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Isotropic Oscillator Under a Magnetic and Spatially Varying Electric Field

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Isotropic Oscillator Under a Magnetic and Spatially Varying Electric Field

David Frost

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Abstract

We investigate the energy levels of a particle confined in the isotropic oscillator potential with a magnetic and spatially varying electric field. Here we are able to exactly solve the Schrodinger equation, using matrix methods, for the first excited states. To this end we find that the spatial gradient of the electric field acts as a magnetic field in certain circumstances. Here we present the changes in the energy levels as functions of the electric field, and other parameters.

1   Introduction

The idea of quantum dots arises out of the quantization of energy from a particle being confined. Knowing the exact way the energy levels are quantized gives one control to "tune" the energies of the system to meet any need. An example of this is the particle in a box formalism that is presented in introductory quantum mechanics. In this system the energies are proportional to $\frac{1}{L}$, so one can change the length of the box to yield different energy levels, and "tune" the system. This feature of nature is extremely useful in optics, quantum computing, and material science. However, infinite potential wells are not realistic. More realistic quantum dots are chemically created shells that confine electrons. This is analogous to the particle in the box, but now the bounds are not infinite, and the box can take on any geometry that would be needed to fit the application. Here we will discuss a similar structure to the infinite square well, the isotropic oscillator. However, since this does not involve infinite potentials, it is more realistic. We will introduce several perturbations on the system, and determine their impact, and ways in which the system can be "tuned". We consider only the time independent solution. Moreover, this is a theoretical investigation and some liberties are taken, although the results are to be seen as justifiable approximations to the exact treatment.

1.1 One Dimensional Harmonic Oscillator

To begin, it will be wise to first consider the 1 dimensional analog of the isotropic oscillator, the harmonic oscillator. Recall the mass and spring system from classical mechanics, this system has potential energy $V(x) = \frac{1}{2}kx^2$ where $k = m\omega^2$ is the so called spring constant, with m as the mass, and ω as the oscillation frequency. Further, x is the distance from the equilibrium point of the spring mass system. This potential energy is called the harmonic oscillator potential.

Now we consider this potential energy in a quantum setting. We will closely follow David J Griffith's derivation in *Introduction to Quantum Mechanics* [1]. We will first constrain ourselves to one dimension, and to a free particle with no other potentials acting on it. Consequently, the Hamiltonian for this system is,

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$$

Now we are tasked with the problem of solving the stationary Schrödinger equation,

$$\hat{H}\psi = -\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\Psi = E\Psi$$

Dividing both sides by $\frac{-\hbar}{2}$ thus yielding

$$\frac{\hbar}{m\omega}\frac{d^2\psi}{dx^2} - \frac{m\omega}{\hbar}x^2\psi = \frac{-2mE}{\hbar}\psi$$

Now, adding in the quantity $\xi = \sqrt{\frac{m\omega}{\hbar}}x$, and express the energy in units of $\frac{1}{2}\hbar\omega$ to give $K = \frac{2E}{\hbar\omega}$ Now we can rewrite our differential equation as

$$\frac{d^2\Psi}{d\xi^2} = (\xi^2 - K)\Psi$$

Now, we consider solutions for $\xi \gg K$ for this we can approximate the differential equation by,

$$\frac{d^2\Psi}{d\xi^2} \approx \xi^2\Psi$$

Checking the characteristic polynomial of this second degree homogeneous linear differential equation, we get solutions of ± 1 so we get that

$$\Psi(\xi) \approx Ae^{\frac{-\xi^2}{2}} + Be^{\frac{\xi^2}{2}}$$

Checking the asymptotic behavior of these approximate solutions we see that $Be^{\frac{\xi^2}{2}}$ must be thrown out, in other words $B = 0$. This is due to the fact that this solution goes to infinity as $\xi \to \infty$, thus this is not a physically viable solution.

Now, we assume that the exact solution is of the form,

$$\Psi(\xi) = h(\xi)e^{\frac{-\xi^2}{2}}$$

Then it follows from differentiation,

$$\frac{d\Psi}{d\xi} = \left(\frac{dh}{d\xi} - \xi h\right)e^{\frac{-\xi^2}{2}}$$

further, differentiating again we get,

$$\frac{d^2\Psi}{d\xi^2} = \left(\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (\xi^2 - 1)h\right)e^{\frac{-\xi^2}{2}}$$

Now, since we have already obtained an approximate asymptotic solution it suffices to solve,

$$\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (K^2 - 1)h = 0$$

To do this we will use the Frobenius method of solving differential equations. By Taylor's theorem we know that any "well behaved" function can be expanded as a power series. We use this to our advantage here in assuming that $h(\xi)$ can be expanded in terms of a power series, in terms of ξ. Thus

$$h(\xi) = \sum_{n=0}^{\infty} a_n \xi^n$$

Now, differentiating the power series we can get that

$$\frac{dh}{d\xi} = \sum_{n=0}^{\infty} n a_n \xi^{n-1}$$

Differentiating once more we find that

$$\frac{d^2h}{d\xi^2} = \sum_{n=0}^{\infty} (n+1)(n+2)a_{n+2}\xi^n$$

Collecting all of the terms into one grand sum, we have that

$$\sum_{n=0}^{\infty} [(n+1)(n+2)a_{n+2} - 2na_n + (K-1)a_n]\xi^n$$

Since this whole sum is equal to zero, the coefficients of the power series must be zero. So then we have that

