BINDING OF A CHARGED PARTICLE TO AN ELECTRIC DIPOLE IN THE PRESENCE OF A MAGNETIC FIELD

MASTER OF SCIENCE (2008) McMaster University

Physics and Astronomy Hamilton, Ontario

TITLE : Binding of a Charged Particle in the Presence of an Electric Dipole and a Magnetic Field

AUTHOR : Arindam Chatterjee

SUPERVISOR : Dr. Rajat K. Bhaduri

NUMBER OF PAGES : XIII, 109

BINDING OF A CHARGED PARTICLE TO AN ELECTRIC DIPOLE IN THE PRESENCE OF A MAGNETIC FIELD

By

ARINDAM CHATTERJEE, B.Sc. (Hons.)

A Thesis

Submitted to the School of Graduate Studies

in Partial Fulfillment of the Requirements

for the Degree

Master of Science

McMaster University

Abstract

We formulate a variational method to obtain the binding energies of a charged particle in presence of an electric dipole and a magnetic field aligned along the dipole. First, we test the method by obtaining the critical dipole moment for a point dipole, as well as a finite dipole in the absence of a magnetic field. A few larger dipole moments supporting a zero energy bound state are also obtained. Adding a magnetic field of $\sim$ 20 - 100 T, we show that for a rigid and stationary dipole of moment 2.54 D, the electron binding energy increases by 15% - 66%. Our approach also shows the absence of a critical dipole moment in presence of an aligned magnetic field.

Acknowledgements

I thank the following people for walking me through the positive experiences in my past two years of graduate studies :

My supervisor Dr. Rajat K. Bhaduri, his expertise, encouragement and support have inspired me to strive to be a better student and person as a whole. I extend my sincere appreciation towards his patient guidance that made my study stimulating and fulfilling.

My committee members, Dr. Donald Sprung and Dr. Duncan O'Dell, for their insightful reviews of my work. I would like to appreciate the patience and understanding of my committee members have shown towards me. Dr. Sprung also suggested the algorithms I have used to solve the Schrodinger - like equation for the case of a finite dipole binding an electron in the presence of a magnetic field in Section 3.3.

Prof. M.V.N. Murthy, for fruitful discussions during my stay at IMSc, Chennai in December, 2007.

My friend Rahul Gandhi, for helping me with Matlab, which I have used to minimize the energy expression in Section 3.2.

All my friends in Hamilton, who made my stay in Hamilton beautiful.

Contents

List of Important Symbols

m : Mass of the charged particle.

q : Charge of an external particle.

e : Magnitude of an electron charge.

Q : The magnitude of the charge at each pole of the dipole.

2 d : The separation between the poles of the finite dipole.

$\vec{p}$: Dipole moment.

p : $|\vec{p}|$.

p_c : The critical value of the dipole moment.

ϵ_0 : The permittivity of the vacuum.

$\vec{B}$: The magnetic field.

γ : The square of the ratio of the Bohr radius to the cyclotron radius.

λ : $\frac{2m}{\hbar^2}\frac{pq}{4\pi\epsilon_0}$.

λ_c : The critical value of λ.

Ψ : Trial wavefunction.

E_0 : Energy of the ground state with the azimuthal quantum number zero.

E_b : Binding energy.

V_p : The potential experienced by a charged particle in the presence of a point dipole at the origin.

V_f : The potential experienced by the charged particle in the presence of a finite sized dipole centered at the origin.

$\tilde{V}_p$: The effective potential (depends only on the radial coordinate r) experienced by a charged particle in the presence of a point dipole at the origin.

$\tilde{V}_f$: The effective potential experienced by a charged particle in the presence of a finite sized dipole centered at the origin.

$V_p^{(B)}$: The potential experienced by a charged particle in the presence of a point dipole at the origin and a magnetic field ($\vec{B} = B\hat{z}$).

$V_f^{(B)}$: The potential experienced by a charged particle in the presence of a finite sized dipole centered at the origin and a magnetic field $\vec{B}$.

$\tilde{V}_p^{(B)}$: The effective potential experienced by a charged particle in the presence of a point dipole at the origin and a magnetic field $\vec{B}$.

$\tilde{V}_f^{(B)}$: The effective potential experienced by a charged particle in the presence of a finite dipole centered at the origin and a magnetic field $\vec{B}$.

List of Figures

List of Tables

1 Introduction

The binding of a charged particle by an electric dipole has attracted a lot of attention in the past [1]. The critical dipole moment for a point dipole required to bind an electron was first calculated by Fermi and Teller [2, 3]. For a stationary finite dipole the same problem was addressed in references [4, 5]. In reference [6] the eigenenergies of an electron in the potential of a finite dipole have been calculated. The critical moment is affected strongly by consideration of rotation of the molecule. The minimum dipole moment necessary to support at least one bound state increases by 10% to 30% compared to that of the stationary dipole [7, 8]. Also in such a situation the critical moment depends on the effective dipole length, the rotational state and the moment of inertia [7, 8]. In this thesis, a stationary dipole is considered, without taking dynamical effects into account. For several molecules, dipole bound anionic states exist. Reference [9] discusses the dipole bound anionic states of CH_3CN, C_3H_2, and $(HF)_2$. Excitons also possess permanent dipole moments. For example, in the InAs quantum dots in GaAs the electron hole separation is about 0.4 nm [10, 11]. In reference [8] the mobility of excess electrons in polar hydrogen cyanide gas (dipole moment 2.985D) was measured. The process involved short-lived dipole-bound electron ground states. It may be interesting to study the effect of a magnetic field on such systems and also to investigate if there is any critical value for the electric dipole in such a situation. However, unlike the case of a pure dipole potential, the Schrodinger equation can no longer be solved analytically using the variable separation method. We, in the present work,

have therefore devised a variational method to obtain the energy levels of a charged particle in such a situation. Both the point and the finite dipole are considered. Considering a polar molecule as a dipole and an electron as the charged particle to be bound, it is not unreasonable to assume the dipole to be stationary. We also assume the dipole to be rigid. To test our method, in chapter 2, we consider the problem of a charged particle experiencing only the electric dipole potential. We reproduce the critical dipole moments required to bind a charged particle and compare our results with previously obtained values [12]. In chapter 3 we discuss the variational method in presence of the electric dipole and a magnetic field along the dipole moment. Using our variational method, we obtain the ground state energy for the azimuthal quantum number $m_l = 0$ of an electron in such a situation. Also, we investigate the critical dipole moment, if any, required to bind the electron in such a situation. In references [13, 14] a similar problem has been addressed considering a very strong magnetic field (10^6T). Such strong magnetic fields may be found in astronomical objects like neutron stars. However, in a laboratory set up, usually the highest uniform magnetic fields are of the order of 10-100 T. Our method, as will be discussed in chapter 3, is expected to work better than the method formulated in [13] in this regime. In the following chapters several results related to the inverse square potential will be used. Before proceeding to the second chapter, we, therefore, briefly discuss the inverse square potential from references [15, 16] in the following subsection.

1.1 The $\frac{1}{r^2}$ Potential

It is well-known that the inverse square potential is anomalous in quantum mechanics [15, 16, 17]. The physical system of our interest, the point electric dipole, gives rise to an inverse square potential. Even for the finite dipole, the potential experienced by a charged particle at large distances compared to the dipole length is of inverse square nature. In this section, we discuss some of the previously established results related to such a potential which we have used in the subsequent chapters. The radial part of the Schrodinger equation for a particle (mass m) in an inverse square potential V is given by

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2}u(r) + \frac{\alpha}{r^2}u(r) = Eu(r). \tag{1.1}$$

Here u(r) is related to the radial wavefunction $\Phi(r)$ as $u(r) = r\Phi(r)$ and the coefficient of $\frac{1}{r^2}$ in the centrifugal term, $\frac{\hbar^2 l(l+1)}{2m}$, is included in α. Note that the Hamiltonian is scale invariant. The existence of any bound state implies instability for such a system. We show this following the argument in [15]. Consider equation (1.1) with $E < 0$. In terms of $\tilde{r} = br$, where $b > 0$, this equation implies

$$b^2\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \tilde{r}^2}u(\tilde{r}) + \frac{\alpha}{\tilde{r}^2}u(\tilde{r})\right) = b^2 Eu(\tilde{r}).$$

Thus a bound state (u(r)) with energy E implies a bound state (u(br)) with energy b^2E. Taking b to be any positive number, as $b \to \infty$ the system becomes unstable. However, denoting $\frac{2m}{\hbar^2}\alpha$ by a, it may be shown [15, 16] that the Hamiltonian in equation (1.1) does not support a negative energy

state for $a > -\frac{1}{4}$. For $a > 0$ the potential is evidently repulsive and hence does not support any bound state. For $-\frac{1}{4} < a < 0$ we sketch the proof as given in reference [15]. Let $a = \nu(\nu - 1)$, where ν is any real number. Note that the minimum of a is $-\frac{1}{4}$ and the corresponding ν is $\frac{1}{2}$. For an arbitrary function g(r) we have,

$$\begin{aligned} -\frac{\partial^2}{\partial r^2}g(r) + \frac{a}{r^2}g(r) &= -\left(\frac{\partial^2}{\partial r^2}g(r) + \frac{\nu(1-\nu)}{r^2}g(r)\right) \\ &= -\left(\frac{\partial}{\partial r} + \frac{\nu}{r}\right)\left(\frac{\partial}{\partial r} - \frac{\nu}{r}\right)g(r). \end{aligned} \tag{1.2}$$

Let u(r) and v(r) be any two functions defined over $r \in \{0, \infty\}$ which go to 0 as $r \to 0$ and $r \to \infty$. In the domain of such functions $\left(\frac{\partial}{\partial r} + \frac{\nu}{r}\right)$ and $\left(-\frac{\partial}{\partial r} + \frac{\nu}{r}\right)$ are Hermitian conjugates of each other,

$$\begin{aligned} \left\langle v(r)\left|\frac{\partial}{\partial r} + \frac{\nu}{r}\right|u(r)\right\rangle &= \int_0^\infty v^*\left(\frac{du}{dr} + \frac{\nu}{r}u\right)dr \\ &= v^*u|_0^\infty - \int_0^\infty \left(\frac{dv}{dr}\right)udr + \int_0^\infty \frac{\nu}{r}v^*udr \\ = \left\langle\left(-\frac{d}{dr} + \frac{\nu}{r}\right)v|u\right\rangle. \end{aligned} \tag{1.3}$$

Therefore,

$$\begin{aligned} \left\langle\Phi|\hat{H}|\Phi\right\rangle &= \frac{\hbar^2}{2m}\int_0^\infty \left|\frac{du}{dr} - \frac{\nu}{r}u\right|^2 dr \\ &\geq 0. \end{aligned} \tag{1.4}$$

This shows that equation (1.1) does not have negative energy solutions for $-\frac{1}{4} < a < 0$. For $a < -\frac{1}{4}$, however, negative energy solutions exist but the quantum system is anomalous. The negative energy normalizable solution $\Phi_\kappa(r)$ corresponding to the energy $-\frac{\hbar^2}{2m}\kappa^2$ is given by [15],

$$\Phi_\kappa(r) = \kappa\sqrt{\frac{2\sinh(\pi(-a-\frac{1}{4}))}{\pi(-a-\frac{1}{4})}}\frac{K_{i(-a-\frac{1}{4})}(\kappa r)}{\sqrt{r}}, \tag{1.5}$$

where $K_{i(-a-\frac{1}{4})}$ denotes the modified Bessel function of order $i(-a-\frac{1}{4})$. The allowed values of κ, as usual, are to be determined by the boundary condition that the wavefunction vanishes at the origin. As $r \to 0$, for a real g [16, 15],

$$K_{ig}(\kappa r) \approx -\sqrt{\frac{\pi}{g\sinh(\pi g)}}\ \sin\{g\ln\left(\frac{\kappa r}{2}\right) - arg\Gamma(1+ig)\}. \tag{1.6}$$

Evidently, as $r \to 0$, the wavefunction goes through infinitely many nodes hinting the existence of infinitely many bound states of even lower energies. As we have already discussed the system is, therefore, unstable. However, renormalizing the potential by modifying its short range part, it is possible to show that it supports infinitely many negative energy states as $a \to -\frac{1}{4}$ from the left, that is $E \to 0$ from the negative side [15]. The successive energies are related by,

$$\frac{E_{n+1}}{E_n} = e^{\frac{-2\pi}{(-a-\frac{1}{4})}}. \tag{1.7}$$

For $a < -\frac{1}{4}$, even the positive energy (scattering) states show unusual features. The general solution of equation (1.1) is given by,

$$u_k(r) = \sqrt{r}[AH^{(1)}_{i(-a-\frac{1}{4})} + BH^{(2)}_{i(-a-\frac{1}{4})}], \tag{1.8}$$

where $H^{(1)}$ and $H^{(2)}$ are Hankel functions, $k = \sqrt{\frac{2m}{\hbar^2}E}$ [15]. The boundary condition $u_k(0) = 0$ does not determine the ratio $\frac{A}{B}$. As discussed in [15], as a consequence there is no formula for the phase shift of the scattered wave $(\delta(k))$ and the probability conservation is not implied.

2 Critical Electric Dipole Moment

As pointed out in chapter 1, an electric dipole moment must have a minimum value in order to bind a charged particle. The critical dipole moment (p_c) is the minimum dipole moment required to bind a particle. It may be found analytically. In this chapter, to test our variational method in absence of the magnetic field, we calculate the critical dipole moment of both the point and the finite electric dipole. A few higher dipole moments, which also allow for zero-energy bound states, are also obtained. For a finite dipole (Figure 1), the dipole moment is defined as $\vec{p} = 2d\, Q\hat{z}$, where Q denotes the magnitude of charge at each pole and 2d is the separation between them. For a point dipole, $d \to 0$ and $Q \to \infty$, keeping the dipole moment p finite (Figure 2). Such a situation is an idealization. The critical value p_c depends on the charge q and the mass m of the particle, but only in the combination $p_c mq$ [12, 18]. We therefore use the dimensionless quantity,

$$\lambda = \frac{2m}{\hbar^2}\frac{pq}{4\pi\epsilon_0}, \tag{2.1}$$

throughout this chapter. We obtain the critical value of λ, denoted by λ_c. Our method reproduces the known result [12] that the critical dipole moment does not depend on the short range regularization methods of the inverse square potential [15, 16]. It therefore is the same for both, the point dipole and the finite dipole [12, 18]. In passing we also show that in two dimensions any value of the electric dipole moment binds the charged particle [18].

