langle r^2 \rangle \equiv \gamma \hbar.$$ (3.29)

If we can, somehow, relate $\gamma$ to $E'$ and/or $\omega$ we will have a differential equation for $E'(\omega)$ which we might be able to solve. Therefore, we will first investigate some limits. The first limit is when $\omega \to \infty$. In a previous section we reasoned that in this limit the Coulomb part of the potential is negligible and that we end up with a regular harmonic oscillator for which we know that $E' = (2k + l + \frac{3}{2}) \hbar \omega$. Moreover, since we know the wave functions in every eigenstate of the harmonic oscillator we can also predict the value of $\gamma$ in this limit. Per the virial theorem applied to the harmonic oscillator we know:

$$\gamma = \frac{\mu \omega}{\hbar} \langle r^2 \rangle = \frac{2}{\hbar \omega} \langle V(r) \rangle = \frac{1}{\hbar \omega} \langle E' \rangle = 2k + l + \frac{3}{2}.$$ (3.30)

Another limit is when $\omega$ becomes (relatively) small. In that case, we expect that the Coulombic part of the potential has a relatively large contribution and consequently the eigenenergies have a large deviation from the harmonic oscillator eigenenergies. Because the energies are so high, the classical upper bound of $r$, which is (approximately) given by $r_* = \sqrt{\frac{2E'}{\mu \omega^2}}$, is also high. An estimation of $\langle r^2 \rangle$ can now be made by assuming that the probability density is constant on $[0, r_*)$ and 0 elsewhere:

$$P(r) = \begin{cases} \frac{1}{r_*} & \text{for } 0 \leq r \leq r_*, \\ 0 & \text{for } r > r_* \end{cases}.$$ (3.31)

A problem with this assumption is that we ignore the Coulomb part of the potential around small $r$. However, this contribution will become smaller and smaller for growing energies. With this assumption we have

$$\langle r^2 \rangle \sim \int_0^\infty r^2 P(r) dr = \frac{1}{3} r_*^2 = \frac{2E'}{3\mu \omega^2},$$ (3.32)

which yields

$$\gamma \sim \frac{2E'}{3\hbar \omega}.$$ (3.33)
Let us now assume that this behavior is valid for every $\omega$. Using the definition of $\gamma$ this results in a differential equation for $E'(\omega)$,

$$\frac{dE'}{d\omega} = \gamma \hbar = \frac{2E'}{3}\omega,$$

which has the solution

$$E'(\omega) = A\omega^{\frac{2}{3}},$$

where $A$ is an integration constant. This is the same asymptote as we found in section 3.4, so that we can for example put $A = C = \frac{3}{2} \left( \frac{\mu k^2}{\hbar} \right)^{1/3}$ or we can find the integration constant by fitting to the exact solutions from Taut. However we find that $\lim_{\omega \to \infty} \frac{E'}{\hbar \omega} = 0$ (independent of the choice for $A$) while we should find $\lim_{\omega \to \infty} \frac{E'}{\hbar \omega} = 2k + l + \frac{3}{2}$. So the energy given by (3.35) has the incorrect asymptotic behaviour for $\omega \to \infty$ thus we are still missing some terms. For example, the extrapolation of the low $\omega$ limit of $\gamma$ is inconsistent with the high $\omega$ limit. To correct for this we assume

$$\gamma = a + \frac{2E'}{3\hbar \omega}.$$  

This is a reasonable assumption since (3.33) gives only the leading order. By requiring that the high $\omega$ limit is correct we find

$$a = \frac{1}{3} \left( 2k + l + \frac{3}{2} \right).$$

Solving the differential equation corresponding to this $\gamma$ gives the solution

$$E'(\omega) = \left( 2k + l + \frac{3}{2} \right) \hbar \omega + A\omega^{\frac{2}{3}},$$

where $A$ is again an integration constant. This solution now does indeed have the correct asymptotic behavior for $\omega \to \infty$. However, we cannot expect our Ansatz for $\gamma$ to be perfect. Using the eigenstates from section 3.2 we have a number of $\gamma$’s which are calculated analytically. These can be fitted with

$$\gamma = \frac{1}{3} \left( 2k + l + \frac{3}{2} \right) + \frac{2E'}{3\hbar \omega} + \frac{B}{1 + \alpha \omega^{\beta}},$$

where $B$, $\alpha$ and $\beta$ are fitting parameters. This fitting form has only been chosen because it fits the data very well and has no clear theoretical background. This extra term is an inhomogeneous term in the corresponding differential equation. It still can be solved to find

$$E'(\omega) = \left( 2k + l + \frac{3}{2} \right) \hbar \omega + A\omega^{\frac{2}{3}} + 3B\hbar\omega_{2F1}\left( \frac{1}{3\beta}, 1, \frac{1}{3\beta} + \frac{1}{\alpha \omega^{\beta}} \right),$$

where $_2F_1(a, b, c, d)$ is the Gaussian or ordinary hypergeometric function. Since $\beta > 0$ and $\alpha > 0$ we still find the correct asymptotic behaviour for $E'(\omega)$, but the behaviour for lower $\omega$ has been improved, as can be seen in figure 3.4.
Figure 3.4: Ground state energy \((k = 0, l = 0)\) as function of \(\omega\), where \(\omega_0\) is a reference frequency of 1 Hz. The dots correspond to the exact analytical calculation by Taut, the two lines are calculated by using equations (3.38) and (3.40), which are based on predictions for \(\gamma\). The integration constant \(A\) has been fitted to the analytical points from Taut. We see a very close resemblance of the lines with the analytical points.
3.6 Truncated polynomials

When we write the solution of the differential equation (3.6) as a power series, we find a recurrence relation for the coefficients of the polynomial. In section 3.2 we saw that solutions can be found by assuming that the power series terminates. However this only finds solutions at certain values of \( \omega \). At other values the recurrence relation is still valid, but instead of terminating, the power series is now infinite. This makes it difficult (if not impossible) to find the eigenenergies \( E' \). Let us now assume that higher order terms are relatively small so that only the first \( n \) monomials are relevant. This is certainly the case for those \( \omega \)'s found by Taut’s method so it probably is a reasonable assumption for frequencies that are close to these values. If we assume that this truncated polynomial is the solution, we want to find the corresponding energies. To do this we evaluate the expectation value of the Hamiltonian and put it equal to the eigenenergy. As the coefficients of the polynomial also depend on the energy we will get an equation which can be solved for \( E(\overline{k}) \), either analytically or numerically. In other words, we want to solve

\[
\langle H \rangle = \int \frac{u^* H u \ d\rho}{\int u^* u \ d\rho} = E. \tag{3.41}
\]