$$(n+1)(n+2)a_{n+2} - 2na_n + (K-1)a_n = 0$$

then through simple algebraic means, we arrive at a recursion relation,

$$a_{n+2} = \frac{(2n - (K-1))}{(n+1)(n+2)}a_n$$

Now, for large n, we see that this recursion relation gives

$$a_{n+2} \approx \frac{2}{n}a_n$$

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Therefore, we can say that

$$a_n \approx \frac{C}{(n/2)!}$$

and thus,

$$h(\xi) \approx C \sum \frac{1}{n!} \xi^{2n} \approx Ce^{\xi^2}$$

Seeing this, we must declare that this sum must terminate at some point. Consequently, we say that $K = 2N + 1$ for $N \in \mathbb{Z}$ this will give a termination in the series.

From the recursion relation in the solution of ψ we can find the energies of the one dimensional harmonic oscillator. Since, $K = \frac{2E}{\hbar\omega}$ we can solve the equation $2N + 1 = \frac{2E}{\hbar\omega}$ for E. Doing this, we arrive at the quantized energies of

$$E_N = \left(N + \frac{1}{2}\right)\hbar\omega$$

Then, noticing that when $n = 0$, $h(\xi) = a_0$ and therefore, $\Psi_0(\xi) = a_0 e^{\frac{-\xi^2}{2}}$. Furthermore, through more iterations of this process we get that

$$\Psi_n(\xi) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^N N!}} H_N(\xi) e^{\frac{-\xi^2}{2}}$$

Where $H_N(\xi)$ are Hermite polynomials, which are a collection of orthogonal functions. The constant in front is the normalization constant of the general solution.

This is the one dimensional analog of the isotropic oscillator, it is the most basic part of the rest of our discussion, and forms a basic one dimensional quantum dot. With corresponding energies, $E_N = \left(N + \frac{1}{2}\right)\hbar\omega$.

1.2   The Isotropic Oscillator

The isotropic oscillator is a 3 dimensional form of the harmonic oscillator. Here we make one simplifying assumption, that the frequency is the same in all direction. That is, it is isotropic. We start by converting to spherical coordinates. This means,

$$x = r\sin(\theta)\cos(\phi)$$
$$y = r\sin(\theta)\sin(\phi)$$
$$z = r\cos(\theta)$$

Here, we closely follow the derivation presented by Timothy D. Jones. [2] Since this is three dimensions we take the Schrödinger equation to be

$$\frac{-\hbar}{2m}\nabla^2\Psi(r,\theta,\phi) + \frac{1}{2}m\omega^2 r^2\Psi(r,\theta,\phi) = E\Psi(r,\theta,\phi).$$

In spherical coordinates we have that the Laplacaican,

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial \theta}\left(\sin(\theta)\frac{\partial}{\partial \theta}\right) + \frac{1}{r^2\sin^2(\theta)}\frac{\partial^2}{\partial \phi^2}.$$

Therefore, the Schrödinger equation is

$$\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial \theta}\left(\sin(\theta)\frac{\partial}{\partial \theta}\right) + \frac{1}{r^2\sin^2(\theta)}\frac{\partial^2}{\partial \phi^2}\right)\Psi(r,\theta,\phi) + \frac{1}{2}m\omega^2r^2\Psi(r,\theta,\phi) = E\Psi(r,\theta,\phi).$$

This is a homogeneous linear partial differential equation, to solve this we implement the use of separation of variables. We assume that the solution can be separated into a radial part and an angular part, such that

$$\Psi(r,\theta,\phi) = \Gamma(r)\Omega(\theta,\phi)$$

therefore, the Schódinger equation becomes:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Gamma(r)}{\partial r}\right)\Omega(\theta,\phi) + \frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial \theta}\left(\sin(\theta)\frac{\partial\Omega(\theta,\phi)}{\partial \theta}\right)\Gamma(r)$$

$$+ \frac{1}{r^2\sin^2(\theta)}\frac{\partial^2\Omega(\theta,\phi)}{\partial \phi^2}\Gamma(r) + \frac{1}{2}m\omega^2r^2\Gamma(r)\Omega(\theta,\phi)$$

$$= E\Gamma(r)\Omega(\theta,\phi).$$

Now, we multiply by $\frac{-2mr^2}{\hbar^2}$, and divide by $\Gamma(r)\Omega(\theta,\phi)$ to get,

$$\left[\frac{1}{\Gamma(r)}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Gamma(r)}{\partial r}\right) - \frac{2mr^2}{\hbar^2}\left(\frac{1}{2}m\omega^2r^2 - E\right)\right]$$

$$+ \frac{1}{\Omega(\theta,\phi)}\left[\frac{1}{\sin(\theta)}\frac{\partial}{\partial \theta}\left(\sin(\theta)\frac{\partial\Omega(\theta,\phi)}{\partial \theta}\right) + \frac{1}{\sin^2(\theta)}\frac{\partial^2\Omega(\theta,\phi)}{\partial \phi^2}\right] = 0$$