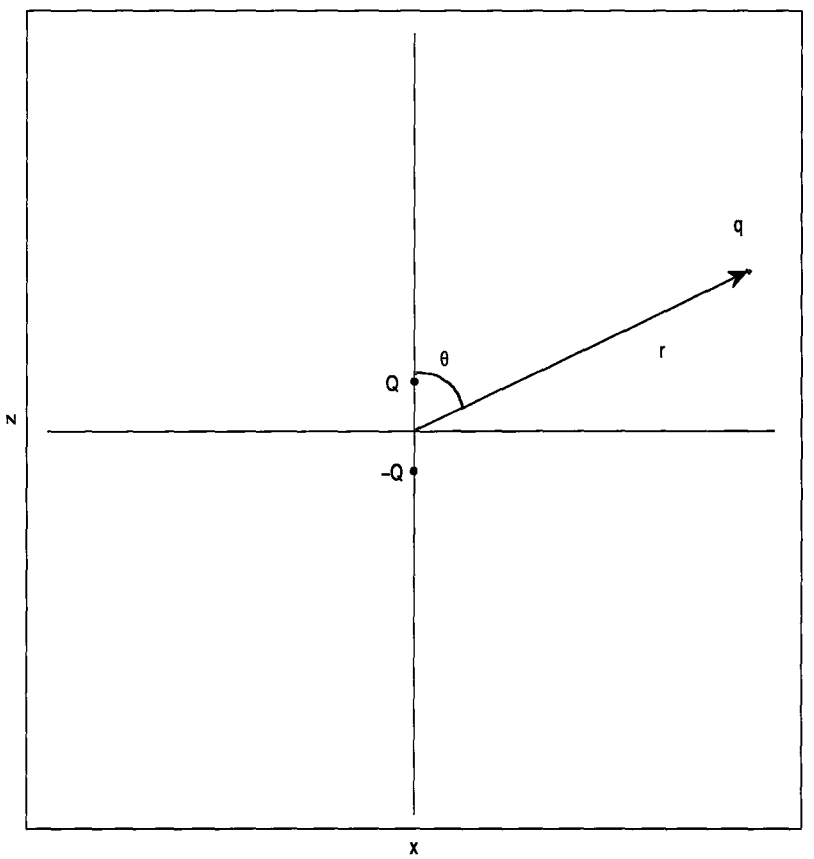

Figure 1: The charge q at (r, θ) in the presence of a finite dipole centered at the origin.

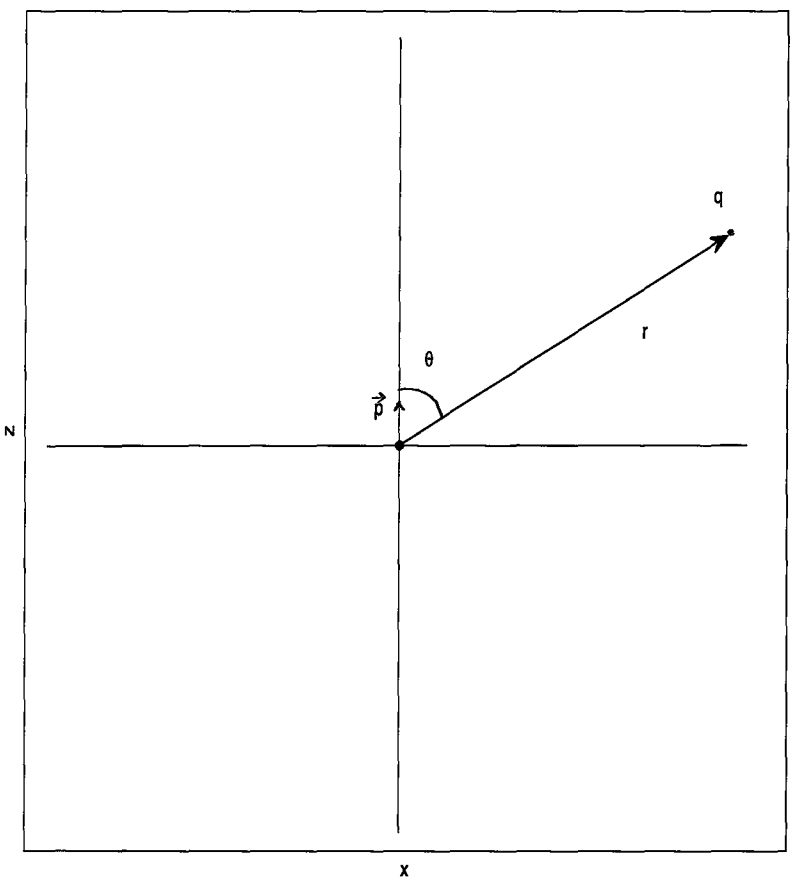

Figure 2: The charge q at (r, θ) in the presence of a point dipole $\vec{p}$ at the origin.

2.1 The Point Dipole

2.1.1 The Critical Dipole Moment

First we consider a point electric dipole. As shown in Figure 2, we assume that the dipole moment $\vec{p} = p\hat{z}$ and $p > 0$. A point charge (q) at position $\vec{r}$, in the presence of a stationary point dipole (Figure 2), experiences a potential V_p (the subscript p stands for the point dipole) given by,

$$V_p(r,\theta) = \frac{pq}{4\pi\epsilon_0}\frac{\cos\theta}{r^2}. \tag{2.2}$$

In spherical polar coordinates the Hamiltonian of the charged particle has azimuthal symmetry, and is given by

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \frac{pq}{4\pi\epsilon_0}\frac{\cos\theta}{r^2}. \tag{2.3}$$

The sign of q may be arbitrarily chosen. We note that changing the sign of q changes the sign of the potential energy term in the Hamiltonian. Reversing the orientation of the dipole moment $\vec{p}$, that is assuming $\vec{p'} = -p\hat{z}$, the new potential $V_p'(r,\theta)$ becomes,

$$V_p'(r,\theta) = \frac{pq}{4\pi\epsilon_0}\frac{\cos(\pi-\theta)}{r^2} = -\frac{pq}{4\pi\epsilon_0}\frac{\cos\theta}{r^2} = -V_p(r,\theta).$$

Thus changing the sign of q or reversing the orientation of the dipole moment both have the same effect on the Hamiltonian. It follows that changing the sign of q and reversing the orientation of the dipole moment simultaneously leave the Hamiltonian unaltered. From physical considerations it is clear

that each of these should not affect the energy eigenvalue and hence also the critical dipole moment. As will be discussed, a similar situation occurs in the case of a finite dipole. We comment (comment b) on this issue in detail at the end of this section. We consider λ to be positive throughout the section unless otherwise mentioned. Because of the azimuthal symmetry m_l is a good quantum number, although l-values get mixed. Since we are interested in the ground state supported by the critical dipole moment, we may take the azimuthal quantum number $m_l = 0$. We consider the following trial wave function with $m_l = 0$,

$$\Psi(r,\theta) = \frac{1}{\sqrt{2\pi}}\Phi(r)\,\Theta(\theta). \tag{2.4}$$

We expand $\Theta(\theta)$ in terms of Legendre polynomials, truncating the series after the first three terms for simplicity. In this approximation,

$$\Theta(\theta) = N_2\left(P_0(\cos\theta) + \alpha_1 P_1(\cos\theta) + \alpha_2 P_2(\cos\theta)\right). \tag{2.5}$$

The normalization constant N_2 is given by,

$$N_2 = \sqrt{\frac{15}{2\left(15 + 5\alpha_1^2 + 3\alpha_2^2\right)}}. \tag{2.6}$$

The ground state wavefunction, given by equation (2.4), is real. Without loss of generality, we assume that the variational parameters α_1 and α_2 are real. We perform a variation with respect to the radial wavefunction $\Phi(r)$,

without specifying its form :

$$\delta\left(\langle\Psi|\hat{H}-E_0|\Psi\rangle\right)=0, \tag{2.7}$$

where E_0 is the ground state energy eigenvalue of $\hat{H}$. This gives the following equation.

$$\delta\left(\int_0^\infty r^2 dr I\right)=0, \tag{2.8}$$

where I is given by

$$I=\frac{\hbar^2}{2m}\left(\left(\frac{\partial\Phi}{\partial r}\right)^2+\frac{10\alpha_1^2+18\alpha_2^2}{15+5\alpha_1^2+3\alpha_2^2}\frac{\Phi^2}{r^2}\right)+\frac{pq}{4\pi\epsilon_0}\frac{4\alpha_1\alpha_2+10}{15+5\alpha_1^2+3\alpha_2^2}\frac{\Phi^2}{r^2}-E_0\Phi^2. \tag{2.9}$$

Using the Euler-Lagrange equation,

$$\frac{\partial}{\partial r}\frac{\partial(r^2I)}{\partial\Phi'}-\frac{\partial(r^2I)}{\partial\Phi}=0, \tag{2.10}$$

where $\Phi'=\dfrac{d\Phi}{dr}$, we obtain,

$$-\frac{\hbar^2}{2m}\frac{d}{dr}\left(r^2\Phi'\right)+\left(\frac{\hbar^2}{2m}\frac{10\alpha_1^2+18\alpha_2^2}{15+5\alpha_1^2+3\alpha_2^2}+\frac{pq}{4\pi\epsilon_0}\frac{4\alpha_1\alpha_2+10}{15+5\alpha_1^2+3\alpha_2^2}\right)\Phi=E_0r^2\Phi. \tag{2.11}$$

With $u(r)=r\Phi(r)$ the above equation simplifies to the following,

$$-\frac{d^2}{dr^2}u+\frac{2m}{\hbar^2}\tilde{V_p}(r)u=\frac{2m}{\hbar^2}E_0u. \tag{2.12}$$

The effective potential $\tilde{V_p}(r)$ (where the subscript p stands for the point dipole) is given by,

$$\tilde{V_p}(r) = \left(\frac{\hbar^2}{2m}\frac{10\alpha_1^2 + 18\alpha_2^2}{15 + 5\alpha_1^2 + 3\alpha_2^2} + \frac{pq}{4\pi\epsilon_0}\frac{4\alpha_1\alpha_2 + 10}{15 + 5\alpha_1^2 + 3\alpha_2^2}\right)\frac{1}{r^2}. \tag{2.13}$$

As we have discussed in the previous chapter, for a zero energy bound state the coefficient of $\frac{1}{r^2}$ in $\tilde{V_p}(r)$ must be $-\frac{1}{4}$ [15, 16]. This leads to the following equation.

$$\frac{10\alpha_1^2 + 18\alpha_2^2}{15 + 5\alpha_1^2 + 3\alpha_2^2} + \lambda\frac{4\alpha_1\alpha_2 + 10}{15 + 5\alpha_1^2 + 3\alpha_2^2} = -\frac{1}{4}, \tag{2.14}$$

where $\lambda = \frac{2m}{\hbar^2}\frac{pq}{4\pi\epsilon_0}$ as defined before. Simplifying,

$$45\alpha_1^2 + 75\alpha_2^2 + 16\lambda\alpha_1\alpha_2 + 40\lambda\alpha_1 + 15 = 0, \tag{2.15}$$

or,

$$\alpha_1 = \frac{1}{90}\left(-40\lambda - 16\lambda\alpha_2 \pm \sqrt{256\lambda^2\alpha_2^2 - 13500\alpha_2^2 + 1280\lambda^2\alpha_2 + 1600\lambda^2 - 2700}\right). \tag{2.16}$$

Since there is only one zero energy bound state, the variational parameters α_1 and α_2 must be unique. For a unique value of α_1 the discriminant must vanish, which yields a quadratic equation in α_2. This implies that

$$256\lambda^2\alpha_2^2 - 13500\alpha_2^2 + 1280\lambda^2\alpha_2 + 1600\lambda^2 - 2700 = 0. \tag{2.17}$$

Therefore,

$$\alpha_2 = \frac{(5(-32\lambda^2 \pm 9\sqrt{-1125 + 688\lambda^2}))}{(-3375 + 64\lambda^2)}. \tag{2.18}$$

For unique α_2,

$$688\lambda^2 - 1125 = 0. \tag{2.19}$$

We also note that equations (2.16) and (2.17) together imply that α_1 changes sign with the sign of λ. However, from (2.18), (2.19) and (2.16), α_2 remains the same even if λ undergoes a sign change. Denoting the critical value of λ by λ_c, therefore,

$$\lambda_c = \sqrt{\frac{1125}{688}} = \frac{15}{4}\sqrt{\frac{5}{43}} \approx 1.27874, \tag{2.20}$$

(considering the positive sign only) or,

$$p_c = \frac{\hbar^2}{2m}\frac{4\pi\epsilon_0}{q}\lambda_c = 1.27874\frac{\hbar^2}{2m}\frac{4\pi\epsilon_0}{q}. \tag{2.21}$$

The corresponding values of the variational parameters are given by

$$\begin{aligned} \alpha_1 &= -\sqrt{\frac{43}{125}} \approx -0.5865 \\ \alpha_2 &= \frac{2}{25} = 0.0800. \end{aligned} \tag{2.22}$$

From equation 2.21, in atomic unit the critical dipole moment ($p_c = \frac{\lambda_c}{2}$) required to bind an electron is 0.63937 which is about 1.625 D. As should be evident from the analytical solution [12, 18], the critical dipole moment is determined by the angular part of the wavefunction assuming that the coefficient of $\frac{\hbar^2}{2mr^2}$ in the radial equation is $-\frac{1}{4}$. In our method the variational parameters in the angular part of the wavefunction determine the critical dipole moment. Considering more terms in the angular part of the trial

n	λ_c
1	1.2990381057
2	1.2787393865
3	1.2786299390
4	1.2786297545
5	1.2786297544

Table 1: The highest order of the Legendre polynomial (n) in the trial wavefunction and the corresponding λ_c

wavefunction yields lower values of λ_c. Table 1 lists the highest order of the Legendre polynomial (n) in the angular part of the trial wavefunction and the corresponding λ_c obtained by our method. For given n the corresponding $\Theta(\theta)$ is given by,

$$\Theta(\theta) = N_n \Sigma_{i=1}^{n} (1 + \alpha_i P_i(\cos\theta)). \tag{2.23}$$

N_n is the corresponding normalization constant. It is not surprising that our λ_c is very close to the very accurate value (1.2786297544 up to ten decimal places) obtained in reference [18]. This is because the angular part of the trial wave function closely resembles the actual wavefunction for the zero energy state [12, 18]. For the critical value λ_c, the minimum of the strength of $\frac{2m}{\hbar^2}\tilde{V}_p(r)$ in equation (2.12),

$$\frac{10\alpha_1^2 + 18\alpha_2^2}{15 + 5\alpha_1^2 + 3\alpha_2^2} + \lambda \frac{4\alpha_1\alpha_2 + 10}{15 + 5\alpha_1^2 + 3\alpha_2^2},$$

goes to $-\frac{1}{4}$. With $\lambda = 1.27874$, we numerically minimized this and obtained exactly $-\frac{1}{4}$. The corresponding values of the variational parameters, up to four decimal places, are given by, $\alpha_1 = -.5865$ and $\alpha_2 = .0800$. This is shown in figures 3 and 4. In figures 3 and 4, we plot the strength of the effective

potential with the critical dipole moment against the variational parameters α_1 and α_2 respectively.