First we assume that only the constant term is relevant so that we find

\[
u(\rho) = a_0 \rho^{l+1} \exp \left( -\frac{1}{2} \rho^2 \right). \tag{3.42}
\]

Putting this back into (3.41) we find that

\[
2l + 3 + \frac{\overline{k}}{\sqrt{\pi}} \frac{4l^{l+1}l!(l + 1)!}{(2l + 2)!} = E, \tag{3.43}
\]

so that we find

\[
\frac{E'(\omega)}{\hbar \omega} = \frac{1}{2} E = l + \frac{3}{2} + 2k \sqrt{\frac{\mu}{\hbar^2 \omega \pi}} \frac{4l^{l+1}l!(l + 1)!}{(2l + 2)!}. \tag{3.44}
\]

We see that in the limit of \( \omega \to \infty \), which corresponds to \( \overline{k} \to 0 \), the correct asymptotic behaviour is reproduced. This can be explained by the fact that the wave functions in this limit (which is just the harmonic oscillator) are exactly of the form in equation (3.42) so that these wave functions are exact eigenstates. Next we truncate the polynomial after two terms:

\[
u(\rho) = a_0 \rho^{l+1} \left( 1 + \frac{\overline{k}}{2(l + 1)} \right) \exp \left( -\frac{1}{2} \rho^2 \right). \tag{3.45}
\]

Again \( \langle H \rangle \) is independent of \( E \) so that the energy can be found to be

\[
\frac{E'(\omega)}{\hbar \omega} = \frac{(8(1 + l)^2(3 + 2l) + \overline{k}^2(19 + 20l + 4l^2)) \Gamma \left( \frac{3}{2} + l \right) + 2\overline{k} \left( \overline{k}^2 + 8(1 + l)(2 + l) \right) \Gamma(2 + l)}{16\overline{k}(1 + l)^2 \Gamma(1 + l) + 2 \left( 8(1 + l)^2 + \overline{k}^2(3 + 2l) \right) \Gamma \left( \frac{3}{2} + l \right)}. \]
Figure 3.5: Ground state energies as calculated analytically by Taut and as found by solving equation (3.41), where $n$ is degree of the truncated polynomial. $\omega_0$ is a reference frequency of 1 Hz and we see that as $n$ increases the method of truncated polynomials works well on an increasingly large domain.

In general when the polynomial is truncated after $n + 1$ terms (so $a_{n+1}$ is taken to be 0) we can solve the equation $\langle H \rangle = E$ exactly for $E$ for $n = 0, 1, 2, 3$ and only numerically for all higher $n$. Excited states with $k \neq 0$ can also be found by looking at the second, third or even more solutions of equation (3.41) (note that this requires a high $n$). The solutions for $k = 0$ and $n = 0, 1, 2, 3$ are plotted in figure 3.5 together with the analytical solutions of Taut. One can see that for increasing $n$ the energies are correct on an increasingly larger domain. This is also what one should expect since all the analytical solutions calculated by Taut are polynomials of a certain (finite) degree and for a certain $n$ the energy should be at least correct up to the point corresponding with the analytical solution that has that degree $n$. When comparing the exact and approximate energies for the correct $\omega$ we see this behaviour, moreover, we see that in general the approximate energy is correct up to degree $n + 1$. Therefore this is another method to find energies, but also solutions, in the weakly interacting regime.
3.7 Numerical eigenenergies

Instead of trying to solve the Schrödinger equation analytically we may attempt to find numerical solutions, which will be done in this section. The problem we are trying to solve numerically is essentially solving the differential eigenequation (3.4). We thus need to find the eigenenergy $E'$ and the wave function $u$. This is done by splitting the domain in two parts: (i) $\varepsilon \leq r \leq r_0$ and (ii) $r_0 \leq r \leq \alpha$, where $\varepsilon \ll r_0$ and $\alpha \gg r_0$.\(^8\) This is illustrated in figure 3.6. One can see that $r_0$ has been chosen so that $V_{\text{eff}}(r_0)$ is the minimum of $V_{\text{eff}}(r)$ so that the edge where the two subdomains are connected always lies in the classically allowed region. Next, the differential equation is numerically solved on both subdomains for a certain energy.\(^9\) If that energy happens to be an eigenenergy the solutions on both subdomains should connect perfectly, that is, their values as well as their derivatives should be equal. This can be measured by the Wronskian defined by

$$W = u_{(i)}(r_0)u'_{(ii)}(r_0) - u'_{(i)}(r_0)u_{(ii)}(r_0).$$ \hspace{1cm} (3.46)

The Wronskian depends on the chosen energy and will in general not be equal to zero, except at eigenenergies. The problem of finding the eigenenergies thus has been reduced to finding the zeros of the Wronskian. An example for the Wronskian is plotted in figure 3.7, for $\omega = 10^{16}$ Hz. The zeros can now be found numerically for every $\omega$ and this results in the spectrum shown in figure 3.8. We see that the numerical results match with the analytical energies found by Taut. We also see that both asymptotes match the predicted asymptotes.

Figure 3.6: Potential for $\omega = 10^{16}$ Hz with a possible split of the domain in subdomains (i) and (ii).

\(^8\)We would like to find a solution on $0 \leq r \leq \infty$ but we have to bound our domain on both sides. First because of the fact that numerical methods cannot use infinite domains and second because of the fact that at $r = 0$ the potential is in fact infinite so that we need to exclude the point $r = 0$ from our domain.

\(^9\)Regarding the boundary conditions, we chose values for $u$ in both classically forbidden domains and chose these values such that they match the exponential behaviour we expect in these forbidden domains.
CHAPTER 3. EIGENENERGIES

Figure 3.7: Wronskian as function of energy $E$ for $\omega = 10^{16}$ Hz. The eigenenergies are the zeros of the Wronskian which are shown too.