1.2.1 The Angular Equation

Using the separation constant, χ, and multiplying by $\Omega(\theta,\phi)\sin^2(\theta)$, to get

$$\sin(\theta)\frac{\partial}{\partial \theta}\left(\sin(\theta)\frac{\partial\Omega(\theta,\phi)}{\partial \theta}\right) + \frac{\partial^2\Omega(\theta,\phi)}{\partial \phi^2} = \chi\sin^2(\theta)\Omega(\theta,\phi)$$

Now, we must use separation of variables on this, hence let $\Omega(\theta,\phi) = \Phi(\phi)\Theta(\theta)$. Now, with this substitution we get,

$$\sin(\theta)\frac{\partial}{\partial \theta}\left(\sin(\theta)\frac{\partial\Theta(\theta)}{\partial \theta}\right)\Phi(\phi) + \frac{\partial^2\Phi(\phi)}{\partial \phi^2}\Theta(\theta) = \chi\sin^2(\theta)\Theta(\theta)\Phi(\phi)$$

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Now, we divide by $\Theta(\theta)\Phi(\phi)$ and subtract by $\chi \sin^2(\theta)$ to get

$$\frac{\sin(\theta)}{\Theta(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial\Theta(\theta)}{\partial\theta}\right) + \chi\sin^2(\theta) + \frac{1}{\Phi(\phi)}\frac{\partial^2\Phi(\phi)}{\partial\phi^2} = 0.$$

Now, we can separate these by a constant, say k. We will first solve the $\Phi(\phi)$ equation.

We now have that,

$$-\frac{1}{\Phi(\phi)}\frac{\partial^2\Phi(\phi)}{\partial\phi^2} = k.$$

This then leads us to

$$\frac{\partial^2\Phi(\phi)}{\partial\phi^2} + k\Phi(\phi) = 0,$$

this yields the characteristic equation of

$$x^2 + k = 0$$

giving us 2 roots namely, $\pm\sqrt{k}i$, therefore we have that,

$$\Phi(\phi) = e^{\pm i\sqrt{k}\phi}.$$

Noticing that the azimuthal angle's function must be 2π periodic, we must impose the condition that

$$e^{\pm i\sqrt{k}\phi + 2\pi} = e^{\pm i\sqrt{k}\phi}.$$

This then implies that

$$e^{\pm i2\pi\sqrt{k}} = 1$$

therefore by Euler's formula, we have that

$$\cos(2\pi\sqrt{k}) + i\sin(2\pi\sqrt{k}) = 1$$

For this to be the case, $\sqrt{k}$ must be an integer. Since this is the case, we will relabel $\sqrt{k} = m$. Thus, we have that

$$\Phi(\phi) = e^{\pm im\phi}$$

Now we proceed to the longitudinal equation:

$$\frac{\sin(\theta)}{\Theta(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial\Theta(\theta)}{\partial\theta}\right) + \chi\sin^2(\theta) = m^2$$

Now, carrying out the differentiation, using the product rule, and multiplying by $\Theta(\theta)$, and dividing by $\sin(\theta)$ we find,

$$\sin(\theta)\frac{\partial^2\Theta(\theta)}{\partial\theta^2} - \cos(\theta)\frac{\partial\Theta(\theta)}{\partial\theta} + (\chi\sin^2(\theta) - m^2)\Theta(\theta) = 0$$

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This differential equation is solved by the associated Legendre polynomials. Due to the boundary conditions placed on these solutions, we see that $\chi = l(l+1)$ where l is a non-negative integer. Therefore, putting these two solutions together and normalizing we get the spherical harmonics, $Y_l^m(\theta, \phi)$. These are given by,

$$Y_l^m(\theta, \phi) = (-1)^m \sqrt{\frac{(2l+1)l - |m|}{4\pi(l + |m|)}} e^{im\phi} P_l^m(cos(\theta))$$

where $P_l^m(cos(\theta))$ is an associated Legendre polynomial. These associated Legendre polynomials are given by,

$$P_l^m(x) = (1 - x^2)^{\frac{|m|}{2}} \left(\frac{d}{dx}\right)^{|m|} P_l(x)$$

here, $P_l(x)$ is the Legendre polynomial. The Legendre polynomial is given by the formula,

$$P_l(x) = \frac{1}{2l!} \left(\frac{d}{dx}\right)^l (x^2 - 1)^l.$$

1.2.2 The Radial Equation [2]

Now we solve the radial equation

$$\frac{1}{\Gamma(r)} \frac{\partial}{\partial r}\left(r^2 \frac{\partial \Gamma(r)}{\partial r}\right) - \frac{2mr^2}{\hbar^2}\left(\frac{1}{2}m\omega^2 r^2 - E + \frac{\hbar^2}{2mr^2}l(l+1)\right) = 0$$

Now multiplying by $\Gamma(r)$, carrying out the differentiation, and dividing by r^2 we get

$$\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right)\Gamma(r) + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}m\omega^2 r^2 - \frac{\hbar^2}{2mr^2}l(l+1)\right)\Gamma(r) = 0$$

Looking at the asymptotic behavior of this, we see that towards infinity, the r^2 terms will monopolize, and the other terms may be neglected. In addition, let $b^2 = \frac{m^2\omega^2}{\hbar^2}$. Now we have that this first asymptotic behavior implies that

$$\frac{\partial^2}{\partial r^2}\Gamma(r) \propto b^2 r^2 \Gamma(r) \rightarrow \Gamma(r) \propto e^{\frac{-br^2}{2}}$$