As shown in Figure 5, the minimum value of the coefficient of the $\frac{1}{r^2}$ in the effective potential, when minimized with respect to α_1 and α_2 for a given λ, decreases with increasing λ. However, since for a point dipole the effective potential is purely inverse square, no negative energy state exists for $\lambda > \lambda_c$ [12, 15]. For specific dipole moments, which are higher than the critical value, zero energy bound states do exist. We proceed to obtain a few of these using our method in the next subsection.

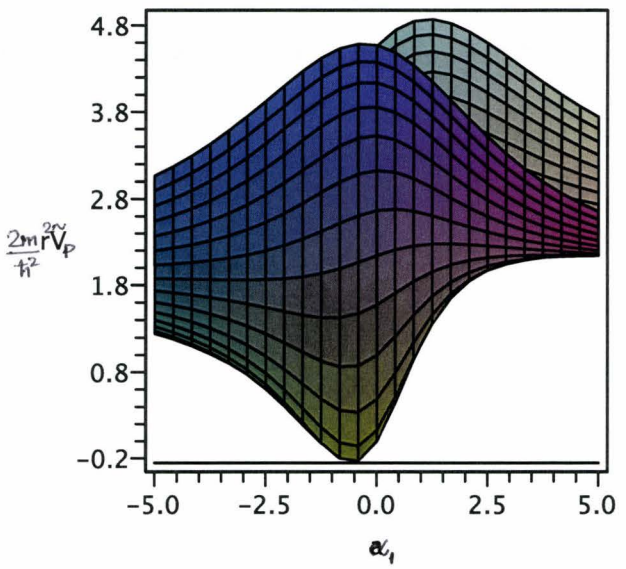

Figure 3: $\frac{2m}{\hbar^2}r^2\tilde{V}_p$ with $\lambda = \lambda_c$ vs. α_1. The effective potential $\tilde{V}_p$ is defined in equation (2.13) with λ replaced by λ_c. The graph shows the projection of the 3D plot $\frac{2m}{\hbar^2}r^2\tilde{V}_p$ vs. α_1 and α_2.

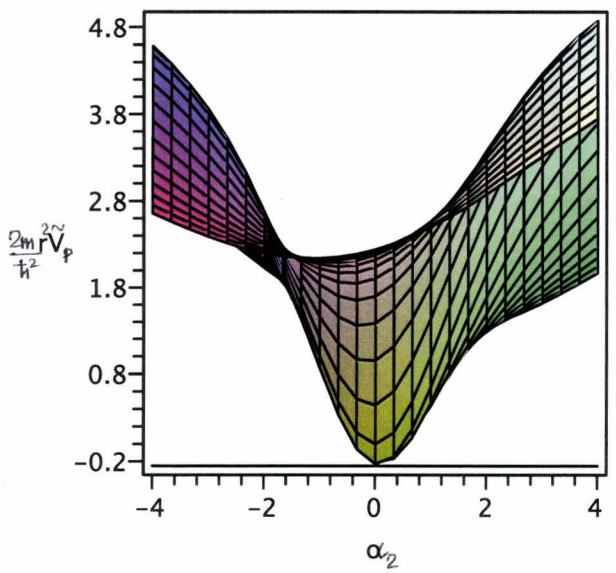

Figure 4: $\frac{2m}{\hbar^2}r^2\tilde{V}_p$ with $\lambda = \lambda_c$ vs. α_2. The graph shows the projection of the 3D plot $\frac{2m}{\hbar^2}r^2\tilde{V}_p$ vs. α_1 and α_2.

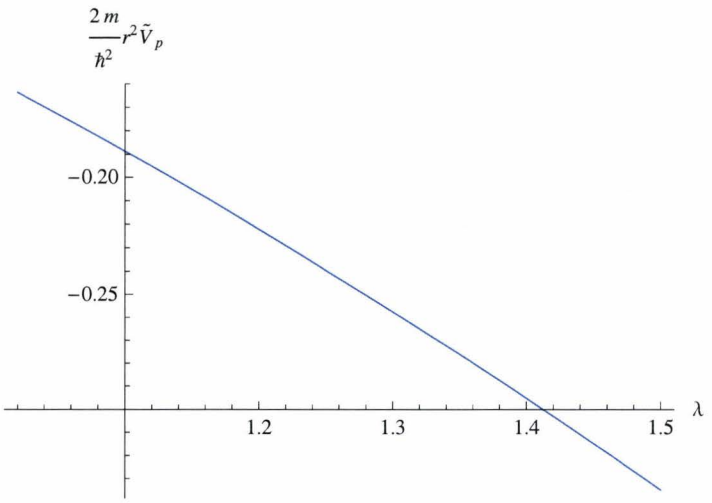

Figure 5: The minimum of $\frac{2m}{\hbar^2} r^2 \tilde{V}_p$ with respect to the variational parameters α_1 and α_2 vs. the corresponding λ.

2.1.2 Larger Dipole Moments Supporting Zero Energy Bound States

Now we obtain a few of the dipole moments which are greater than the critical dipole moment but which also support a zero energy bound state. We then compare the values we obtain with the values obtained in references [12, 19]. First we consider the bound states with azimuthal quantum number $m_l = 0$. From the analytical solution it may be evident that we need to consider more Legendre polynomials in the angular part of the trial wavefunction to get a few higher values of λ. To keep calculations simple we assume that $n = 5$ in equation (2.25). As before, assume that the wavefunction is given by,

$$\Psi(r,\theta) = \frac{1}{\sqrt{2\pi}}\Phi(r)\Theta(\theta), \tag{2.24}$$

$$\Theta(\theta) = N_n\left(1 + \Sigma_{i=1}^{n}\alpha_i P_i(\cos\theta)\right), \tag{2.25}$$

with N_n being the corresponding normalization constant. For n = 2 we had obtained only one value of λ supporting a zero energy bound state. As before, we perform a variation of $\langle\Psi|\hat{H} - E_0|\Psi\rangle$ with respect to the radial part of the wavefunction, $\Phi(r)$,

$$\delta\langle\Psi|\hat{H} - E_0|\Psi\rangle = 0.$$

With $u(r) = r\Phi(r)$, the Euler-Lagrange equation now gives,

$$-\frac{d^2}{dr^2}u(r) + \frac{2m}{\hbar^2}\tilde{V}_p(r)u(r) = \frac{2m}{\hbar^2}E_0 u(r), \tag{2.26}$$

(for a detailed calculation see appendix A). The modified effective potential $\tilde{V}_p(r)$ is given by,

$$\begin{aligned}\tilde{V}_p(r) = &\frac{\hbar^2}{2m}\frac{(2310\alpha_1^2 + 4158\alpha_2^2 + 5940\alpha_3^2 + 7700\alpha_4^2 + 9450\alpha_5^2)}{1155\alpha_1^2 + 693\alpha_2^2 + 5\,(693 + 99\alpha_3^2 + 77\alpha_4^2 + 63\alpha_5^2)}\frac{1}{r^2} \\ &+\frac{\hbar^2}{2m}\frac{(462\alpha_1(5+2\alpha_2) + 594\alpha_2\alpha_3 + 440\alpha_3\alpha_4 + 350\alpha_4\alpha_5)\lambda}{1155\alpha_1^2 + 693\alpha_2^2 + 5\,(693 + 99\alpha_3^2 + 77\alpha_4^2 + 63\alpha_5^2)}\frac{1}{r^2}.\end{aligned} \tag{2.27}$$

For a zero energy bound state $E_0 = 0$, we demand that the coefficient of $\frac{1}{r^2}$ in equation (2.26) to be equal to $-\frac{1}{4}$. Therefore,

$$\begin{aligned}&\frac{(2310\alpha_1^2 + 4158\alpha_2^2 + 5940\alpha_3^2 + 7700\alpha_4^2 + 9450\alpha_5^2)}{1155\alpha_1^2 + 693\alpha_2^2 + 5\,(693 + 99\alpha_3^2 + 77\alpha_4^2 + 63\alpha_5^2)} \\ &+\frac{(462\alpha_1(5+2\alpha_2) + 594\alpha_2\alpha_3 + 440\alpha_3\alpha_4 + 350\alpha_4\alpha_5)\lambda}{1155\alpha_1^2 + 693\alpha_2^2 + 5\,(693 + 99\alpha_3^2 + 77\alpha_4^2 + 63\alpha_5^2)} = -\frac{1}{4}.\end{aligned} \tag{2.28}$$

Now we claim that for a non-degenerate zero energy bound state the variational parameters must be unique. Solving for the variational parameter α_1 from the above equation and demanding the discriminant to be zero, we get

$$\alpha_1 = \frac{1}{20790}\left(-9240\lambda - 3696\alpha_2\lambda\right). \tag{2.29}$$

Following similar arguments, as discussed in the previous subsection (2.1.1), for the other variational parameters α_i, $i \in 2, 3, 4, 5$, we obtain,

$$\alpha_2 = \frac{35640\alpha_3\lambda - 24640\lambda^2}{2\left(-259875 + 4928\lambda^2\right)}, \tag{2.30}$$

$$\alpha_3 = \frac{8316000\alpha_4\lambda + 532224\lambda^3 - 157696\alpha_4\lambda^3}{2\left(-114604875 + 2558160\lambda^2\right)}, \tag{2.31}$$

$$\alpha_4 = \frac{9(-23152500\alpha_5\lambda + 516800\alpha_5\lambda^3 + 67584\lambda^4)}{11\,(843908625 - 19701360\lambda^2 + 16384\lambda^4)}, \tag{2.32}$$

$$\alpha_5 = \frac{-450560\lambda^5}{21\,(17829244125 - 423580320\lambda^2 + 510208\lambda^4)}. \tag{2.33}$$

We note that equations (2.29), (2.31) and (2.33) imply that α_1, α_3 and α_5 change signs with λ. However equations (2.30), (2.32) imply that α_2 and α_4 remain the same even if λ changes sign. Obviously it is required that the denominators in the expressions obtained for the variational parameters are non-zero. For unique α_5, we obtain the following solutions for λ,

$$\lambda = \{\pm 57.167, \pm 34.0293, \pm 15.1034, \pm 6.66936, \pm 1.27863\}. \tag{2.34}$$

However, among these values $\pm 34.0293, \pm 6.66936$ are the roots of the following equation which appears in the denominator of α_4,

$$843908625 - 19701360\lambda^2 + 16384\lambda^4 = 0. \tag{2.35}$$

Thus these correspond to the singularities of the coefficient α_4. Eliminating these values from the list we obtain the first three values of λ which support zero-energy bound states,

$$\lambda = \{\pm 57.167, \pm 15.1034, \pm 1.27863\}. \tag{2.36}$$

As may be evident, these values of λ may also be obtained by substituting the expressions for α_1,α_2,α_3,α_4,α_5 obtained above in equation (2.28). The detailed calculation is shown in appendix A. The corresponding values of the

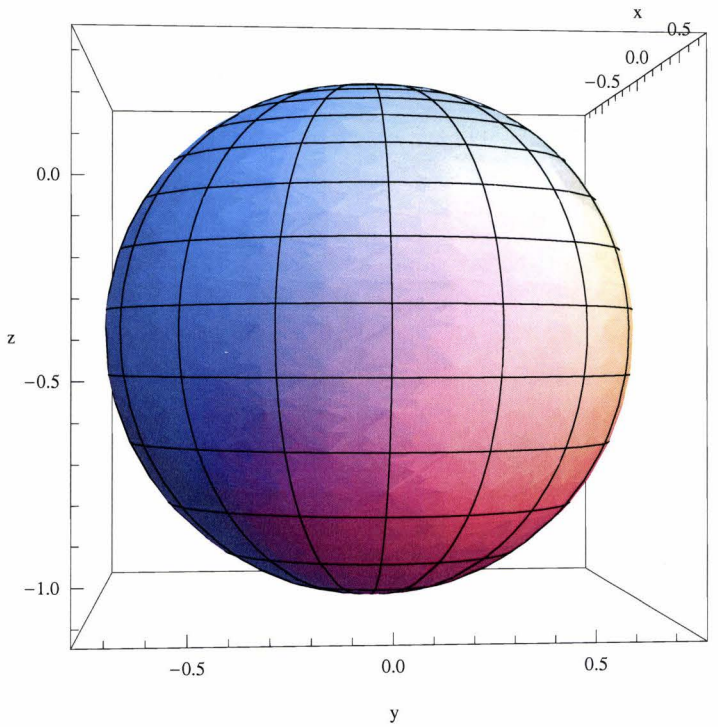

Figure 6: A 3D plot of $\Theta(\theta)$ given by equation (2.25) corresponding to $\lambda = 1.27863$.

variational parameters, rounded up to the fourth decimal place, are tabulated in Table 2. $\Theta(\theta)$ corresponding to $\lambda = 1.27863$ and $\lambda = 15.1034$ are plotted in figures 6 and 7 respectively.