Figure 3.8: Numerical eigenenergies in terms of $\hbar \omega$ as function of $\omega$ ($\omega_0$ is again the reference frequency of 1 Hz). The dots correspond to the set of eigenenergies found by Taut, where we can see that our numerical results match these energies. We also see both asymptotes which we predicted in previous sections.
3.8 General states

As promised, we will now investigate the energies of more general states. For this, we will use the energies we found using the Hellmann-Feynman theorem including inhomogeneous term since they resemble the analytical energies the closest and are relatively easy to calculate. We will subtract the asymptotic behaviour described by equation (3.27) for a better view on the results. This is shown in figure 3.9. On the right-hand side, in the weakly interacting regime, we recognize the harmonic oscillator limit in which the levels are evenly spaced with spacing $1\hbar\omega$. When $\omega$ is lowered from the harmonic oscillator limit we see that the degeneracy is (partially) lifted, every set of $k$ and $l$ now has its own energy. When $\omega$ is decreased further we see that the energy is mainly determined by the principal quantum number $k$ and only slightly modulated by the azimuthal quantum number $l$. Moreover, when extrapolating to $\omega \approx 0$ we expect from the figure that the energy is only determined by the quantum number $k$. This is also what we found in section 3.4. We have thus found that in both limits, the extremely weakly and extremely strongly interacting regime, the problem can be described by a harmonic oscillator.

Figure 3.9: Energies of excited states as function of $\omega$, where $\omega_0 = 1$ Hz. Asymptotic behaviour ($E \sim C\omega^{2/3}$ for $\omega \downarrow 0$) has been subtracted for a clearer plot. All lines are calculated using the Hellmann-Feynman theorem (equation (3.40)).
CHAPTER 3. EIGENENERGIES

The weakly interacting limit we already explained, since then the Coulomb repulsion is negligible with respect to the harmonic oscillator. In the strongly interacting limit the opposite is true, now the harmonic oscillator is negligible. When we only take the Coulomb repulsion into effect we will end up with the problem of Coulomb scattering (which has no bound states). In this problem, not only s-wave scattering is relevant but also p-wave, d-wave etc. We also see this in the figure, namely, when $\omega \downarrow 0$ we see that all values of $l$ are important when considering the ground state energy.

Even when we are not completely in the strongly interacting limit we should be able to make a quantitative prediction of the eigenenergies by using the centrifugal barrier as a perturbation on the harmonic Taylor approximation. This was not executed here and might be interesting to do in a future research.

3.8.1 Many-particle systems

Our research, and more in specific figure 3.9, can be used to predict the behaviour of many-particle systems. To do so we assume that these particles only interact in pairs and that these pairs are independent. When we are in the quantum degenerate regime we only need to fill the eigenenergies from the bottom, up to the Fermi energy. When filling up the energy levels we also need to take into account the spin-states and the Pauli exclusion principle. The total wave function can be found by combining the spatial- and the spin-part:

$$\psi(1, 2) = \Psi(\mathbf{r}) \phi(\mathbf{R}) \chi(s_1, s_2).$$  \hfill (3.47)

Now since electrons are fermions the wave function needs to be antisymmetric under particle exchange. For this exchange, $\phi(\mathbf{R})$ has parity 1, $\Psi(\mathbf{r})$ has parity $(-1)^l$ and $\chi(s_1, s_2)$ has parity $(-1)^S$, where $S$ is the total spin. This means that a state with even $l$ is in a triplet spin-state ($S = 1$) and a state with odd $l$ is in a singlet state ($S = 0$). This means that the Pauli exclusion principle does not add any constraints on the occupation of certain energy levels, one just needs to “choose” the correct spin-state. As a result we can fill all the eigenstates where each state has a certain degeneracy. In the weakly interacting limit we just get the problem of $2N$ particles in a three-dimensional harmonic oscillator. This problem can solved to find as Fermi level [12]

$$E_F = (6N)^{1/3} \hbar \omega.$$

In the other limit, the strongly interacting limit, we find that all $N$ particle-pairs are in a state with energy equal to the ground state energy. Therefore we find that

$$E_{\text{total}} = N E_{\text{gs}} \sim \frac{3N}{2} \left(\mu k^2 \omega^2\right)^{1/3}$$  \hfill (3.49)

for $\omega \downarrow 0$, where $E_{\text{gs}}$ is the ground state energy, and thus

$$E_F = E_{\text{gs}} \sim \frac{3}{2} \left(\mu k^2 \omega^2\right)^{1/3}.$$  \hfill (3.50)
It is remarkable that the electrons, which are fermions, behave a lot like bosons (they all are in a state with ground state energy). The precise reason is unknown and could be the subject of a further research. In the transition zone between the strongly interacting and the weakly interacting regime we expect some sort of a phase transition in which the occupation numbers of the different states as well as the complete behaviour of the system changes. This all shows that a system consisting of many trapped electrons is very interesting. It can be studied much more extensively, but due to a lack of time this was not done here.
4. Wave functions

In this chapter we will investigate the wave functions corresponding to the eigenenergies that we found in the previous chapter. Note that not every method used for calculating the eigenenergies is also suitable to provide the associated wave function.

4.1 Numerical solutions

The first method that can provide wave functions at any eigenenergy is when the differential equation is solved numerically. An example of the wave functions for $\omega = 10^{16}$ Hz is shown in figure 4.1. The shown potential and associated wave functions are for $l = 0$. Note that none of the wave-functions is normalized properly but rather satisfy

$$\int_0^\infty \int_0^{2\pi} \int_0^{\pi} |\psi|^2 r^2 \sin(\theta) d\theta dr = \alpha,$$

where $\alpha \neq 1$. The found wave functions behave as we expected. They are much like the wave functions for a regular harmonic oscillator except for the higher amplitude at low $r$ which is caused by the Coulomb repulsion. We also see the characteristic penetration into the classically forbidden regions as well as the approximate equidistant spacing of the energy levels which was already found in the previous chapter. We will use the eigenstates as presented in figure 4.1 as “benchmark”; we can compare the wave functions found by other methods with these wave functions and make observations about the quality of these other methods.

\footnote{$\alpha$ is chosen so that the wave functions are clearly visible and is the same for each wave function.}
CHAPTER 4. WAVE FUNCTIONS

Figure 4.1: Numerically determined eigenstates for $\omega = 10^{16}$ Hz. The wave functions look a lot like the wave functions for the harmonic oscillator which is also what we expected.