Considering the second asymptote, when $r \rightarrow 0$, and the $\frac{1}{r^2}$ terms control the equation, allowing the other parts to be neglected the differential equation becomes,

$$\frac{\partial^2 \Gamma(r)}{\partial r^2} + \frac{2}{r}\frac{\partial \Gamma(r)}{\partial r} \propto \frac{l(l+1)}{r^2}\Gamma(r).$$

To solve this equation we assume that there is a function $\zeta(r)$ that will simplify the equation. Then we have that

$$\frac{d\Gamma^2}{dr^2}\left(\frac{d\zeta}{dr}\right)^2 + \frac{d\Gamma}{dr}\left(\frac{d^2\zeta}{dr^2} + \frac{2}{r}\frac{d\zeta}{dr}\right) - \frac{l(l+1)}{r^2}\Gamma = 0$$

Now that is simplified, we can see that this will have solutions when

$$\frac{d\zeta}{dr} = \frac{l(l+1)}{r}$$

Letting this be true, we can then see that the radial equation becomes

$$\frac{d\Gamma^2}{dr^2} + \sqrt{l(l+1)}\frac{d\Gamma}{dr} - \sqrt{l(l+1)}\Gamma$$

This has solutions,

$$\Gamma(\zeta(r)) = Ae^{\frac{-l+1}{l(l+1)}\zeta(r)} + Be^{\frac{l}{l(l+1)}\zeta(r)}$$

Then, solving for $\zeta(r)$ we find

$$\zeta(r) = 1(l+1)\ln(r)$$

Therefore, we have that

$$\Gamma(r) = Ar^{-(l+1)} + Br^l.$$

Now, applying the condition that this solution must be finite at the origin, we see that $A = 0$, and we are left with the asymptotic solution

$$\Gamma(r) = Br^l.$$

Putting the asymptotic solutions together and assuming that the solution can be written in terms of a power series we get that

$$\Gamma(r) = Ar^l e^{-\frac{br^2}{2}} \sum_k a_k r^k.$$

Solving for the recursion relation of a_k, we find that

$$a_{k+2} = \frac{\frac{-2mE}{\hbar^2} + b(2k + 2l + 3)}{(k+2)(k+2l+3)}a_k.$$

Now, requiring for the series to terminate, at k_f we find the energies of this system to be

$$E_l = \left(k_f + l + \frac{3}{2}\right)\hbar\omega$$

Here, one can see that we still only need to "tune" ω to change the energies of the isotropic oscillator. Further, putting the solutions together we have that the full wave function for this system is given by

$$Ar^l e^{-\frac{br^2}{2}} \sum_k a_k r^k Y_m^l(\theta, \phi)$$

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1.3 The Schrödinger Equation in terms of linear algebra

Recall the Schödinger equation: $\hat{H}\Psi = E\Psi$. This can be framed in the language of linear algebra. Here, we can note that the Hamiltonian operator is a linear transformation on a Hilbert space, representing the space of all wave functions. Then, it becomes clear that the energies of a system are the real valued eigenvalues of the Hamiltonian. Since the Hamiltonian is a linear operator, it has a matrix representation. We define an element of a matrix representation of the Hamiltonian as,

$$H_{ij} = \langle \varphi_i | \hat{H} | \varphi_j \rangle = \int \varphi_i^* \hat{H} \varphi_j$$

where the integral is over all space, and φ_n is one basis function for the Hilbert space in question. In addition, φ^* denotes the complex conjugate of φ. Further, we require that these basis functions be orthogonal, hence $\langle \varphi_i | \varphi_j \rangle = \delta_{i,j}$ where $\delta_{i,j}$ is the Dirac delta function.

Then, the Schrödinger equation becomes an eigenvalue problem [3], where we have

$$\begin{pmatrix} H_{11} & H_{12} & \dots \\ H_{21} & H_{22} & \dots \\ \vdots & \vdots & \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \vdots \end{pmatrix} = E \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \vdots \end{pmatrix}$$

This is then equivalent to solving the matrix equation [3]:

$$\begin{pmatrix} H_{11} - E & H_{12} & \dots \\ H_{21} & H_{22} - E & \dots \\ \vdots & \vdots & \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \vdots \end{pmatrix} = 0$$

Then, to find the non-trivial solutions of this equation we need to take the determinant of the resulting matrix. Thus, we need to solve the following equation [3].

$$\begin{vmatrix} H_{11} - E & H_{12} & \dots \\ H_{21} & H_{22} - E & \dots \\ \vdots & \vdots & \end{vmatrix} = 0$$

So, now it becomes an important task to find the matrix representation of the Hamiltonian of a system. Further, each state vector $|\varphi_j\rangle$ will have an associated eigenvalue. If two such state vectors have the same eigenvalue, these states are said to be degenerate. In addition, the collection of all eigenvalues of an operator is called the eigenvalue spectrum of the operator.