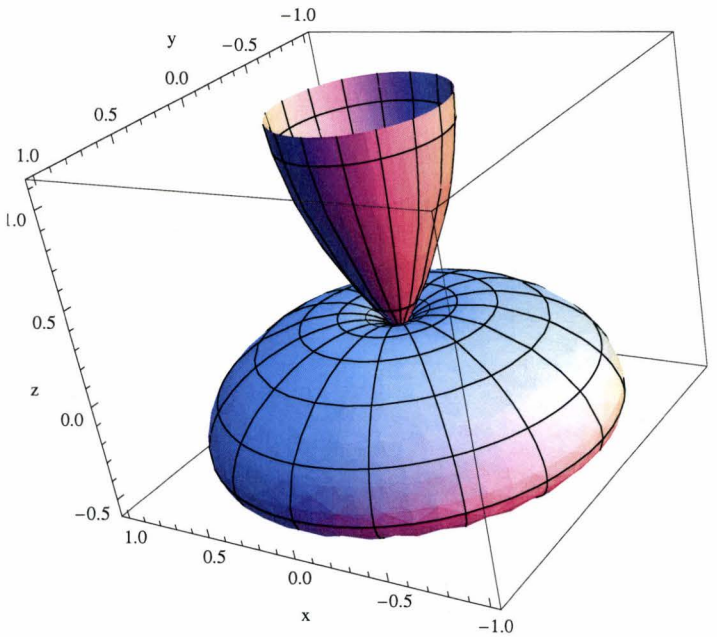

Figure 7: A 3D plot of $\Theta(\theta)$ given by equation (2.25) corresponding to $\lambda = 15.1034$.

λ	α_1	α_2	α_3	α_4	α_5
1.27863	-0.5867	0.0804	-0.0050	0.0002	-0.0000
15.1034	-0.0497	-2.4815	2.4733	-1.16353	0.3227
57.167	-0.0131	-2.4987	0.6578	3.0561	-3.2086

Table 2: The lowest three values of λ which support zero-energy bound states for $m_l = 0$ and the corresponding variational parameters.

n	λ'
1	-
2	-
3	17.5306
4	15.2899
5	15.1034

Table 3: The highest order of the Legendre polynomial in $\Theta(\theta)$ and the corresponding λ'

Comparing the values of λ with the accurate values (rounded off to appropriate significant figures) 1.27863, 15.0939, 42.6018 respectively [12], we find that while the critical value 1.27863 is very accurate and the next higher value 15.1034 is close, but the highest value 57.167 is poor. The increasing values of $|\alpha_{2i}|$ for $i \in \{1,2\}$ and $|\alpha_{2j+1}|$ for $j \in \{0,1,2\}$ corresponding to $\lambda = 57.167$ indicate this as well. Also, even higher values of λ's start appearing as we consider more Legendre polynomials in the trial wavefunction. As an example, in Table 3, we tabulate the highest order of the Legendre polynomial (n) in the trial wavefunction and the corresponding values obtained for the second lowest value of λ, denoted by λ', which supports a zero-energy bound state. For a higher value of λ supporting a zero-energy bound state, the contribution from the kinetic term (the first term in the R.H.S of equation 2.27) in the coefficient of $\frac{\hbar^2}{2mr^2}$ in equation (2.27) increases. However, this is compensated by a decreasing contribution from the potential term (the

second term in the R.H.S of equation (2.27)), satisfying equation (2.28). In Table 4 we tabulate the contributions from the kinetic term (say $\langle V_k \rangle$) and that from the potential term (say $\langle V_\lambda \rangle$) in the coefficient of $\frac{\hbar^2}{2mr^2}$ for different values of λ we have obtained above. Evidently $\langle V_\lambda \rangle$ is the coefficient of $\frac{\hbar^2}{2mr^2}$ in the expectation value of V_p with respect to the angular part $\Theta(\theta)$ and $\langle V_k \rangle$ is the coefficient of $\frac{\hbar^2}{2mr^2}$ in the expectation value of $\hat{p}^2$ with respect to the angular part $\Theta(\theta)$.

λ	$\langle V_k \rangle$	$\langle V_\lambda \rangle$	$\langle V_k \rangle + \langle V_\lambda \rangle$
1.27863	0.212531	-0.462531	-0.25
15.1034	6.48167	-6.73167	-0.25
57.167	13.3201	-13.5701	-0.25

Table 4: The contribution of the kinetic term and the potential term in the coefficient of $\frac{\hbar^2}{2mr^2}$ in the equation (2.27) and the corresponding λ.

We also obtain the lowest two values of λ, for $m_l = 1$ and $m_l = 2$, which support a zero-energy bound state, using our method demonstrated above. We denote these by λ_{m_l} and λ'_{m_l} respectively. We assume the trial wave functions for each m_l as,

$$\Psi(r, \theta, \phi) = \frac{1}{\sqrt{2\pi}} \Phi(r) \Theta(\theta) e^{i m_l \phi}, \tag{2.37}$$

where,

$$\Theta(\theta) = N_n (P_{m_l}^{m_l}(\cos\theta) + \Sigma_{i=1}^{n} \alpha_i P_{i+m_l}^{m_l}(\cos\theta)). \tag{2.38}$$

$P_{i+m_l}^{m_l}$ is the associated Legendre polynomial, N_n is the normalization constant. As before, we also assume the variational parameters to be real. Again we take $n = 5$. In Table 5 we display our result. The accurate values ob-

tained in [12] approximated to the fourth decimal place are mentioned in parentheses for comparison. The details of the calculations for $m_l = 1$ and

m_l	λ_{m_l}	λ'_{m_l}
1	7.5839(7.5839)	28.3094(28.2242)
2	19.0581(19.0581)	47.2378(46.7971)

Table 5: The lowest two values of λ which support zero-energy bound states for $m_l = 1$ and $m_l = 2$.

$m_l = 2$ are given in appendices B and C respectively.

2.1.3 Absence of the Critical Dipole Moment in Two Dimensions

We apply our method to show the absence of any critical dipole moment for a point electric dipole in two dimensions [18]. Using only one parameter α_1, the radial equation for a zero-energy bound state is given by,

$$-\frac{d^2u}{dr^2} + \left(\frac{\alpha_1^2 + 2\alpha_1\lambda}{2+\alpha_1^2} - \frac{1}{4}\right)\frac{u}{r^2} = 0. \tag{2.39}$$

For a zero energy bound state the coefficient of $\frac{1}{r^2}$ has to be $-\frac{1}{4}$ [15, 16]. Therefore,

$$\left(\frac{\alpha_1^2 + 2\alpha_1\lambda}{2+\alpha_1^2} - \frac{1}{4}\right) = -\frac{1}{4}$$

$$\Rightarrow \alpha_1^2 + 2\alpha_1\lambda = 0, \tag{2.40}$$

or,

$$\alpha_1 = -\lambda \pm \lambda. \tag{2.41}$$

For the critical dipole moment, we claim that there will be a unique ground state. Hence the discriminant of the above equation must vanish. Therefore, $\lambda_c = 0$. It is known that in two dimensions any attractive potential has a bound state. So this result is expected [18].

2.2 The Finite Dipole

Now we consider a finite electric dipole (Figure 1). We assume that the dipole is rigid and stationary. Hence the kinetic energy of the dipole is neglected. The dipole moment $\vec{p} = p\hat{z}$. For a charged particle, with mass m and charge q, in the finite electric dipole potential V_f (the subscript f stands for finite dipole) is given by,

$$V_f(r,\theta) = \frac{Qq}{4\pi\epsilon_0}\left(\frac{1}{\sqrt{r^2+d^2-2rd\cos\theta}} - \frac{1}{\sqrt{r^2+d^2+2rd\cos\theta}}\right). \quad (2.42)$$

In the above 2 d is the separation between the charges $\pm Q$ in the dipole. The Hamiltonian for the charged particle is

$$\hat{H} = \frac{-\hbar^2}{2m}\nabla^2 + V_f(r,\theta).$$

Here we note that unlike the point dipole potential V_p, at short range V_f is well behaved. As $r \to 0$, $V_f \to 0$. Unlike the case of a point dipole, the Hamiltonian above is not scale invariant any more and there is no anomaly. Hence for $p > p_c$ negative energy bound states exist. The sign of q may be arbitrary. We note, however, that a change in the sign of q also changes

the sign of the potential. For $Q > 0$, the dipole moment is aligned along the positive z axis (Figure 1). Interchanging the positions of +Q and -Q reverses the orientation of the dipole moment. In that case denoting the dipole moment by $\vec{p'}$, $\vec{p'} = -p\hat{z}$ in spherical polar coordinates. The potential $V_f'(r)$ becomes,

$$\begin{aligned} V_f'(r,\theta) &= \frac{Qq}{4\pi\epsilon_0}\left(\frac{1}{\sqrt{r^2+d^2-2rd\cos(\pi-\theta)}} - \frac{1}{\sqrt{r^2+d^2+2rd\cos(\pi-\theta)}}\right) \\ &= -\frac{Qq}{4\pi\epsilon_0}\left(\frac{1}{\sqrt{r^2+d^2-2rd\cos\theta}} - \frac{1}{\sqrt{r^2+d^2+2rd\cos\theta}}\right) \\ &= -V_f(r,\theta)\,. \end{aligned} \tag{2.43}$$

Thus, similar to the case of the point dipole, changing the sign of q and reversing the orientation of the dipole moment both have the same effect on the Hamiltonian. This means that changing the sign of q and reversing the orientation of the dipole moment simultaneously leaves the Hamiltonian unaltered. From physical considerations it is clear that each of these operations should not have any effect on the energy eigenvalue and hence also on the critical dipole moment. In comment (b) we discuss this issue in detail for both the point and the finite dipole. Following an argument by Connolly and Griffiths [18], we first show that for a finite electric dipole, the occurrence of a zero energy bound state of a charged particle depends only on the dipole

moment. The Schrodinger equation, at energy E, reads,

$$\frac{-\hbar^2}{2m}\nabla^2\Psi(r,\theta)+\frac{Qq}{4\pi\epsilon_0}\left(\frac{1}{\sqrt{r^2+d^2-2rd\cos\theta}}-\frac{1}{\sqrt{r^2+d^2+2rd\cos\theta}}\right)\Psi(r,\theta) = E\Psi(r,\theta). \tag{2.44}$$

Multiplying both sides by $\frac{2m}{\hbar^2}d^2$ we get,

$$-\tilde{\nabla}^2\Psi(\tilde{r},\theta)+\frac{\lambda}{2}\left(\frac{1}{\sqrt{\tilde{r}^2+1-2\tilde{r}\cos\theta}}-\frac{1}{\sqrt{\tilde{r}^2+1+2\tilde{r}\cos\theta}}\right)\Psi(\tilde{r},\theta) = \frac{2m}{\hbar^2}d^2E\Psi(\tilde{r},\theta), \tag{2.45}$$

where, $\tilde{r}=\frac{r}{d}$. The above equation clearly implies that the presence of a zero energy bound state depends only on the product p= 2d Q. We denote the critical dipole moment by p_c and the corresponding value of λ by λ_c as before. For $p = p_c$ and hence for $\lambda = \lambda_c$, the ground state energy becomes zero. The above argument thus shows that the critical dipole moment is independent of the charge separation of the dipole. Though d is assumed to be non-zero in this case, this hints that the critical dipole moment is the same for point and finite dipoles.

We now obtain the critical dipole moment of a finite dipole using our method. For the ground state (or for s-wave states in general), with $m_l = 0$,

$$\hat{H}=\frac{-\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right)+V_f(r,\theta). \tag{2.46}$$

We consider the following trial wave function.

$$\Psi(r,\theta) = \frac{1}{\sqrt{2\pi}}\Phi(r)\Theta(\theta), \tag{2.47}$$

where,

$$\Theta(\theta) = N_2(P_0(\cos\theta) + \alpha_1 P_1(\cos\theta) + \alpha_2 P_2(\cos\theta)). \tag{2.48}$$

As we will discuss in comment b, the potential $V_f(r,\theta)$ (equation (2.42)) only includes Legendre polynomials of odd orders. Hence, in $\langle\Psi|V_f|\Psi\rangle$, it couples even and odd Legendre polynomials in $\Theta(\theta)$. Therefore we keep Legendre polynomials of both even and odd orders in the trial wavefunction. This issue has been discussed in detail in the next chapter. As before, we assume α_1 and α_2 to be real. The normalization constant N_2 is given by equation (2.6).

Now we consider,

$$\delta\langle\Psi|\hat{H} - E_0|\Psi\rangle = 0,$$

or,

$$\int_0^\infty r^2 dr I = 0, \tag{2.49}$$

where,

$$I = \frac{\hbar^2}{2m}\left(\frac{\partial\Phi}{\partial r}\right)^2 + (\tilde{V_f}(r) - E_0)\Phi^2. \tag{2.50}$$

The effective potential $\tilde{V_f}(r)$, for $r \leq d$ is,

$$\tilde{V_f}(r) = \frac{\hbar^2}{2m}\frac{2(5\alpha_1^2+9\alpha_2^2)}{15+5\alpha_1^2+3\alpha_2^2}\frac{1}{r^2} + \frac{\hbar^2}{2m}\frac{\lambda}{d^2}\left(\frac{(10\alpha_1+4\alpha_1\alpha_2)}{15+5\alpha_1^2+3\alpha_2^2}\frac{r}{d} + \frac{18}{7}\frac{\alpha_1\alpha_2}{15+5\alpha_1^2+3\alpha_2^2}\left(\frac{r}{d}\right)^3\right), \tag{2.51}$$

and for $r > d$ it is,

$$\tilde{V_f}(r) = \frac{\hbar^2}{2m}\frac{2(5\alpha_1^2+9\alpha_2^2)}{15+5\alpha_1^2+3\alpha_2^2}\frac{1}{r^2} + \frac{\hbar^2}{2m}\frac{\lambda}{d^2}\left(\frac{(10\alpha_1+4\alpha_1\alpha_2)}{15+5\alpha_1^2+3\alpha_2^2}\left(\frac{d}{r}\right)^2 + \frac{18}{7}\frac{\alpha_1\alpha_2}{15+5\alpha_1^2+3\alpha_2^2}\left(\frac{d}{r}\right)^4\right), \quad (2.52)$$

Note that the effective potential is continuous at r = d.