4.2 Harmonic approximation

The harmonic approximation was investigated in section 3.4. There we also already stated that this method will give us analytical expressions for the wave functions. In figure 4.2 these wave functions are shown as well as the potentials. A first observation we can make is that the leading edge of the potential is wrongly situated. This is caused by the fact that the harmonic potential is a Taylor approximation of $V_{\text{eff}}$ and therefore it only works well around the minimum. As a result we see that the found wave functions are not spatially extended enough. This of course also causes incorrect eigenenergies. Another result of the Taylor approximation is that the divergence of the potential caused by the Coulomb repulsion is not caught in the harmonic potential. This amounts to incorrect behaviour of the wave functions around $r = 0$, for example none of the excited states shows the exponential penetration into the classically forbidden region. These are all errors in the harmonic approximation, however we see that the ground state is predicted quite well. This has the same reason as why this method is so powerful when $\omega$ is relatively low, namely that the Taylor expansion is very close. For lower frequencies the harmonic approximation also works better for excited states. Moreover, in section 3.8 we saw that for low $\omega$ only the ground state is relevant and this method provides an analytical expression for that state.
4.2. HARMONIC APPROXIMATION

Figure 4.2: Eigenstates of the Taylor approximation of the potential. We see incorrect behaviour for small $r$ and also around the leading edge of the oscillator. We also see that the ground state is approximately correct and this is caused by the fact that the Taylor approximation only has a small error around the minimum.

Figure 4.3: Wave functions found by the method of truncated polynomials. $n$ denotes the degree of the truncated polynomial. We see that the found wave functions are very close to the numerically found states.
4.3 Truncated polynomials

Another method that provides wave functions is that of the truncated polynomials, where the wave functions are given by these truncated polynomials. The wave functions are not eigenfunctions of the Hamiltonian, but instead they satisfy equation (3.41). We saw that the prediction of the eigenenergies was very good in the weakly interacting regime and the explanation of this also predicts that the wave functions should be very good. The wave functions that were found for $\omega = 10^{16}$ Hz are shown in figure 4.3. When comparing this figure with figure 4.1 we immediately see that indeed the wave functions are very close to the real wave functions. As a result, this method is one of the most powerful methods to predict the wave functions in the weakly interacting regime. Moreover, an increase in $n$ also leads to an expansion of the domain in which this method works well.\(^\text{11}\)

Another method to calculate the wave functions that is very much like the method of truncated polynomials is as follows. First one calculates the eigenenergy with a suitable method from chapter 3, for example numerically. This eigenenergy is then put into a power series using recurrence relation (3.10). This infinite polynomial then describes the exact wave function but since it is infinitely long one has to terminate this polynomial. This actually is a different method than the method of truncated polynomials as described in section 3.6 since the energy is not determined the same way. This last method is the most reliable and stable method to give an analytical expression of the wave function at any value $\omega$. It even works in the strongly interacting regime where the method of truncated polynomials as described in section 3.6 does not work well (as was visible from figure 3.5).

\(^{11}\)This is somewhat trivial since an infinite $n$ gives the exact solutions of equation (3.6) at any $\omega$ because this is what the power series method essentially does.
5. Conclusion

In this research the problem of two interacting electrons in a harmonic trap was studied. The main task was to solve the Schrödinger equation that describes this problem, or at least to be able to make quantitative and analytical statements about the eigenenergies and eigenstates. As a starting point we used the set of particular analytical solutions provided by Taut. These solutions already lifted a corner of the veil about the complete eigenenergies. For example, they already showed a weakly interacting regime, where the problem can be described by ignoring the Coulomb repulsion, and a strongly interacting regime where the relative interaction energy diverges. It also showed that the correlation between the interaction strength and the density was precisely reversed with respect to what we see for normal plasmas. This was the first of several remarkable features of this problem that we discovered.

Taut’s solutions were studied thoroughly but as we wanted an expression for the eigenenergies for every frequency \( \omega \) these were not sufficient. Therefore, we tried a number of other methods. The first method was by using the Coulomb potential as a perturbation. Using the perturbation theory this gives a prediction of the eigenenergies which was shown to work well in the weakly interacting regime. The second method that was used to find eigenenergies was by making a Taylor approximation of the potential around its minimum. We showed that this method is extremely powerful in the strongly interacting regime. This was also one of those remarkable features and something that is not clear on first hand. With this method we found an analytical expression for the asymptote of the eigenenergy namely \( E' \sim \omega^{2/3} \). With this method we also found a characteristic spacing of \( \sqrt{3} \hbar \omega \) between energy levels in the strongly interacting limit.

Another method that is perhaps the most analytically based method was the one that used the Hellmann-Feynman theorem. With this theorem we were able to derive a differential equation for \( E' (\omega) \). We found that the solution of this differential equation is in agreement with the previous two methods as well as that it closely resembles the solutions found by Taut. With this method we were able to calculate the spectrum, and we showed the bottom part of it. This also showed the remarkable feature we found earlier: in a strongly interacting regime the problem reduces to one of a simple harmonic oscillator.

We also tried two other methods, namely the method of truncated polynomials and numerical solutions. These were to a smaller extent able to give an analytical prediction of the energies although the numerical solutions were very good non-analytical solutions. Both methods however did give good results for the wave functions. Also the harmonic approximation was able to predict the wave functions but these were only good in the...
strongly interacting regime.

Concluding, we have found some methods to find the eigenenergies, but most of them work only well in a specific regime. The one exception to this are the eigenenergies found by using the Hellmann-Feynman theorem. However this last method was not able to give a prediction of the wave functions. Furthermore we investigated the spectrum for general states and saw that this harbours interesting behaviour. In this context we were also able to draw a link to Coulomb scattering. Finally we shortly investigated the many-particle problem. Here we found another remarkable feature namely the bosonic behaviour of fermions in the strongly interacting limit. Also we suggested that the system should undergo a phase transition.