2 Building the Confined System

Now we consider a state space, using the wave functions of the isotropic oscillator as the basis functions. In addition, we will truncate the space at the first excited state. This makes the Schrödinger equation exactly solvable in this space. This alters the final results as the first excited states eventually couple with higher excited states. However, this coupling is small and the solutions presented here will be very accurate. For clarity, we only make use of the states with $l = 0, 1$:

$$\Psi_{00} \quad \Psi_{01} \quad \Psi_{11} \quad \Psi_{1,-1}$$

Consequently, the matrix representation of our Hamiltonian is the following:

$$\begin{pmatrix} \langle\Psi_{00}|\hat{H}|\Psi_{00}\rangle & \langle\Psi_{00}|\hat{H}|\Psi_{01}\rangle & \langle\Psi_{00}|\hat{H}|\Psi_{11}\rangle & \langle\Psi_{00}|\hat{H}|\Psi_{1,-1}\rangle \\ \langle\Psi_{01}|\hat{H}|\Psi_{00}\rangle & \langle\Psi_{01}|\hat{H}|\Psi_{01}\rangle & \langle\Psi_{01}|\hat{H}|\Psi_{11}\rangle & \langle\Psi_{01}|\hat{H}|\Psi_{1,-1}\rangle \\ \langle\Psi_{11}|\hat{H}|\Psi_{00}\rangle & \langle\Psi_{11}|\hat{H}|\Psi_{01}\rangle & \langle\Psi_{11}|\hat{H}|\Psi_{11}\rangle & \langle\Psi_{11}|\hat{H}|\Psi_{1,-1}\rangle \\ \langle\Psi_{1,-1}|\hat{H}|\Psi_{00}\rangle & \langle\Psi_{1,-1}|\hat{H}|\Psi_{01}\rangle & \langle\Psi_{1,-1}|\hat{H}|\Psi_{11}\rangle & \langle\Psi_{1,-1}|\hat{H}|\Psi_{1,-1}\rangle \end{pmatrix}$$

Notice, that if the Hamiltonian is a combination of two or more elements under addition, $\hat{H} = H_1 + H_2$ this matrix can be written as a combination of the individual matrices for the individual components of the Hamiltonian. Consequently, one can find the matrix representation of a complex Hamiltonian by first finding the individual matrix representation of the Hamiltonian's components, and then summing them. We now will consider three separate effects on the isotropic oscillator, the addition of a magnetic field, the addition of a constant electric field, and the addition of a spatially varying electric field. In doing this, we can find the matrix for the combined system, by finding the individual matrix representations and then adding them to find the complete matrix representation of the Hamiltonian in this function space.

2.1 Zeeman Effect

The change of the eigenvalues, or the energies, of a system due to the addition of a magnetic field is referred to as the Zeeman effect. We will now see if the Zeeman effect is present in the isotropic oscillator confined system, and if so see how much of an impact it will make. The addition of a magnetic field is handled by adding the term $\vec{\mu} \cdot \vec{B}$ to the Hamiltonian, where $\vec{\mu} = \mu_B \hat{L}$, where $\hat{L}$ is the angular momentum operator, and $\vec{B}$ is the magnetic field vector. Now, we determine the matrix representation for this element in the Hamiltonian, recalling that the basis functions for this space are the isotropic oscillator wave functions, we have that the ith, j^{th} position in the matrix is given by,

$$\langle\Psi_{ml}|\vec{\mu} \cdot B|\Psi_{m'l'}\rangle$$

for $m \in \{-1, 0, 1\}$ and $l \in \{0, 1\}$. Taking these integrals we find that the final matrix is:

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\mu_B}{\sqrt{2}}(B_x - iB_y) & \frac{\mu_B}{\sqrt{2}}(B_x + iB_y) \\ 0 & \frac{\mu_B}{\sqrt{2}}(B_x + iB_y) & B_z\mu_B & 0 \\ 0 & \frac{\mu_B}{\sqrt{2}}(B_x - iB_y) & 0 & -B_z\mu_B \end{pmatrix}$$