Using the Euler-Lagrange equation we get,

$$\frac{\partial}{\partial r}\frac{\partial(r^2 I)}{\partial \Phi'} - \frac{\partial(r^2 I)}{\partial \Phi} = 0, \quad (2.53)$$

where $\Phi'(r) = \frac{d}{dr}\Phi(r)$. With $\Phi(r) = \frac{u(r)}{r}$, $E_0 = 0$ we get,

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + \tilde{V_f}(r)\right)u(r) = 0. \quad (2.54)$$

Solving the above equation is not straight forward. However, for determining the critical value λ_c, this may be avoided. Let us consider the long range part of $\tilde{V_f}$. For $r \gg d$, in $\tilde{V_f}(r)$ evidently the $\frac{1}{r^2}$ term dominates. Multiplying the above equations by $\frac{2m}{\hbar^2}$ we get,

$$\left(-\frac{\partial^2}{\partial r^2} + \frac{2(5\alpha_1^2+9\alpha_2^2)}{15+5\alpha_1^2+3\alpha_2^2}\frac{1}{r^2} + \lambda\frac{(10\alpha_1+4\alpha_1\alpha_2)}{15+5\alpha_1^2+3\alpha_2^2}\frac{1}{r^2}\right)u(r) = 0 \quad (2.55)$$

This equation is the same radial equation obtained in case of the point dipole. This is a consequence of the fact that for large r a finite dipole may be well-approximated as a point dipole. For a normalizable solution, u(r) must vanish as $r \to \infty$. This equation has a normalizable solution only if

the coefficient of the $\frac{1}{r^2}$ is less than $-\frac{1}{4}$ [16, 18]. Hence for the critical dipole moment we obtain the following equation,

$$\frac{2(5\alpha_1^2+9\alpha_2^2)}{15+5\alpha_1^2+3\alpha_2^2}+\lambda\frac{(10\alpha_1+4\alpha_1\alpha_2)}{15+5\alpha_1^2+3\alpha_2^2}=-\frac{1}{4}. \tag{2.56}$$

Simplifying we get,

$$45\alpha_1^2+75\alpha_2^2+16\lambda\alpha_1\alpha_2+40\lambda\alpha_1+15=0, \tag{2.57}$$

or,

$$\alpha_2=-\frac{8}{75}\lambda\alpha_1\pm\frac{1}{75}\sqrt{64\lambda^2\alpha_1^2-3375\alpha_1^2-3000\lambda\alpha_1-1125.} \tag{2.58}$$

The critical dipole moment supports only one bound state. So the parameter α_2 must be unique. This implies that the discriminant of the above expression must vanish. Thus we get,

$$\frac{1}{75}\sqrt{64\lambda^2\alpha_1^2-3375\alpha_1^2-3000\lambda\alpha_1-1125}=0, \tag{2.59}$$

or,

$$64\lambda^2\alpha_1^2-3375\alpha_1^2-3000\lambda\alpha_1-1125=0. \tag{2.60}$$

This is a quadratic equation in α_1. By the same argument α_1 must also be unique. Hence the discriminant must vanish. This gives,

$$10320\lambda_c^2-16875=0, \tag{2.61}$$

or,

$$\lambda_c = \frac{15}{4}\sqrt{\frac{5}{43}} \approx 1.27874. \tag{2.62}$$

The corresponding values of α_1 and α_2 are given by,

$\alpha_1 = -\sqrt{\frac{45}{125}} \approx .5865, \quad \alpha_2 = .08.$

This value is close to the value of λ obtained in references [12, 18], which is 1.27863 (rounded up to the fifth decimal place).

As we have noticed, the long range part of the effective potential in case of the finite dipole is the same as the effective potential obtained for the point dipole. The critical dipole moment obtained in this case also becomes more accurate as we consider more P_l's in the trial wavefunction. Also, similar to the point dipole case, for the critical λ and hence for the critical dipole moment, the minimum of the coefficient of $\frac{1}{r^2}$,

$$\frac{10\alpha_1^2 + 18\alpha_2^2}{15 + 5\alpha_1^2 + 3\alpha_2^2} + \lambda\frac{4\alpha_1\alpha_2 + 10}{15 + 5\alpha_1^2 + 3\alpha_2^2},$$

goes to $-\frac{1}{4}$. Figures 2 and 3 illustrate this. We plot the coefficient of $\frac{1}{r^2}$ vs. α_1 and vs. α_2 respectively for $\lambda = \lambda_c$. With $\lambda = 1.27874$, we numerically minimized the coefficient and obtained exactly $-\frac{1}{4}$. As shown in Figure 5 above, for a given λ, the coefficient of $\frac{1}{r^2}$ in the effective potential, when minimized with respect to the variational parameters α_1 and α_2, decreases with increasing λ. As we have already mentioned, unlike the case of a point dipole, a finite dipole, with dipole moment $p > p_c$ has a ground state with negative energy [6]. Like V_f, the contribution of the finite dipole to the effective potential $\tilde{V}_f$ is also well-behaved near the origin. The coefficient of

$\frac{1}{r^2}$ in the long range part of the effective potential exceeds $-\frac{1}{4}$ as the dipole moment increases beyond the critical value producing ground states with negative energies.

Comments:

a. For our variational method to be meaningful it is essential that the expectation value, $< \Psi|\hat{H} - E_0|\Psi >$ is well defined. This demands that the domain of Ψ is the space of square integrable functions. However, the zero energy wavefunction is not normalizable. To determine the critical strength (λ_c) using our method, for the sake of mathematical consistency one may work with $\lambda_c + \epsilon$, $\epsilon > 0$. This holds good in the case of a finite dipole. However, such a scheme does not work for the point dipole, since a pure inverse square potential has no negative energy bound states [15, 16]. To circumvent this shortcoming, there are several regularization methods [15, 16], as mentioned in the previous chapter. We may regularize the pure inverse square potential with a hard sphere of radius R [12] and still obtain the same critical value [12]. This happens because the long range part of the potential supports a normalizable bound state only if the coefficient of $\frac{1}{r^2}$ is more attractive than $-\frac{1}{4}$ [15, 16]. Therefore all our arguments still hold good. Moreover, our method reflects the already established result [12] that the critical dipole moment is independent of the short range modification necessary to regularize the inverse square potential.

b. We have mentioned that for the point as well as the finite dipole, reversing the orientation of the dipole moment, or changing the sign of q, both change

the sign of λ, and hence the sign of the potential. We note that, in both cases, the potentials $V(r,\theta)$ may be expanded in terms of odd Legendre polynomials. The expansion is trivial in case of the point dipole. For the finite dipole, the following relation holds.

$$V_f(r,\theta) = \frac{2Qq}{4\pi\epsilon_0}\Sigma_{i=0}^{\infty}\frac{r^{2i+1}}{d^{2i+2}}P_{2i+1}(\cos\theta), \tag{2.63}$$

for $r < d$,

$$V_f(r,\theta) = \frac{2Qq}{4\pi\epsilon_0}\Sigma_{i=0}^{\infty}\frac{d^{2i+1}}{r^{2i+2}}P_{2i+1}(\cos\theta), \tag{2.64}$$

for $r \geq d$. As a consequence under the parity transformation ($\hat{\mathcal{P}}$) both the potentials also change signs. This is also evident from the explicit forms of the potentials V_p and V_f given by equations (2.2) and (2.42) respectively.

We now consider the equation,

$$\hat{H}\Psi = E\Psi.$$

Then,

$$\hat{\mathcal{P}}\hat{H}\Psi = E\hat{\mathcal{P}}\Psi,$$

or,

$$\hat{\mathcal{P}}\hat{H}\hat{\mathcal{P}}^{-1}\hat{\mathcal{P}}\Psi = E\hat{\mathcal{P}}\Psi.$$

Thus $\hat{\mathcal{P}}\Psi$ is an eigenstate of the parity transformed Hamiltonian $\hat{\mathcal{P}}\hat{H}\hat{\mathcal{P}}^{-1}$ with the same energy E. The parity transformed Hamiltonians for both the point and the finite dipole has the same form as the corresponding original Hamiltonians $\hat{H}$ with the orientations of the dipole moments being reversed

or the sign of q being altered. This justifies our claim that the energy eigenvalues should not change if we change the sign of q or reverse the orientation of the dipole moment. Evidently the corresponding wavefunction Ψ changes to $\hat{\mathcal{P}}\Psi$. This implies that, if we change the sign of p or reverse the orientation of the dipole, the variational parameters appearing as the coefficients of odd Legendre polynomials will change sign, the variational parameters appearing as the coefficients of the even Legendre polynomials will remain unaltered. This is why we have observed that the variational parameters appearing as the coefficients of odd Legendre polynomials change signs with λ.

3 A Charged Particle in the Potential of an Electric Dipole in the Presence of a Magnetic Field

In this section, we use our variational method to estimate the energy levels of a charged particle (charge q, mass m) in the presence of an electric dipole, and a magnetic field aligned along the dipole moment. We first explain why our method is expected to work well in determining energy levels of a charged particle in such a situation. Both the point and the finite electric dipoles are considered. We also investigate whether there is critical dipole moment required to bind a charged particle in the presence of a magnetic field. As discussed in the previous chapter, the critical dipole moment binds a state with the azimuthal quantum number $m_l = 0$. Therefore we consider states with $m_l = 0$. We determine the ground state energies with $m_l = 0$ of the charged particle in such systems. The variation in binding energy of the charged particle with the charge separation (2 d) of the finite dipole is also studied. All physical quantities listed in different tables are expressed in atomic unit (See appendix E for a detailed description).

3.1 Description of The Variational Method

We consider the potential experienced by the charged particle, in the presence of rigid and stationary finite electric dipole and a magnetic field as shown in Figure 8. The particle is assumed to be spinless. We discuss the effect of spin later in this chapter. Because of the azimuthal symmetry, m_l is a good

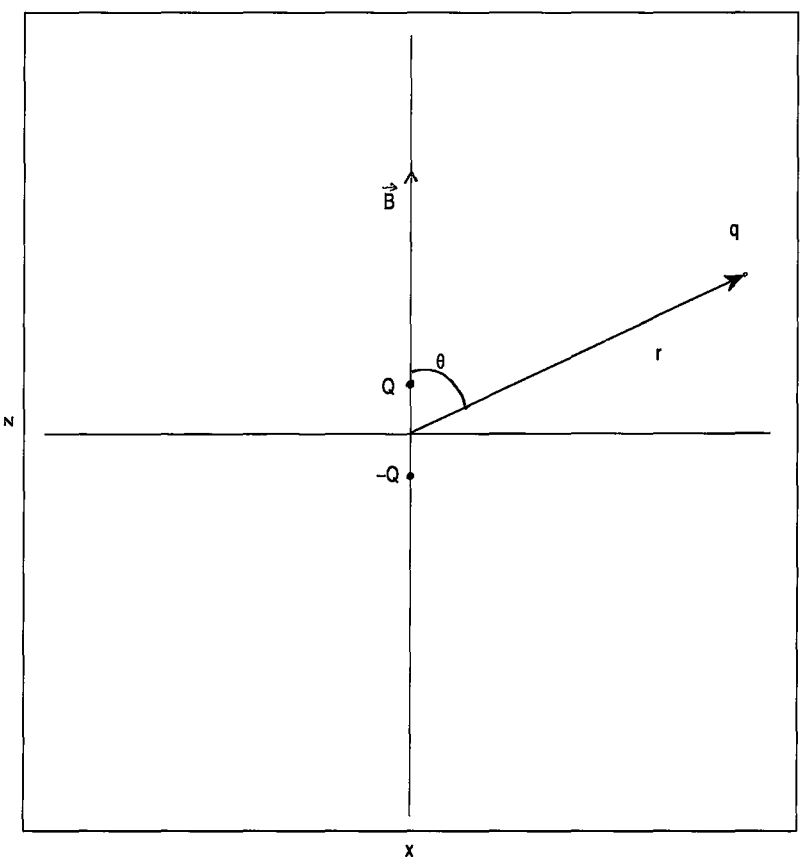

Figure 8: A charge q in presence of a finite dipole centered at the origin a magnetic field $\vec{B}$.

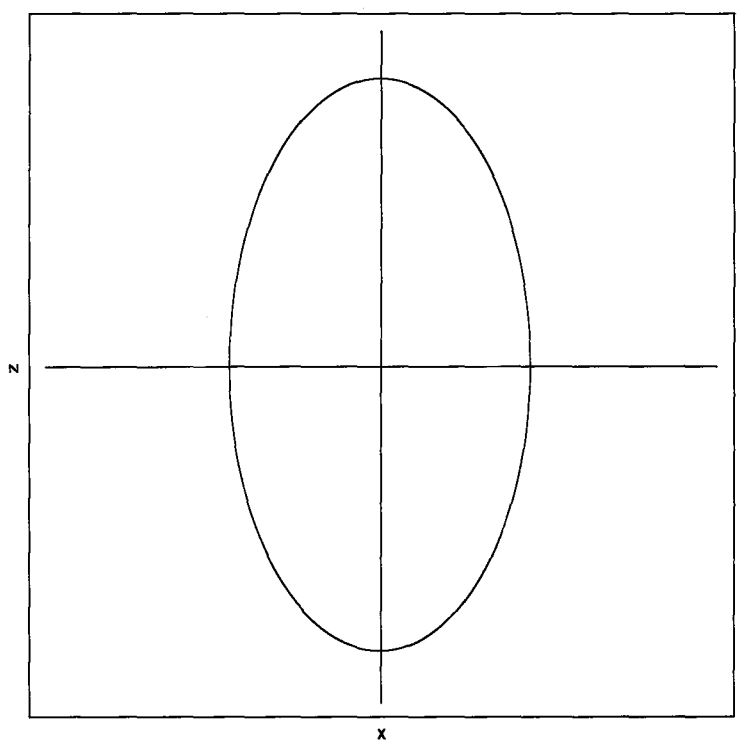

Figure 9: Constant R in x - z plane. In cylindrical coordinate system R is defined in equation (3.13).