We want to state that work on this subject is not necessarily done. For example, a perturbation approach to the strongly interacting limit most likely will be able to make a more quantitative prediction of the eigenenergies in this regime. Another lead might be the ladder operators. When these can be found the calculation of eigenenergies simplifies a lot. Also a big part of the many-particle problem has been left unexplored. These can be topics of a future research on this problem and finally one might also be able to observe some of the predicted effects in a real-life experiment.
BIBLIOGRAPHY

Bibliography


A. Appendix

A.1 Ladder operators for the three-dimensional harmonic oscillator

The wave functions for the three-dimensional harmonic oscillator are

\[ \psi_{klm}(r, \theta, \phi) = N_{kl} r^l \exp(-\nu r^2) L_k^{(l+\frac{1}{2})}(2\nu r^2) Y_m^l(\theta, \phi) \]  
(A.1)

where \( \nu = \frac{\mu \omega}{2\hbar} \) and

\[ N_{kl} = \sqrt{\frac{2\nu^3}{\pi} \frac{2k+3l+4k!(k+l+1)!}{(2k+2l+2)!}}. \]  
(A.2)

while the corresponding eigenenergies are

\[ E_{kl} = \left(2k + l + \frac{3}{2}\right) \hbar \omega. \]  
(A.3)

Since the eigenproblem is a differential equation we will search a relation between \( \frac{\partial \psi_{klm}}{\partial r} \), \( \psi_{klm} \) and \( \psi_{k\pm 1,l,m} \). So using (A.1) we find

\[
\frac{1}{\psi_{klm}} \frac{\partial \psi_{klm}}{\partial r} = \frac{l}{r} - 2\nu r + \frac{1}{L_k^{(l+\frac{1}{2})(2\nu r^2)}} \frac{d}{dr} \left(L_k^{(l+\frac{1}{2})(2\nu r^2)}\right)
= \frac{l}{r} - 2\nu r + \frac{4\nu r}{L_k^{(l+\frac{1}{2})(2\nu r^2)}} \frac{d}{dx} \left(L_k^{(l+\frac{1}{2})(x)}\right),
\]  
(A.4)

where \( x = 2\nu r^2 \). Next we use two recurrence relations for the derivative of a Laguerre polynomial [13]:

\[
\frac{d}{dx} \left(L_k^{(l+\frac{1}{2})}(x)\right) = \begin{cases} 
k L_k^{(l+\frac{1}{2})}(x) - (k + l + \frac{1}{2}) L_k^{(l+\frac{1}{2})}(x), \\
(k+1) L_{k+1}^{(l+\frac{1}{2})}(x) - (k + l + \frac{3}{2} - x) L_k^{(l+\frac{1}{2})}(x). \end{cases}
\]  
(A.5)
First we fill in the first recurrence relation to find the lowering operator. After some
manipulation we find
\[
\frac{1}{\psi_{klm}} \frac{\partial \psi_{klm}}{\partial r} = \frac{l + 2k}{r} - 2\nu r - \frac{2}{r} \left( k + l + \frac{1}{2} \right) \frac{L^{(l+\frac{1}{2})}_{k-1}(x)}{L^{(l+\frac{1}{2})}_{k}(x)} \]
(A.6)

or rewritten:
\[
\left( \frac{1}{2} r \frac{\partial}{\partial r} + \nu r^2 - k - \frac{1}{2} \right) \psi_{klm} = - \left( k + l + \frac{1}{2} \right) \frac{N_{kl}}{N_{k-1,l}} \psi_{k-1,l,m}, \quad (A.7)
\]
so we identify
\[
\hat{\mathcal{L}}_- = \frac{1}{2} r \frac{\partial}{\partial r} + \nu r^2 - \hat{k} - \frac{1}{2} l \quad (A.8)
\]
and
\[
l_-(k) = - \left( k + l + \frac{1}{2} \right) \frac{N_{kl}}{N_{k-1,l}} = - \sqrt{k(k + l + \frac{1}{2})}, \quad (A.9)
\]
where we used the operator \( \hat{k} \), defined by \( \hat{k} \psi_{klm} = k \psi_{klm} \). Likewise, we fill in the second
recurrence relation to find the raising operator. After manipulation we find
\[
\frac{1}{\psi_{klm}} \frac{\partial \psi_{klm}}{\partial r} = - \frac{l + 2k + 3}{r} + 2\nu r + \frac{2}{r} \left( k + l + \frac{1}{2} \right) \frac{L^{(l+\frac{1}{2})}_{k+1}(x)}{L^{(l+\frac{1}{2})}_{k}(x)} \]
(A.10)

or:
\[
\left( \frac{1}{2} r \frac{\partial}{\partial r} - \nu r^2 + k + \frac{1}{2} l + \frac{3}{2} \right) \psi_{klm} = (k + 1) \frac{N_{kl}}{N_{k+1,l}} \psi_{k+1,l,m}, \quad (A.11)
\]
so that we can identify
\[
\hat{\mathcal{L}}_+ = \frac{1}{2} r \frac{\partial}{\partial r} - \nu r^2 + \hat{k} + \frac{1}{2} l + \frac{3}{2} \quad (A.12)
\]
and
\[
l_+(k) = (k + 1) \frac{N_{kl}}{N_{k-1,l}} = \sqrt{(k + 1)(k + l + \frac{1}{2})}, \quad (A.13)
\]
Now we need to find an explicit expression for $\hat{k}$. We do this using the radial wave equation:

$$
\left(-\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial r^2} + \frac{1}{2} \mu \omega^2 r^2 + \frac{\hbar^2 l(l+1)}{2\mu r^2}\right) u(r) = \hbar \omega \left(2k + l + \frac{3}{2}\right) u(r),
$$

(A.14)

with $u(r) = \frac{r \psi(r,\theta,\phi)}{Y^m_l(\theta,\phi)}$ the radial wave function and where we filled in the energy from equation (A.3). But since the operators on the left-hand side do not operate on functions of $\theta$ and $\phi$ we can include the spherical harmonics as well to find

$$
\left(-\frac{1}{4\nu} \frac{\partial^2}{\partial r^2} + \nu r^2 + \frac{l(l+1)}{4\nu r^2}\right) (r \psi_{klm}) = \left(2k + l + \frac{3}{2}\right) (r \psi_{klm}).
$$

(A.15)

Isolating $k$ we find that

$$
k(r \psi_{klm}) = \left(-\frac{1}{8\nu} \frac{\partial^2}{\partial r^2} + \frac{1}{2} \nu r^2 + \frac{l(l+1)}{8\nu r^2} - \frac{1}{2} l - \frac{3}{4}\right) \psi_{klm} \equiv \hat{R}(r \psi_{klm}).
$$

(A.16)