Where μ_B is the Bohr magneton, and has the value $5.788*10^{-5}\frac{ev}{T}$. This is then the contribution from the magnetic field. Notice that the factor on the magnetic field is in the order of $10^{-5}\frac{ev}{T}$, so it is a very small contribution. In order to get a large response, one must use comparatively large magnetic fields. There is an effect for small magnetic fields, but this effect is along the same order of magnitude as the Bohr magneton. To see the effect of a magnetic field on the system, we can graph the eigenvalues as a function of a changing magnetic field. To demonstrate this effect we use incredibly high magnetic fields, of order $10^3 T$, this is solely to show the effect. Using smaller magnetic fields will give much smaller energy contributions, these are on the same order as the Bohr magneton. Since these are much smaller than the excitation energy of, $1ev$ we can say that our model is producing reasonably accurate results, in spite of it's truncated function space. This will demonstrate the deviation from the original system as a function of the magnitude of the magnetic field. This is shown below.
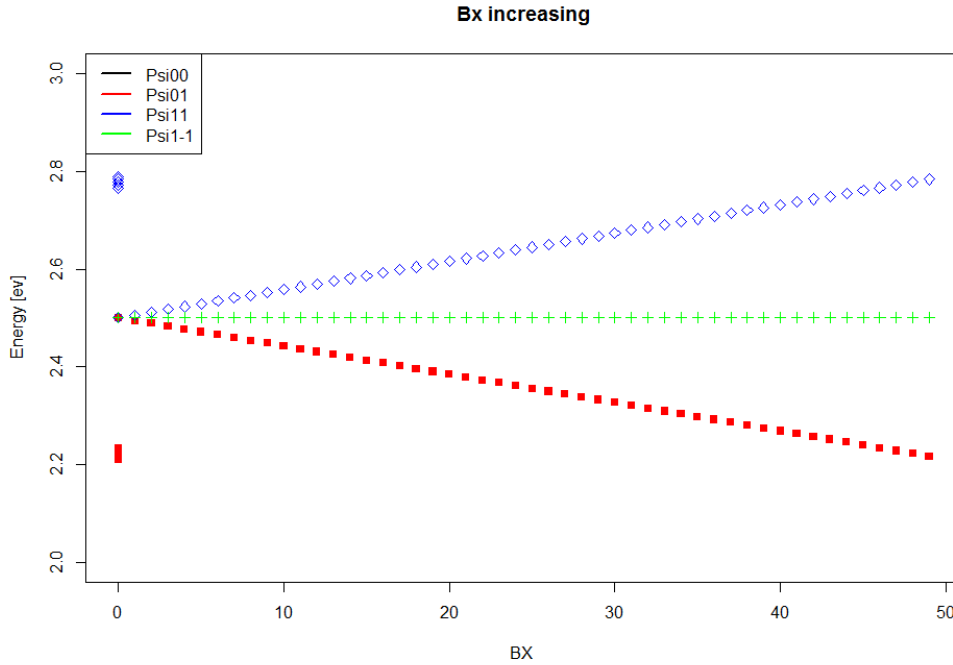

Figure 1: Eigenvalues of the first excited state as a function of $B_x[T]$, with $E_1 = 2.5ev$

One can clearly see that the first excited states split, and grow to increasingly different energies.

This is contrary to the behavior in the unperturbed isotropic oscillator. Therefore, the addition of a magnetic field does impact the system. In the uninterrupted setting, we have that $\Psi_{1,1}$ and $\Psi_{1,-1}$ are degenerate. Here, with the addition of the Zeeman effect, these states are non-degenerate. Further, one can note that the difference in energies of these two states are symmetric, as one goes up, the other goes down by the same factor.

2.2 Stark Effect

A change in the eigenvalues of a system due to the presence of a constant electric field is referred to as the Stark effect. Now, we consider a constant electric field acting on the isotropic oscillator confined system, we wish to see if the Stark effect will impact the system, and if so to what degree. To do this we add the term for electric potential energy,

$$
\begin{pmatrix} E_x & E_y & E_z \end{pmatrix} \begin{pmatrix} r\sin(\theta)\cos(\phi) \\ r\sin(\theta)\sin(\phi) \\ r\cos(\theta) \end{pmatrix}
$$

to our Hamiltonian, and then find the matrix that represents this contribution. In doing this we find that the matrix representation of the static electric part of the Hamiltonian is given by,

$$
\begin{pmatrix} 0 & \frac{E_z}{4\sqrt{\pi b}} & 0 & 0 \\ \frac{E_z}{4\sqrt{\pi b}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}
$$

and we see that only the z component of the electric field causes any addition to the Hamiltonian matrix. From this matrix we can see that the addition of a static electric field should affect the $m = 0$ excited state, while leaving the other two alone. To see this we conduct the same graphing as used with the magnetic field. Here we use a ground state of $1.5ev$, and set $b = 10.0\frac{1}{\overset{\circ}{A}^2}$.
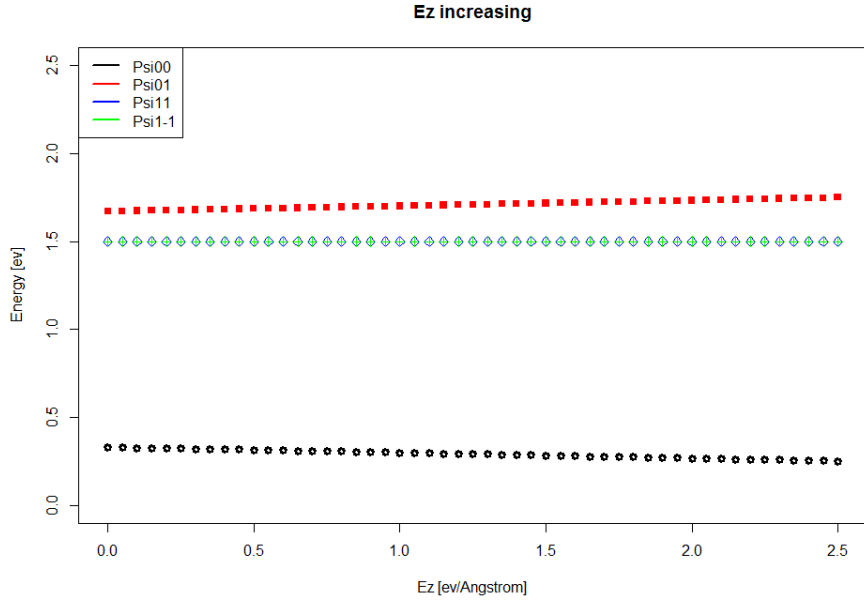
Figure 2: Eigenvalues of the system as a function of E_z

One can see the state with the most energy is, Ψ_{01}, and the states with $m \pm 1$ are intertwined, as the states with the second most energy. Here one can see that with the addition of an electric field the $m = 0$ excited state gains more energy, and becomes non-degenerate. Therefore, the Stark effect is present. In addition, the Stark effect alters the ground state energy as well, giving it a downward trend as E_z increases. The effect of these perturbations on the ground state will be addressed in a later section.