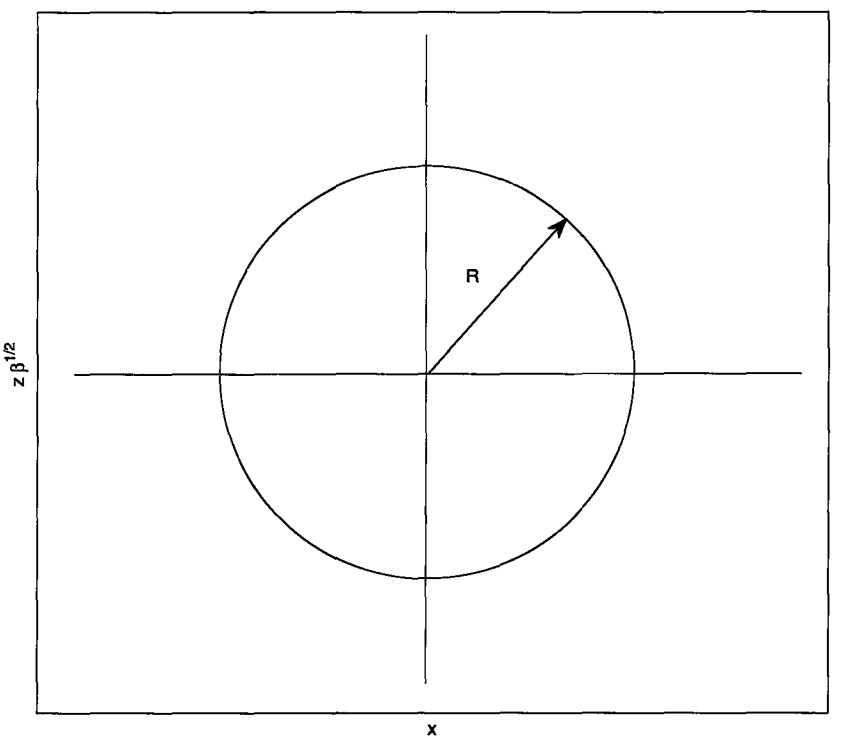

Figure 10: Constant R in x - $\sqrt{\beta}$ z plane. In cylindrical coordinate system R is defined in equation (3.13).

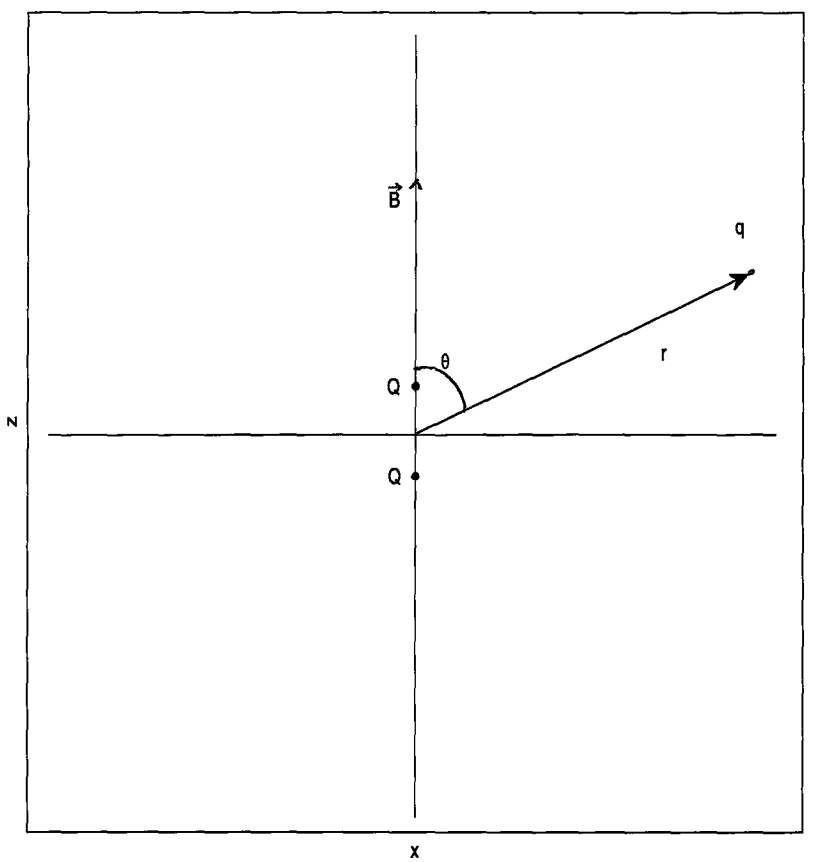

Figure 11: A charge q in presence of a H_2^+ centered at the origin and a magnetic field $\vec{B}$.

quantum number. We consider the ground state with $m_l = 0$. In spherical polar co-ordinate system, the potential $V_f^{(B)}(r,\theta)$ (the subscript f and the superscript B stand for the finite dipole and the magnetic field respectively) takes the following form :

$$V_f^{(B)}(r,\theta) = V_f(r,\theta) + \frac{e^2B^2}{8m}r^2\sin^2\theta, \tag{3.1}$$

where $V_f(r,\theta)$ is given by equation (2.42). The contribution from the finite dipole to $V_f^{(B)}(r,\theta)$ may be written as,

$$V_f(r,\theta) = \frac{Qq}{4\pi\epsilon_0}\frac{1}{\sqrt{r^2+d^2}}\left(\frac{1}{\sqrt{1-\frac{2rd}{r^2+d^2}\cos\theta}} - \frac{1}{\sqrt{1+\frac{2rd}{r^2+d^2}\cos\theta}}\right). \tag{3.2}$$

Each term on the R.H.S above may be expanded in terms of both even and odd powers of $\cos\theta$. Clearly even powers of $\cos\theta$ get canceled and only the terms with odd powers of $\cos\theta$ survive. Hence $V_f(r,\theta)$ may be expanded in terms of Legendre polynomials of odd orders (equations (2.63) and (2.64)). On the other hand, the contribution from the magnetic field in $V_f^{(B)}(r,\theta)$ may be expanded in terms of the first two Legendre polynomials of even orders. Hence we get

$$V_f^{(B)}(r,\theta) = \frac{2Qq}{4\pi\epsilon_0}\Sigma_{i=0}^{\infty}\frac{r^{2i+1}}{d^{2i+2}}P_{2i+1}(\cos\theta) + \frac{q^2B^2}{8m}r^2\frac{2}{3}(P_0(\cos\theta) - P_2(\cos\theta)), \tag{3.3}$$

for $r < d$ and

$$V_f^{(B)}(r,\theta) = \frac{2Qq}{4\pi\epsilon_0}\Sigma_{i=0}^{\infty}\frac{d^{2i+1}}{r^{2i+2}}P_{2i+1}(\cos\theta) + \frac{q^2B^2}{8m}r^2\frac{2}{3}(P_0(\cos\theta) - P_2(\cos\theta)), \tag{3.4}$$

for $r > d$. It has already been discussed that at short range $V_f(r,\theta)$ is well-behaved. As a consequence $V_f^{(B)}$ is also well-behaved at short range. As $r \to 0$, $V_f^{(B)} \approx V_f \propto r$. However, as we mentioned before, when $r \to \infty$, the contribution of the electric dipole (V_f) to the potential $V_f^{(B)}(r,\theta)$ goes as $\frac{1}{r^2}$. Hence the contribution from the magnetic field to $V_f^{(B)}$ dominates for large r. In cylindrical polar coordinates $V_f^{(B)}$ may be written as,

$$V_f^{(B)}(\rho,z) = \frac{Qq}{4\pi\epsilon_0}\left(\frac{1}{\sqrt{\rho^2+(z-d)^2}} - \frac{1}{\sqrt{\rho^2+(z+d)^2}}\right) + \frac{q^2B^2}{8m}\rho^2. \tag{3.5}$$

The Schrodinger equation for the charged particle is given by

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(r,\theta) + V_f^{(B)}(r,\theta)\Psi(r,\theta) = E_0\Psi(r,\theta). \tag{3.6}$$

For the point dipole, on the other hand, the corresponding potential $V_p^{(B)}$ (the subscript p stands for the point dipole) is given by,

$$V_p^{(B)}(r,\theta) = \frac{pq}{4\pi\epsilon_0}\frac{\cos\theta}{r^2} + \frac{e^2B^2}{8m}r^2\sin^2\theta \tag{3.7}$$

This also may be expanded in terms of Legendre polynomials as follows :

$$V_p^{(B)}(r,\theta) = \frac{pq}{4\pi\epsilon_0}\frac{P_1(\cos\theta)}{r^2} + \frac{2}{3}\frac{e^2B^2}{8m}r^2(P_0(\cos\theta) - P_2(\cos\theta)). \tag{3.8}$$

The Schrodinger equation for the ground state ($m_l = 0$) of the charged particle is obtained by replacing $V_f^{(B)}$ with $V_p^{(B)}$ in equation (3.6)

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(r,\theta) + V_p^{(B)}(r,\theta)\Psi(r,\theta) = E_0\Psi(r,\theta), \tag{3.9}$$

where E_0 denotes the corresponding ground state energy. The Hamiltonian for the finite dipole, unlike the case of the point dipole, is not scale invariant. The Schrodinger equations equations (3.6) and (3.9) do not have analytical solutions. Hence approximate methods are needed to study such systems. In our approach, we assume that the trial wavefunction for the ground state ($m_l = 0$) is a function of the variables R and η. In spherical polar coordinates, these variables are given by,

$$R = r\sqrt{\sin^2\theta + \beta\cos^2\theta} = r\sqrt{1-(1-\beta)\cos^2\theta}, \tag{3.10}$$

$$\eta = \arctan\left(\frac{\tan\theta}{\sqrt{\beta}}\right) = \arccos\frac{\sqrt{\beta}\cos\theta}{\sqrt{1-(1-\beta)\cos^2\theta}}. \tag{3.11}$$

In cylindrical polar coordinates the variables R and η are given by,

$$R = \sqrt{\rho^2 + \beta z^2}, \tag{3.12}$$

$$\eta = \arctan\frac{\rho}{\sqrt{\beta}z}, \tag{3.13}$$

$$\eta \in \{0, \pi\}. \tag{3.14}$$

where β is a variational parameter such that $0 < \beta < 1$. $\beta < 0$ is excluded since it clearly makes both R and η imaginary. We exclude $\beta > 1$ from physical considerations which will become clear after we write down the trial

wavefunction.

The trial wavefunction for the ground state of the charged particle is taken to be

$$\Psi(R) = \Phi(R)\Theta(\eta), \tag{3.15}$$

$$\Theta(\eta) = N_n(1 + \Sigma_{i=1}^{n}\alpha_i P_i(\cos\eta). \tag{3.16}$$

As before, the only requirement is that the trial wave function is normalizable. We do not assume any explicit form for $\Phi(R)$. In the presence of a magnetic field, the charged particle feels an attraction towards the z axis. Therefore, with the electric dipole, when a magnetic field is added, we expect an increment in the probability density at points on the z axis. With $0 < \beta < 1$, $\Phi(R)$ meets this expectation, and $\beta > 0$ with a fixed R denotes an ellipsoid. Since $\beta < 1$, the major axis of the ellipsoid is along the z axis. A cross section of the ellipsoid in the x- z plane is shown in Figure 9. Apart from allowing complex values for R and η, $\beta < 0$ also permits non-normalizable $\Phi(R)$. These physical considerations influence the choice of β in the range between 0 and 1.

R is invariant under parity transformation and may be expressed in terms of even Legendre polynomials. However, $\cos\eta$ changes sign under parity transformation and may be expressed in terms of the odd Legendre polyno-

mials.

$$R = r\Sigma_{i=0}^{\infty} c_i^R P_i(\cos\theta), \tag{3.17}$$

$$c_i^R = \frac{\int_{-1}^{1}(1-(1-\beta)t^2)P_i(t)dt}{\int_{-1}^{1} P_i^2(t)dt}, \tag{3.18}$$

$$\cos\eta = \sqrt{\beta}\Sigma_{i=0}^{\infty} c_i^\eta P_i(\cos\theta), \tag{3.19}$$

$$c_i^\eta = \frac{\int_{-1}^{1}\sqrt{\beta}\arccos\frac{\sqrt{\beta}t}{\sqrt{1-(1-\beta)t^2}}P_i(t)dt}{\int_{-1}^{1} P_i^2(t)dt}. \tag{3.20}$$

As we mentioned, $c_{2n+1}^R = 0$, $c_{2n}^\eta = 0$, where n is any positive integer. We explicitly work out the first two non-zero coefficients in each case below.

$$c_0^R = \frac{1}{2}\left(\sqrt{\beta} + \frac{\arccos\left[\sqrt{\beta}\right]}{\sqrt{1-\beta}}\right), \tag{3.21}$$

$$c_2^R = \frac{5\left((-1+\beta)\sqrt{\beta}(1+2\beta) + \sqrt{1-\beta}(-1+4\beta)\arccos\left[\sqrt{\beta}\right]\right)}{16(-1+\beta)^2}, \tag{3.22}$$

$$c_1^\eta = \frac{3}{2}\left(1 + \frac{1}{-1+\beta} + \sqrt{-\frac{\beta}{(-1+\beta)^3}}\arccos\left[\sqrt{\beta}\right]\right), \tag{3.23}$$

$$c_3^\eta = \frac{7}{2}\left(-\frac{\beta(13+2\beta)}{8(-1+\beta)^2} + \frac{3}{8}\left(5\sqrt{-\frac{\beta}{(-1+\beta)^5}} - 4\sqrt{-\frac{\beta}{(-1+\beta)^3}}\right)\right.$$
$$\left.\arccos\left[\sqrt{\beta}\right]\right). \tag{3.24}$$

It is now clear that the trial wavefunction $\Psi(R,\eta)$ implicitly contains infinitely many of both even and odd powers of $\cos\theta$. We determine $\Phi(R)$ and the corresponding ground state energy E_0 by performing a variation of the quantity $\langle\Psi|\hat{H} - E_0|\Psi\rangle$, with respect to $\Phi(R)$. Since we explicitly choose $\Theta(\eta)$, the η integral may be performed analytically. We know that Legendre

polynomials satisfy the following relation [21].

$$\int_{-1}^{1} P_{i_1}(t)P_{i_2}(t)P_{i_3}(t)dt = \frac{2}{2i_1+1}C(i_2 i_3 i_1|000)^2 \tag{3.25}$$

Here C denotes the Clebsch- Gordan coefficient. Also we know that, for the above integral to be non-zero, the following conditions hold ([21]).

$$\Sigma_{n=1}^{n=3} i_n = 2m, \tag{3.26}$$

$$|i_j - i_k| < i_l < i_j + i_k, \tag{3.27}$$

where $n \in \{0, 1, 2, 3, 4, ...\}$, $\{j, k, l\} \in \{1, 2, 3\}$.