Swapping $\hat{R}$ and $r$ introduces a commutator which can be evaluated to find

$$
\left[ \hat{R}, r \right] = -\frac{1}{4\nu} \frac{\partial}{\partial r}
$$

(A.17)

so that

$$
r \hat{k} \psi_{klm} \equiv r k \psi_{klm} = r \left(-\frac{1}{8\nu} \frac{\partial^2}{\partial r^2} - \frac{1}{4\nu r} \frac{\partial}{\partial r} + \frac{1}{2} \nu r^2 + \frac{l(l+1)}{8\nu r^2} - \frac{1}{2} l - \frac{3}{4}\right) \psi_{klm}
$$

(A.18)

and we find

$$
\hat{k} = -\frac{1}{8\nu} \frac{\partial^2}{\partial r^2} - \frac{1}{4\nu r} \frac{\partial}{\partial r} + \frac{1}{2} \nu r^2 + \frac{l(l+1)}{8\nu r^2} - \frac{1}{2} l - \frac{3}{4}.
$$

(A.19)

With this operator we find that

$$
\hat{L}_\pm = \pm \frac{1}{8\nu} \frac{\partial^2}{\partial r^2} + \frac{1}{2} r \frac{\partial}{\partial r} \pm \frac{1}{4\nu r} \frac{\partial}{\partial r} \mp \frac{1}{2} \nu r^2 \pm \frac{l(l+1)}{8\nu r^2} + \frac{3}{4}.
$$

(A.20)

which have the commutator

$$
\left[ \hat{L}_+, \hat{L}_- \right] = 2\hat{k} + l + \frac{3}{2}
$$

(A.21)

and we can therefore write the (radial) Schrödinger equation as

$$
\hat{H} \psi = \hbar \omega \left(\hat{L}_+ \hat{L}_- - \hat{L}_- \hat{L}_+\right) \psi = E \psi.
$$

(A.22)
A.2 Solutions of the Coulomb problem

We have the Schrödinger equation

\[ -\frac{\hbar^2}{2\mu} \frac{d^2 \psi_r}{dr^2} + \frac{k}{r} \psi_r = E_r \psi_r \]  

(A.23)

for which we want to find the eigenenergies and eigenfunctions. We will only regard \( k < 0 \) because otherwise there are no bound states. We now make the substitution \( \rho = \kappa r \) with \( \kappa = \sqrt{-\frac{2\mu E_r}{\hbar^2}} \) (which is allowed since \( E_r < 0 \) for bound states). Then we find the differential equation

\[ \frac{d^2 \psi_r}{d\rho^2} = \left( 1 - \frac{\rho_0}{\rho} \right) \psi_r \]  

(A.24)

where \( \rho_0 = -\frac{2\mu k}{\hbar^2 \kappa} \) (and thus \( \rho_0 > 0 \)). Now, since \( V(\rho) \rightarrow -\infty \) for \( \rho \rightarrow 0 \) we demand that \( \psi_r(\rho = 0) = 0 \). Now we write the solution of this equation as \( \Psi(\rho) \). We thus have a differential equation for \( \Psi \), namely

\[ \frac{d^2 \Psi}{d\rho^2} = \left( 1 - \frac{\rho_0}{\rho} \right) \Psi, \]  

(A.25)

which has solutions

\[ \Psi(\rho) = \rho \exp(-\rho) \left( A \, _1F_1 \left( 1 - \frac{1}{2} \rho_0, 2, 2\rho \right) + B \, U \left( 1 - \frac{1}{2} \rho_0, 2, 2\rho \right) \right) \]  

(A.26)

where \( A \) and \( B \) are integration constants, \( _1F_1 \) is the confluent hypergeometric function of the first kind (Kummer’s function of the first kind) and \( U \) is another confluent hypergeometric function (Tricomi’s). Since \( \psi_r \) needs to be normalizable we need \( A = 0 \), otherwise this function will diverge for \( \rho \rightarrow \infty \). Because we demanded that \( \psi_r(\rho = 0) = 0 \) we need that

\[ \lim_{\rho \downarrow 0} \Psi(\rho) = 0. \]  

(A.27)

This yields the following equation:

\[ \frac{B}{\rho_0 \Gamma \left( -\frac{\rho_0}{2} \right)} = 0. \]  

(A.28)

Since \( B \neq 0 \) (otherwise we have the trivial solution \( \Psi(\rho) = 0 \)) we find a condition for \( \rho_0 \):

\[ \rho_0 = 2n \]  

(A.29)

with \( n = 1, 2, 3, \ldots \). Using the definitions of \( \rho_0 \) and \( \kappa \) we can find the energy \( E_r \) in terms of \( n \):

\[ E_r = -\frac{\mu k^2}{2\hbar n^2}. \]  

(A.30)
The value of $B$ is determined by the normalization-condition:

$$
\int_0^\infty |\psi_{r,n}(r)| \, dr = 1 \Rightarrow \kappa \int_0^\infty |\Psi(\rho)| \, d\rho = 1.
$$

(A.31)

Working out the integration gives

$$
\frac{|B|^2 (n!)^2}{4\kappa} = 1,
$$

(A.32)

which is satisfied for $B = \frac{1}{n!}\sqrt{-\frac{4\mu k}{\hbar^2 n}}$. We thus have

$$
\Psi_n(\rho) = \frac{1}{n!} \sqrt{-\frac{4\mu k}{\hbar^2 n}} \rho \exp(-\rho)U(1 - n, 2, 2\rho).
$$

(A.33)

But since $n \in \mathbb{N}$ we can use a property for the confluent hypergeometric functions:

$$
U(1 - n, 2, 2\rho) = (-1)^{n-1}(n-1)!L_n^{(1)}(2\rho),
$$

(A.34)

where $L_n^{(\alpha)}(z)$ is a generalized Laguerre polynomial and thus that

$$
\Psi_n(\rho) = \sqrt{-\frac{4\mu k}{\hbar^2 n^2}} (-1)^{n-1} \rho \exp(-\rho) L_n^{(1)}(2\rho).
$$

(A.35)

Finally, to find $\psi_r(r)$ we need to substitute $\rho = \kappa r$ back into $\Psi_n(\rho)$. Then we find

$$
\psi_{r,n}(r) = \sqrt{-\frac{4\mu^3 k^3}{\hbar^6 n^3}} (-1)^{n-1} \exp\left(\frac{\mu kr}{\hbar^2 n}\right) L_n^{(1)}\left(\frac{2\mu kr}{\hbar^2 n}\right).
$$