2.3 Adding in a Spatially Varying Electric Field

Now, we consider how the system would react to the presence of a non-homogeneous electric field. This is of prime interest, as this type of electric field is ubiquitous in the world, and determining its effect on our system will yield a way to account for this. To add in a non-homogeneous electric field, we add

$$
\begin{pmatrix} r\sin(\theta)\cos(\phi) & r\sin(\theta)\sin(\phi) & r\cos(\theta) \end{pmatrix}
\begin{pmatrix} v_{xx} & v_{xy} & v_{xz} \\ v_{yx} & v_{yy} & v_{yz} \\ v_{zx} & v_{zy} & v_{zz} \end{pmatrix}
\begin{pmatrix} r\sin(\theta)\cos(\phi) \\ r\sin(\theta)\sin(\phi) \\ r\cos(\theta) \end{pmatrix}
$$

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to the Hamiltonian and determine its contribution's matrix representation. Hence, the matrix representation is,

$$
\begin{pmatrix}
\frac{1}{2b}(v_{xx} + v_{yy} + v_{zz}) & 0 & 0 & 0 \\
0 & \frac{1}{4b}(v_{xx} + v_{yy} + 3v_{zz}) & \frac{3}{4\sqrt{2}b}(v_{xz} - iv_{yz}) & \frac{3}{4\sqrt{2}b}(v_{xz} + iv_{yz}) \\
0 & \frac{3}{4\sqrt{2}b}(v_{xz} + iv_{yz}) & \frac{1}{4b}(v_{xx} + v_{yy} + v_{zz}) & \frac{1}{4b}(v_{xx} + v_{yy} + itv_{xy}) \\
0 & \frac{3}{4\sqrt{2}b}(v_{xz} - iv_{yz}) & \frac{1}{4b}(v_{xx} + v_{yy} - iv_{xy}) & \frac{1}{4b}(v_{xx} + v_{yy} + v_{zz})
\end{pmatrix}
$$

Graphing the dependence of the eigenvalues of the system as a function of the v_{xz} gradient, we notice a very striking behavior.
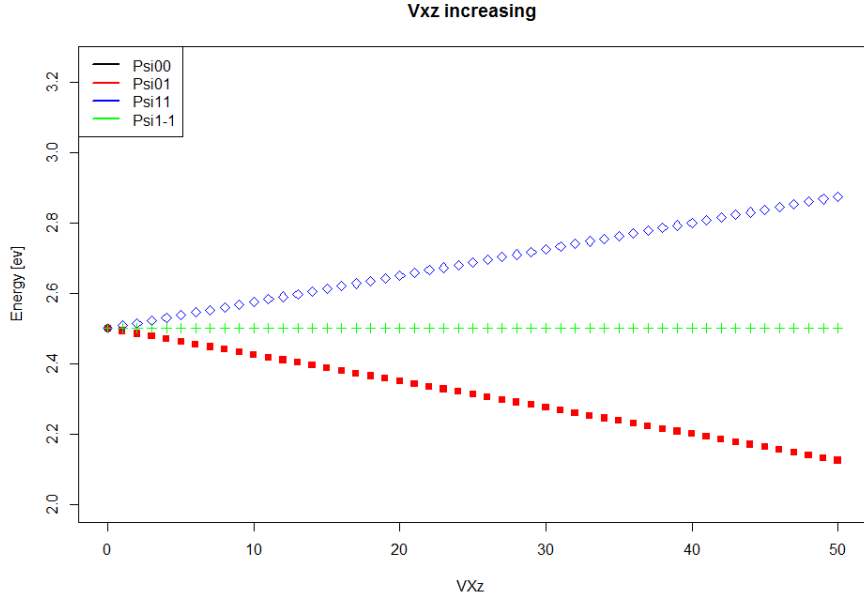

Figure 3: Eigenvalues of the system as a function of $v_{xz}\left[\frac{ev}{\overset{\circ}{A}^2}\right]$

Here one can see that the electric field gradient has very similar behavior to the energy dependence of the magnetic field. They both exhibit the same splitting of the states, and forming symmetric non-degenerate states. This is due to the H_{32} and H_{42} contributions to the Hamiltonian. This becomes more clear when one adds up each contribution. The full matrix is,

$$
\begin{pmatrix}
E_0 + \frac{1}{2b}(v_{xx} + v_{yy} + v_{zz}) & \frac{E_z}{4\sqrt{\pi}b} & 0 & 0 \\
\frac{E_z}{4\sqrt{\pi}b} & E_1 + \frac{1}{4b}(v_{xx} + v_{yy} + 3v_{zz}) & \frac{\mu_B}{\sqrt{2}}(B_x - iB_y) + \frac{3}{4\sqrt{2}b}(v_{xz} - iv_{yz}) & \frac{\mu_B}{\sqrt{2}}(B_x + iB_y) + \frac{3}{4\sqrt{2}b}(v_{xz} + iv_{yz}) \\
0 & \frac{\mu_B}{\sqrt{2}}(B_x + iB_y) + \frac{3}{4\sqrt{2}b}(v_{xz} + iv_{yz}) & E_1 + \frac{1}{4b}(v_{xx} + v_{yy} + v_{zz}) & \frac{1}{4b}(v_{xx} + v_{yy} - iv_{xy}) \\
0 & \frac{\mu_B}{\sqrt{2}}(B_x - iB_y) + \frac{3}{4\sqrt{2}b}(v_{xz} - iv_{yz}) & \frac{1}{4b}(v_{xx} + v_{yy} + iv_{xy}) & E_1 + \frac{1}{4b}(v_{xx} + v_{yy} + v_{zz})
\end{pmatrix}
$$