As we explained earlier, the potential term in the original Hamiltonian contains both even and odd Legendre polynomials. The even polynomials are contributed by the magnetic field and the odd ones are contributed by the electric dipole. With our choice of coordinates (R, η, ϕ), the wavefunction contains infinitely many Legendre polynomials. From equation (3.25), it is evident that the term $\langle\Psi|V|\Psi\rangle$ couples infinitely many even and odd Legendre polynomials coming from $\Psi(R, \eta)$. Thus our method naturally takes into account infinitely many couplings of the Legendre polynomials. To keep the computation simple, we keep only three variational parameters, (β, α_1, α_2), in case of the point dipole and only two, (β, α_1), in case of the finite dipole. Performing the variation of $\langle\Psi|\hat{H} - E_0|\Psi\rangle$ with respect to $\Phi(R)$ we obtain a Schrodinger-like equation for $\Phi(R)$. We solve the equation to determine $\Phi(R)$ and the corresponding ground state energy E_0.

Note that a similar method was used to determine the ground state and

few excited states of a charged particle in the presence of H_2^+ and a magnetic field parallel to the axis of the H_2^+ (Figure 11) [20]. In spherical polar coordinates, the potential $V_H^{(B)}(r,\theta)$ (the subscript H is for H_2^+) experienced by the charged particle at $\vec{r}$ in its ground state is given by

$$V_H^{(B)}(r,\theta) = \frac{Qq}{4\pi\epsilon_0}\left(\frac{1}{\sqrt{r^2+d^2-2rd\cos\theta}} + \frac{1}{\sqrt{r^2+d^2+2rd\cos\theta}}\right) + \frac{q^2B^2}{8m}r^2\sin^2\theta. \tag{3.28}$$

Unlike V_f, here the first '-' sign in equation (3.1) is replaced by a '+'. This leads to the cancellation of the odd powers of $\cos\theta$. The potential $V_H^{(B)}(r,\theta)$ has even parity and may be expanded as a linear combination of even Legendre polynomials. As described in the paper ([20]), a trial wavefunction $\Psi(r,\theta) = \Phi(R)$, where R is defined by equation (3.11), was used. The only variational parameter is β. Such a wavefunction contains only the even Legendre polynomials. Hence the term $\langle\Psi|V_H^{(B)}|\Psi\rangle$ only considers couplings between different even Legendre polynomials coming from the wavefunction. Considering a trial wavefunction $\Psi(r,\eta,\phi) = \Phi(R)\Theta(\eta)$, as we did, does not improve the results. Though it takes into account the odd-odd Legendre couplings as well, such a trial wavefunction is not a parity eigenstate. The Hamiltonian, however, is invariant under parity transformation. In the same paper, the authors also apply this method to determine the ground state energy of a hydrogen atom in a magnetic field. In this case, in comparison to a few other simple variational methods, this method was found to be superior in the presence of a strong magnetic field. We have checked our numerics by replicating a few of the results published in reference [20].

3.2 The Point Dipole and Magnetic Field

In this subsection we will obtain the ground state energy of a particle (charge q, mass m) in the presence of a point electric dipole and a magnetic field. As shown in Figure 12, the dipole moment $\vec{p} = p\hat{z}$ and a uniform magnetic field $\vec{B} = B\hat{z}$ are aligned along the z-axis. In cylindrical coordinates the Hamiltonian for the charged particle is given by,

$$\hat{H} = -\frac{\hbar^2}{2m}(\hat{p} - \frac{q}{2}\vec{B} \times \vec{r})^2 + \frac{pq}{\rho^2 + z^2}\cos\theta. \tag{3.29}$$

Because of the azimuthal symmetry, the azimuthal quantum number m_l is a good quantum number. We choose that $m_l = 0$. We also assume that the ground state wavefunction for $m_l = 0$ may be expressed in the following form.

$$\Psi(R, \eta) = \frac{1}{\sqrt{2\pi}}\Phi(R)\Theta(\eta), \tag{3.30}$$

where

$$\Theta(\eta) = N_2(1 + \alpha_1 P_1(\cos\eta) + \alpha_2 P_2(\cos\eta)), \tag{3.31}$$

$$N_2 = \sqrt{\frac{15}{2}}\sqrt{\frac{1}{15 + 5\alpha_1^2 + 3\alpha_2^2}}\,. \tag{3.32}$$

The variational parameters α_1 and α_2 are considered to be real. We have,

$$R = \sqrt{(\rho^2 + \beta z^2)}, \quad \eta = \arctan(\frac{\rho}{\sqrt{\beta}z}).$$

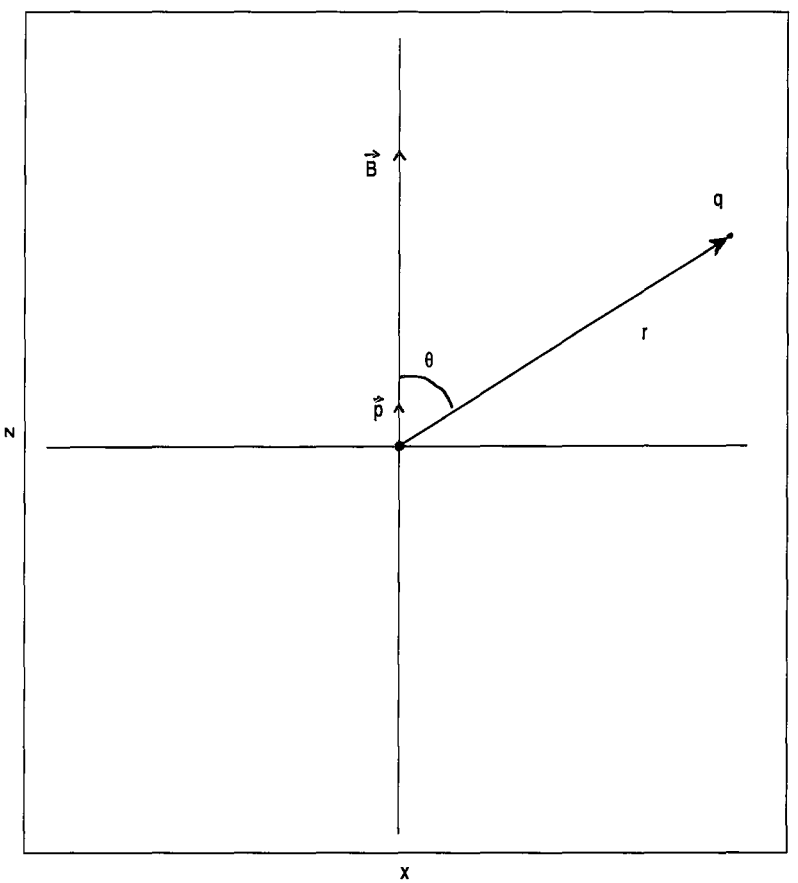

Figure 12: A charge q in presence of a point dipole $\vec{p}$ at the origin and a magnetic field $\vec{B}$.

Inverting these we get,

$$\rho = R\sin\eta, \tag{3.33}$$

$$z = \frac{R}{\sqrt{\beta}}\cos\eta. \tag{3.34}$$

Assuming $\beta > 0$ avoids a singularity in the above relation. Using these relations, in terms of the coordinates (R, η, ϕ), the potential experienced by the charged particle due to the stationary point electric dipole may be expressed as

$$V_p(R,\eta) = \frac{pq}{R^2}\frac{\cos\eta}{(\frac{\cos^2\eta}{\beta} + \sin^2\eta)^{\frac{3}{2}}}. \tag{3.35}$$

For the ground state, the contribution from the magnetic field to the potential experienced by the charged particle is given by

$$V_B(R,\eta) = \frac{q^2B^2}{8m}R^2\sin^2\eta. \tag{3.36}$$

The expectation value $\langle\Psi|\hat{H} - E_0|\Psi\rangle$ now becomes,

$$\begin{aligned}\langle\Psi|\hat{H} - E_0|\Psi\rangle = \frac{2\pi}{\sqrt{\beta}}\int_0^\infty R^2dR[\frac{\hbar^2}{2m}\{I_1\left(\frac{d}{dR}\Phi(R)\right)^2 + I_2\frac{\Phi}{R}\frac{d}{dR}\Phi(R) \\ + I_3\frac{\Phi(R)^2}{R^2}\} + pq\beta\frac{\Phi^2}{R^2}I_d + \frac{q^2B^2}{8m}I_BR^2\Phi(R)^2 - E_0\Phi(R)^2],\end{aligned} \tag{3.37}$$

where,

$$I_1 = \frac{14\alpha_1^2 + 21\beta\alpha_1^2 + 10\alpha_2^2 + 11\beta\alpha_2^2 - 28\alpha_2 + 28\beta\alpha_2 + 35\beta + 70}{7(15 + 5\alpha_1^2 + 3\alpha_2^2)} \quad (3.38)$$

$$I_2 = -\frac{4(1-\beta)(7\alpha_1^2 + 3\alpha_2^2 + 21\alpha_2)}{7(15 + 5\alpha_1^2 + 3\alpha_2^2)}, \quad (3.39)$$

$$I_3 = \frac{2(7\alpha_1^2 + 28\beta\alpha_1^2 + 27\alpha_2^2 + 36\beta\alpha_2^2)}{7(15 + 5\alpha_1^2 + 3\alpha_2^2)}, \quad (3.40)$$

$$I_d = -\frac{15\beta\alpha_1(8(1-\beta)^{\frac{3}{2}} - \alpha_2\sqrt{(1-\beta)}(8\beta + 10)}{4(1-\beta)^{\frac{5}{2}}(15 + 5\alpha_1^2 + 3\alpha_2^2)} + \frac{\ln\frac{(1+\sqrt{(1-\beta)})^2}{\beta}(7\beta\alpha_2 + 4\beta + 2\alpha_2 - 4))}{4(1-\beta)^{\frac{5}{2}}(15 + 5\alpha_1^2 + 3\alpha_2^2)}, \quad (3.41)$$

$$I_B = \frac{2(7\alpha_1^2 + 5\alpha_2^2 - 14\alpha_2 + 35)}{7(15 + 5\alpha_1^2 + 3\alpha_2^2)}. \quad (3.42)$$

Performing a variation of $\langle\Psi|\hat{H} - E_0|\Psi\rangle$ with respect to $\Phi(R)$ and using the Euler-Lagrange equation, we obtain

$$-\frac{\hbar^2}{2m}I_1\left(\Phi''(R) + \frac{2}{R}\Phi'(R)\right) + \left(\frac{\hbar^2}{2m}\left(I_3 - \frac{I_2}{2}\right) + pqI_d\right)\frac{\Phi(R)}{R^2} + \frac{q^2B^2}{8m}I_B R^2\Phi(R) = E_0\Phi(R), \quad (3.43)$$

where $\Phi''(R) = \frac{d^2}{dR^2}\Phi(R)$ and $\Phi'(R) = \frac{d}{dR}\Phi(R)$. For the details of the calculation see appendix D. With $\Phi(R) = \frac{u(R)}{R}$, this reduces to,

$$-\frac{\hbar^2}{2m}I_1\frac{d^2}{dR^2}u(R) + \left(\frac{\hbar^2}{2m}\left(I_3 - \frac{I_2}{2}\right) + pqI_d\right)\frac{u(R)}{R^2} + \frac{q^2B^2}{8m}I_B R^2 u(R) = E_0 u(R). \quad (3.44)$$

Multiplying both sides by $\frac{2m}{\hbar^2 I_1}$, we get,

$$-\frac{d^2}{dR^2}u(R) + \frac{1}{I_1}\left(\left(I_3 - \frac{I_2}{2}\right) + \frac{2m}{\hbar^2}pqI_d\right)\frac{u(R)}{R^2} + \frac{q^2B^2}{8m}\frac{I_B}{I_1}R^2u(R) = \frac{2m}{\hbar^2 I_1}E_0 u(R). \quad (3.45)$$

Note that, I_1 and I_B are positive definite; we show this below.

$$I_1 = \frac{14\alpha_1^2 + 21\beta\alpha_1^2 + 10(\alpha_2 - \frac{7}{5})^2 + 11\beta(\alpha_2^2 + \frac{14}{11})^2 + \frac{189}{11}\beta + \frac{252}{5}}{7(15 + 5\alpha_1^2 + 3\alpha_2^2)} \quad (3.46)$$

$$I_B = \frac{2(7\alpha_1^2 + 5(\alpha_2 - \frac{7}{5})^2 + \frac{126}{5}}{7(15 + 5\alpha_1^2 + 3\alpha_2^2)}. \quad (3.47)$$

These relations imply that the coefficient of the R^2 term is non-negative. To ensure that the energy E_0 is real, we claim that the operator

$$-\frac{\hbar^2}{2m}\frac{d^2}{dR^2} + \frac{1}{I_1}\left(\frac{\hbar^2}{2m}\left(I_3 - \frac{I_2}{2}\right) + pqI_d\right)\frac{u(R)}{R^2} + \frac{q^2B^2}{8m}\frac{I_B}{I_1}R^2,$$

acting on $u(R)$ is hermitian in the domain of the square integrable functions of R. Considering the original Hamiltonian to be hermitian in the domain of square integrable functions in three dimensions, this claim is reasonable. However, similar to the case of the pure $\frac{1}{r^2}$ potential, this implies the following constraint on the coefficient of the $\frac{1}{R^2}$ term of the above equation.