(A.36)
A.3 Ladder operators for the Coulomb problem

We will search for ladder operators in \( \rho \)-space. Searching for ladder operators in the \( r \)-space is much harder (if not impossible) since the argument of the Laguerre polynomials not only is a function of \( r \) but also of \( n \). The eigenvalue problem in \( \rho \)-space is given by the equation

\[
\left( \rho \frac{d^2}{d\rho^2} - \rho \right) \Psi_n = -2n\Psi_n. \tag{A.37}
\]

Now, instead of just postulating the correct ladder operators, we can find them using the factorization method. This will use the solutions we already found:

\[
\Psi_n(\rho) = \tilde{A}_n \rho \exp(-\rho) L_n^{(1)}(2\rho). \tag{A.38}
\]

with \( \tilde{A}_n = \sqrt{-\frac{4\mu k}{n\hbar^2}}(-1)^{n-1} \). We now want to find ladder operators such that

\[
\hat{L}_\pm \Psi_n = l_\pm (n)\Psi_{n \pm 1}. \tag{A.39}
\]

As before, to find \( \hat{L}_+ \) we calculate \( \frac{d\Psi_n}{d\rho} \) and write it in terms of \( \Psi_{n+1} \) (and \( \Psi_n \)). Thus:

\[
\frac{d\Psi_n}{d\rho} = \tilde{A}_n \frac{d}{d\rho} \left( \rho \exp(-\rho) L_n^{(1)}(2\rho) \right)
= \tilde{A}_n \left( \exp(-\rho) L_n^{(1)}(2\rho) - \rho \exp(-\rho) L_n^{(1)}(2\rho) + \rho \exp(-\rho) \frac{d}{d\rho} \left( L_n^{(1)}(2\rho) \right) \right)
= \frac{1}{\rho} \Psi_n - \Psi_n + \tilde{A}_n \rho \exp(-\rho) \frac{d}{d\rho} \left( L_n^{(1)}(2\rho) \right). \tag{A.40}
\]

We make the substitution \( u = 2\rho \) and use the first recurrence relation from equation (A.5) to find

\[
\frac{d\Psi_n}{d\rho} = \frac{1}{\rho} \Psi_n - \Psi_n + \tilde{A}_n \rho \exp(-\rho) \frac{d}{d\rho} \left( L_n^{(1)}(2\rho) \right)
= \frac{1}{\rho} \Psi_n - \Psi_n + \tilde{A}_n \rho \exp(-\rho) \frac{1}{\rho} \left( nL_n^{(1)}(2\rho) - (n+1-2\rho)L_{n-1}^{(1)}(2\rho) \right)
= \frac{1}{\rho} \Psi_n - \Psi_n + \frac{n}{\rho} \tilde{A}_n \rho \exp(-\rho) L_n^{(1)}(2\rho)
- \frac{n+1}{\rho} \tilde{A}_n \rho \exp(-\rho) L_{n-1}^{(1)}(2\rho) + 2\tilde{A}_n \rho \exp(-\rho) L_{n-1}^{(1)}(2\rho) \tag{A.41}
= \frac{1}{\rho} \Psi_n - \Psi_n + \frac{n\tilde{A}_n}{\rho A_{n+1}} \hat{A}_{n+1} \rho \exp(-\rho) L_n^{(1)}(2\rho) - \frac{n+1}{\rho} \Psi_n + 2\Psi_n
= -\frac{n}{\rho} \Psi_n + \Psi_n + \frac{n\tilde{A}_n}{\rho A_{n+1}} \Psi_{n+1}.
\]
This can be rewritten as
\[
\left( -\rho \frac{d}{d\rho} + \rho - n \right) \Psi_n = -\frac{n\hat{A}_n}{\hat{A}_{n+1}} \Psi_{n+1}. \tag{A.42}
\]

We define the operator \( \hat{n} \) by \( \hat{n}\Psi_n = n\Psi_n \) so that we can identify
\[
\hat{L}+ = -\rho \frac{d}{d\rho} + \rho - \hat{n} \tag{A.43}
\]
and
\[
l_+(n) = -\frac{n\hat{A}_n}{\hat{A}_{n+1}} = -n \sqrt{\frac{4\mu k}{4\mu k} (1)^{n-1}n^{-3/2}} = n \frac{(n+1)^{3/2}}{n^{3/2}} - \frac{\sqrt{(n+1)^3}}{n}. \tag{A.44}
\]

Now, to find \( \hat{L}^{-} \) we write \( \frac{d\Psi_n}{d\rho} \) in terms of \( \Psi_{n-1} \) (and \( \Psi_n \)). Here we use the second recurrence relation from (A.5) so that we find ((A.40) stays unchanged)
\[
\frac{d\Psi_n}{d\rho} = \frac{1}{\rho} \Psi_n - \Psi_{n-1} + \frac{\hat{A}_n}{\rho \hat{A}_{n-1}} \rho \exp(-\rho) \left( \frac{1}{\rho} \right) \left( (n-1)L^{(1)}_{n-1}(2\rho) - nL^{(1)}_{n-2}(2\rho) \right)
= \frac{1}{\rho} \Psi_n - \Psi_{n-1} + \frac{n-1}{\rho} \hat{A}_n \rho \exp(-\rho) L^{(1)}_{n-1}(2\rho) - \frac{n}{\rho} \hat{A}_n \rho \exp(-\rho) L^{(1)}_{n-2}(2\rho)
= \frac{1}{\rho} \Psi_n - \Psi_{n-1} + \frac{n-1}{\rho} \Psi_n - \frac{n\hat{A}_n}{\rho \hat{A}_{n-1}} \hat{A}_{n-1} \rho \exp(-\rho) L^{(1)}_{n-2}(2\rho)
= \frac{n-1}{\rho} \Psi_n - \frac{n\hat{A}_n}{\rho \hat{A}_{n-1}} \Psi_{n-1}
\]
which in turn can be rewritten as
\[
\left( \rho \frac{d}{d\rho} + \rho - n \right) \Psi_n = -\frac{n\hat{A}_n}{\hat{A}_{n-1}} \Psi_{n-1}. \tag{A.46}
\]
We thus identify
\[
\hat{L}^- = \rho \frac{d}{d\rho} + \rho - \hat{n} \tag{A.47}
\]
and
\[
l_-(n) = -\frac{n\hat{A}_n}{\hat{A}_{n-1}} = -n \sqrt{\frac{4\mu k}{4\mu k} (1)^{n-2}(n-1)^{-3/2}} = n \frac{(n-1)^{3/2}}{n^{3/2}} - \frac{\sqrt{(n-1)^3}}{n}. \tag{A.48}
\]
To eliminate \( \hat{n} \) we use equation (A.37) and the fact that \( n\Psi_n = \hat{n}\Psi_n \):
\[
-2\hat{n}\Psi_n = \left( \rho \frac{d}{d\rho} + \rho - n \right) \Psi_n \Rightarrow \hat{n} = \frac{1}{2} \frac{d^2}{d\rho^2} + \frac{1}{2}\rho. \tag{A.49}
\]
This leads to the operators
\[ \hat{L}_\pm = \frac{1}{2} \frac{d^2}{d\rho^2} \pm \frac{\rho}{d\rho} + \frac{1}{2} \rho, \] (A.50)
while we already found
\[ l_\pm(n) = \sqrt{\frac{(n \pm 1)^3}{n}}. \] (A.51)