Here one can notice that the $H_{32} = \frac{\mu_B}{\sqrt{2}}(B_x - iB_y) + \frac{3}{4\sqrt{2}b}(v_{xz} - iv_{yz})$, then the magnetic and electric gradient have the same behavior. Notice however, that the coefficient on the electric gradient is

much larger than the one on the magnetic field. This then means that our system is sensitive to the electric gradient. This gradient indeed acts almost identically as the magnetic field when considering the energy levels. Then, the electric gradient can support the magnetic contribution to the energies.

In addition, if we let $v_{xx} = v_{yy} = v_{zz} = 0$, and $E_z = 0$. We can directly solve the determinant of the matrix. Doing this we can find a closed form solution for the resulting energies of the $m = \pm 1$, and letting

$$F = \frac{\mu_B}{\sqrt{2}}(B_x - iB_z) + \frac{3}{4\sqrt{2}b}(v_{xz} - iv_{yz})$$

Finding this we have,

$$E_{(1,1),(1,-1)} = \sqrt{(\mu_B B_z)^2 + \|F\|^2}$$

Using this one could measure the transition from $\Psi_{1,-1}$ to $\Psi_{1,1}$ and determine the magnetic splitting provided the electric field gradient is known.

2.4   Impact of Electric and Magnetic Fields on Ground State

The ground state is least effected by the truncation of our function space. Now we look at the mixture of the states corresponding to the ground state energy. Here, the state of a particle with a given energy is given by a linear combination of the eigenvectors. These are the vectors that are scaled by the eigenvalue under the Hamiltonian operator. This is given by,

$$\Psi = c_{0,0}\psi_{0,0} + c_{0,1}\psi_{0,1} + c_{1,1}\psi_{1,1} + c_{1,-1}\psi_{1,-1}$$

In the following table, we present the values of the coefficients, under certain circumstances. The square of these coefficients correspond to the probability of finding the particle in this state given it has the ground state energy.

	$c_{0,0}$	$c_{0,1}$	$c_{1,1}$	$c_{1,-1}$
$E_z = v_{i,j} = B_i = 0$	1	0	0	0
$E_z = 10.0\frac{ev}{\overset{\circ}{\text{A}}}$	0.9344	-0.3562	0	0
$E_z = 10.0\frac{ev}{\overset{\circ}{\text{A}}}, B_z = 10^3T$	0.9340	-0.3568	$1.248 \cdot 10^{-2}$	$1.248 \cdot 10^{-2}$
$E_z = 10.0\frac{ev}{\overset{\circ}{\text{A}}}, B_z = B_x = 10^3T$	0.9340	-0.3568	$1.3138 \cdot 10^{-2}$	$1.183 \cdot 10^{-2}$
$E_z = 10.0\frac{ev}{\overset{\circ}{\text{A}}}, v_{xz} = v_{xy} = 10\frac{ev}{\overset{\circ}{\text{A}}^2}$	0.8019	-0.4714	0.2063	0.2239

So, one can see that the magnetic and the electric field gradient produce similar mixing of the states, in that all four states are mixed. However, since the electric gradient does not have such a small constant as the Bohr magneton, it produces a higher level of mixing.

3 Conclusions

Here we have seen that in a truncated function space, under the harmonic oscillator potential, that the Zeeman effect is similar to the effect of a electric field gradient, in coupling and in the alteration of the energy levels. Further, due to the truncation of the space, this model holds more traction for its consequences on the ground state than the other states. The effect on the ground state can be is more accurate, since it is correct up to second order. Since the ground state only couples with the first excited states the statements about the ground state energy can be regarded as extremely accurate, and even exact up to second order perturbation. Moreover, the claims on the first excited states, can still be regarded as reasonable approximations, by reason of the validity criterion, $E_1 - E_0 \ll E_p$ where E_p is the magnetic or electric perturbation energy. As previously discussed this is the case for lower magnitude magnetic fields and electric gradients. However, higher level perturbation still remains to be investigated. While the truncated model is exact in it's space, and can be seen as a reasonable approximation to realistic behavior, the validity of this model is limited by the lack of higher states with $l > 1$.

To make this model more accurate, one must investigate higher states, which might be done using perturbation theory. Further, the addition of spin will make for more contributions, and since real electrons have spin, this will make the model more accurate. In addition to spin, it would be interesting to consider spin orbit coupling in this system. Moreover, the addition of time dependent magnetic fields would have many applications, including NMR, in that the support of an electric field gradient could heighten the effects of the magnetic field, and as such simplify measurements.

References

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