The raising and lowering operator have the commutator
\[ [\hat{L}_+, \hat{L}_-] = \rho \frac{d^2}{d\rho^2} - \rho. \] (A.52)

We thus can write (A.37) as
\[ \hat{H} \Psi = (\hat{L}_+ \hat{L}_- - \hat{L}_- \hat{L}_+) \Psi = -\rho_0 \Psi. \] (A.53)

The commutators with the Hamiltonian are
\[ [\hat{H}, \hat{L}_+] = -2 \hat{L}_+, \quad [\hat{H}, \hat{L}_-] = 2 \hat{L}_-, \] (A.54)
so that if \( \Psi_n \) is a solution at eigenvalue \( \rho_0 = \rho_n \), i.e. \( \hat{H} \Psi_n = -\rho_n \Psi_n \), we can show that \( \hat{L}_+ \Psi_n \) is also a solution:
\[ \hat{H} \hat{L}_+ \Psi_n = (\hat{L}_+ \hat{H} + [\hat{H}, \hat{L}_+]) \Psi_n = \hat{L}_+ \hat{H} \Psi_n - 2 \hat{L}_+ \Psi_n \]
\[ = \hat{L}_+ (-\rho_n \Psi_n) - 2 \hat{L}_+ \Psi_n = -(\rho_n + 2) \hat{L}_+ \Psi_n. \] (A.55)

An equivalent equation can be found for \( \hat{L}_- \Psi_n \):
\[ \hat{H} \hat{L}_- \Psi_n = - (\rho_n - 2) \hat{L}_- \Psi_n, \] (A.56)
so indeed \( \hat{L}_+ \) corresponds to a raising operator and \( \hat{L}_- \) corresponds to a lowering operator. Now, by repeatedly applying the lowering operator to a known eigenstate we should eventually get the ground state. Upon applying \( \hat{L}_- \) once more we should find 0, since otherwise we would not have been in the ground state. Thus, we find a differential equation for the ground state \( \Psi_1 \):
\[ \frac{1}{2} \rho \frac{d^2 \Psi_1}{d\rho^2} + \rho \frac{d\Psi_1}{d\rho} + \frac{1}{2} \rho \Psi_1 = 0 \Rightarrow \frac{d^2 \Psi_1}{d\rho^2} + 2 \frac{d\Psi_1}{d\rho} + \Psi_1 = 0. \] (A.57)

The general solution of this differential equation is
\[ \Psi_1(\rho) = (A\rho + B) \exp(-\rho). \] (A.58)
When invoking the boundary condition $\Psi_1(\rho = 0) = 0$ we find that $B = 0$. The constant $A$ then follows from normalization:

$$\int_0^\infty |\psi_1(\kappa x)|^2 \, dx = 1.$$  \hspace{1cm} (A.59)

To find $A$ we need $\kappa$ which is found by evaluating the Hamiltonian which gives $\rho_1 = 2$. Therefore we find $\kappa = -\frac{\mu k}{\hbar^2}$ so that the normalization yields $A = \sqrt{-\frac{4\mu k}{\hbar^2}}$. The found ground state therefore is

$$\Psi_1(\rho) = \sqrt{-\frac{4\mu k}{\hbar^2}} \rho \exp(-\rho),$$  \hspace{1cm} (A.60)

in agreement with (A.36). The energy of this state is given by $E_x = -\frac{\hbar^2 k^2}{2\mu}$ which in turn is in agreement with equation (A.30). All excited states can now be found by application of $\hat{L}$. We know that $\hat{L} \Psi_n = l_+ (n) \Psi_{n+1}$ so that

$$\hat{L}^n \Psi_1(\rho) = \hat{L}^{n-1} l_+ (1) \Psi_2(\rho) = \ldots = \left( \prod_{i=1}^{n-1} l_+(i) \right) \Psi_n(\rho).$$  \hspace{1cm} (A.61)

We know that $l_+(i) = \sqrt{\frac{(i+1)^3}{i}}$ and that therefore

$$l_+(i) l_+(i+1) = \sqrt{\frac{(i+1)^3}{i}} \sqrt{\frac{(i+2)^3}{i+1}} = (i+1) \sqrt{\frac{(i+2)^3}{i}},$$

$$l_+(i) l_+(i+1) l_+(i+2) = (i+1) \sqrt{\frac{(i+2)^3}{i}} \sqrt{\frac{(i+3)^3}{i+2}} = (i+1)(i+2) \sqrt{\frac{(i+3)^3}{i}},$$

$$\vdots$$  \hspace{2cm} (A.62)

$$l_+(i) l_+(i+1) \ldots l_+(i+j) = (i+1)(i+2) \ldots (i+j) \sqrt{\frac{(i+j+1)^3}{i}} = (i+j)! \sqrt{\frac{(i+j+1)^3}{i}}.$$  \hspace{1cm} (A.62)

Thus,

$$\prod_{i=1}^{n-1} l_+(i) = \frac{(n-1)!}{i!} \sqrt{\frac{n^3}{i}} = n! \sqrt{n}$$  \hspace{1cm} (A.63)

and we find that

$$\Psi_n(\rho) = \frac{\hat{L}_+^n \Psi_1(\rho)}{n! \sqrt{n}}.$$  \hspace{1cm} (A.64)