$$Re\left(-\frac{1}{2} + \frac{\sqrt{1 + \frac{4}{I_1}\left(\frac{2m}{\hbar^2}pqI_d + I_3 - \frac{I_2}{2}\right)}}{2}\right) > -\frac{1}{2}, \quad (3.48)$$

or,

$$\sqrt{1+\frac{4}{I_1}\left(\frac{2m}{\hbar^2}pqI_d+I_3-\frac{I_2}{2}\right)}>0, \tag{3.49}$$

or,

$$\frac{1}{I_1}\left(\frac{2m}{\hbar^2}pqI_d+I_3-\frac{I_2}{2}\right)>-\frac{1}{4}. \tag{3.50}$$

We note that $\frac{1}{I_1}\left(\frac{2m}{\hbar^2}pqI_d+I_3-\frac{I_2}{2}\right)$ is the coefficient of $\frac{1}{R^2}$ in the Schrodinger-type equation we obtained. This equation is similar to the Schrodinger equation for a particle in a harmonic potential in three dimensions. The solution is given by [22]

$$u(R)=NR^l e_1^{-\frac{\tau}{2}R^2}F_1(-n_R,l+\frac{3}{2},\tau R^2), \tag{3.51}$$

where N is the normalization constant. ${}_1F_1$ is the confluent hypergeometric function of the first kind. Also,

$$l = -\frac{1}{2}+\frac{\sqrt{1+\frac{4}{I_1}(\frac{2m}{\hbar^2}pqI_d+I_3-\frac{I_2}{2}}}{2}), \tag{3.52}$$

$$\tau = \frac{2m}{\hbar^2}\frac{q^2B^2}{8m}I_B. \tag{3.53}$$

The energy of the n-th excited state with $m_l=0$ is

$$E_n=\frac{\hbar^2}{m}\sqrt{\left(\frac{2m}{\hbar^2}\frac{q^2B^2}{8m}I_BI_1\right)}\left(2n+1+\frac{1}{2}\sqrt{1+\frac{4}{I_1}\left(\frac{2m}{\hbar^2}pqI_d+I_3-\frac{I_2}{2}\right)}\right). \tag{3.54}$$

The ground state energy E_0 may be obtained by putting $n=0$ in the above

expression.

$$E_0 = \frac{\hbar^2}{m}\sqrt{\left(\frac{2m}{\hbar^2}\frac{q^2B^2}{8m}I_B I_1\right)}\left(1+\frac{1}{2}\sqrt{1+\frac{4}{I_1}\left(\frac{2m}{\hbar^2}pqI_d + I_3 - \frac{I_2}{2}\right)}\right). \tag{3.55}$$

We note that, as expected, the condition for hermiticity of the operator

$$-\frac{\hbar^2}{2m}\frac{d^2}{dR^2} + \frac{1}{I_1}\left(\frac{\hbar^2}{2m}\left(I_3 - \frac{I_2}{2}\right) + pqI_d\right)\frac{u(R)}{R^2} + \frac{q^2B^2}{8m}\frac{I_B}{I_1}R^2,$$

in the domain of the normalizable functions in three dimensions, as given by the relation (3.50), and equation (3.47) together assure that the energy E_0 is positive. We note that, E_0, as obtained by our method, is proportional to B. This is analogous to the case when the magnetic field alone is present. Motivated by physical situations, we consider an electron to be the charged particle of our interest. In atomic units, then, $q = -1$, $m = 1$. We take the dipole moment along the negative z direction to keep λ positive. As mentioned earlier, atomic units are used throughout. Corresponding to the parameter $\gamma = 1$, the magnitude of the magnetic field (B) is 2.35×10^5 Tesla (for details see appendix E). E_0 is minimized with respect to the variational parameters α_1, α_2 and β to obtain the ground state energy. In Table 6, we tabulate E_0 for different values of λ and specify the corresponding values of the variational parameters. Taking the spin (say $\vec{S}$) of the electron into account, the ground state energy of the electron (E_0^s, the superscript s stands for spin) is given by,

$$E_0^s = E_0 - \vec{\mu}.\vec{B}, \tag{3.56}$$

where the magnetic moment of the electron $\vec{\mu} \approx -\vec{S}$ in a.u. Therefore the

actual ground state energy of an electron with $S_z = \frac{1}{2}$ is given by $(E_0 + .5)$. For $S_z = -\frac{1}{2}$, the actual ground state energy is $(E_0 - .5)$. The corresponding binding energy (say E_b^s) is given by,

$$E_b^s = E_b + \vec{\mu}.\vec{B}, \tag{3.57}$$

where,

$$E_b = \frac{\gamma}{2} - E_0. \tag{3.58}$$

To show that even weaker dipoles bind, we consider the values of λ which are smaller than λ_c, which is the critical value of λ in the absence of a magnetic field. The corresponding binding energies (E_b) are also tabulated.

As expected, in presence of the dipole, the ground state energies are lower than the minimum energy of an electron (without considering its spin for the moment) in presence of only $\vec{B}$, which is .5 in atomic units for $\gamma = 1$. We plot the ground state energy of the electron as a function of λ (Figure 13). The energy E_0 decreases as λ increases. Considering that stronger dipole moments offer greater binding, one expects the binding energy of the electron to increase as λ increases. In Figure 14 we plot the binding energy as a function of λ which reveals this. In Figure 15 β against λ has been plotted which shows that β becomes larger as λ increases. This implies that the curves in the ρ-z plane, along which $\Phi(R)$ does not change, tend to become fatter ellipses as we increase λ. Recall that in presence of only $\vec{B}$, the curves are straight lines parallel to the z axis. The presence of an electric dipole allows binding.

λ	β	α_1	α_2	E_0	E_b
0.70	0.1171	-0.4064	0.0367	0.4987	0.0013
0.72	0.1302	-0.4276	0.0385	0.4978	0.0022
0.74	0.1429	-0.4465	0.0398	0.4968	0.0032
0.76	0.1554	-0.4635	0.0408	0.4957	0.0043
0.78	0.1677	-0.4790	0.0416	0.4945	0.0055
0.80	0.1801	-0.4933	0.0422	0.4933	0.0067
0.82	0.1926	-0.5064	0.0426	0.4919	0.0081
0.84	0.2052	-0.5185	0.0428	0.4904	0.0096
0.86	0.2179	-0.5297	0.0429	0.4888	0.0112
0.88	0.2309	-0.5402	0.0429	0.4872	0.0128
0.90	0.2442	-0.5499	0.0429	0.4854	0.0146
0.92	0.2578	-0.5589	0.0428	0.4835	0.0165
0.94	0.2718	-0.5672	0.0426	0.4815	0.0185
0.96	0.2863	-0.5750	0.0425	0.4793	0.0207
0.98	0.3012	-0.5822	0.0423	0.4770	0.0230
1.00	0.3168	-0.5889	0.0422	0.4746	0.0254
1.02	0.3330	-0.5951	0.0420	0.4720	0.0280
1.04	0.3500	-0.6007	0.0420	0.4693	0.0307
1.06	0.3679	-0.6059	0.0419	0.4664	0.0336
1.08	0.3869	-0.6105	0.0420	0.4632	0.0368
1.10	0.4000	-0.6150	0.0409	0.4599	0.0401
1.12	0.4290	-0.6183	0.0424	0.4562	0.0438
1.14	0.4528	-0.6213	0.0428	0.4523	0.0477
1.16	0.4790	-0.6237	0.0434	0.4480	0.0520
1.18	0.5084	-0.6254	0.0443	0.4432	0.0568
1.20	0.5423	-0.6262	0.0456	0.4378	0.0622
1.22	0.5829	-0.6258	0.0474	0.4316	0.0684
1.24	0.6350	-0.6236	0.0502	0.4241	0.0759
1.26	0.7120	-0.6178	0.0550	0.4141	0.0859
1.275	0.8338	-0.6050	0.0642	0.4015	0.0985

Table 6: Various values of λ and their corresponding binding energies for $\gamma = 1$ along with the variational parameters. γ denotes the strength of the magnetic field in atomic unit.

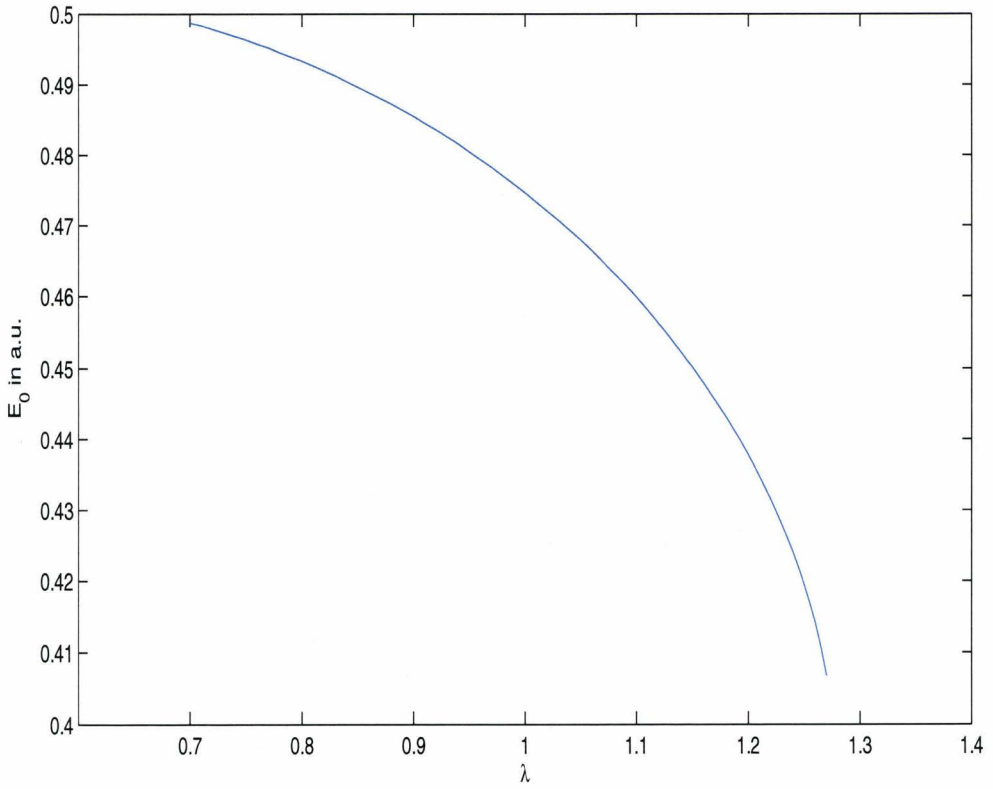

Figure 13: The ground state energy of an electron in the potential of a magnetic field $\vec{B} = 2.35 \times 10^5$ T, and the point dipole, vs. λ.

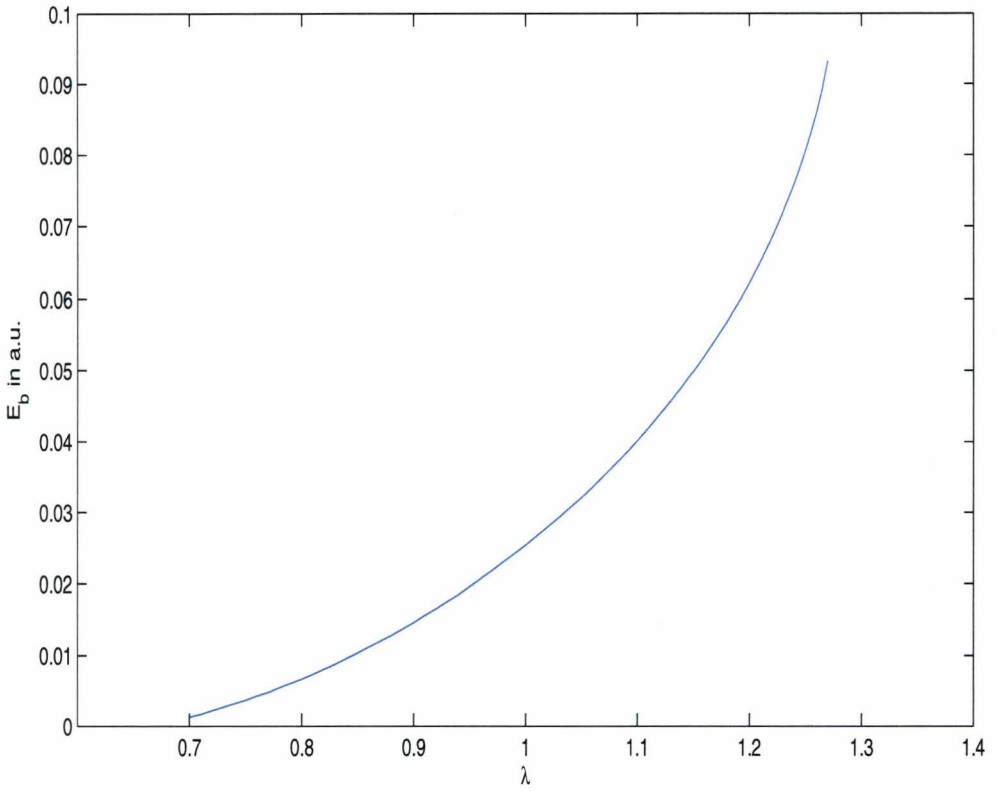

Figure 14: The binding energy of an electron in the potential of a magnetic field $\vec{B} = 2.35 \times 10^5$ T, and the point dipole, vs. λ.

It is already evident that in the presence of the magnetic field $\vec{B}$, a point electric dipole of any strength binds a charge. There is no critical dipole moment. This is not surprising considering the facts that the magnetic field supports bound states in the x-y plane and an attractive potential of any strength supports bound state in one dimension. The magnetic field prevents the wavefunction from diverging at large ρ and the dipole takes care of that as $z \longrightarrow \infty$. As before, for the critical value of the dipole moment without the

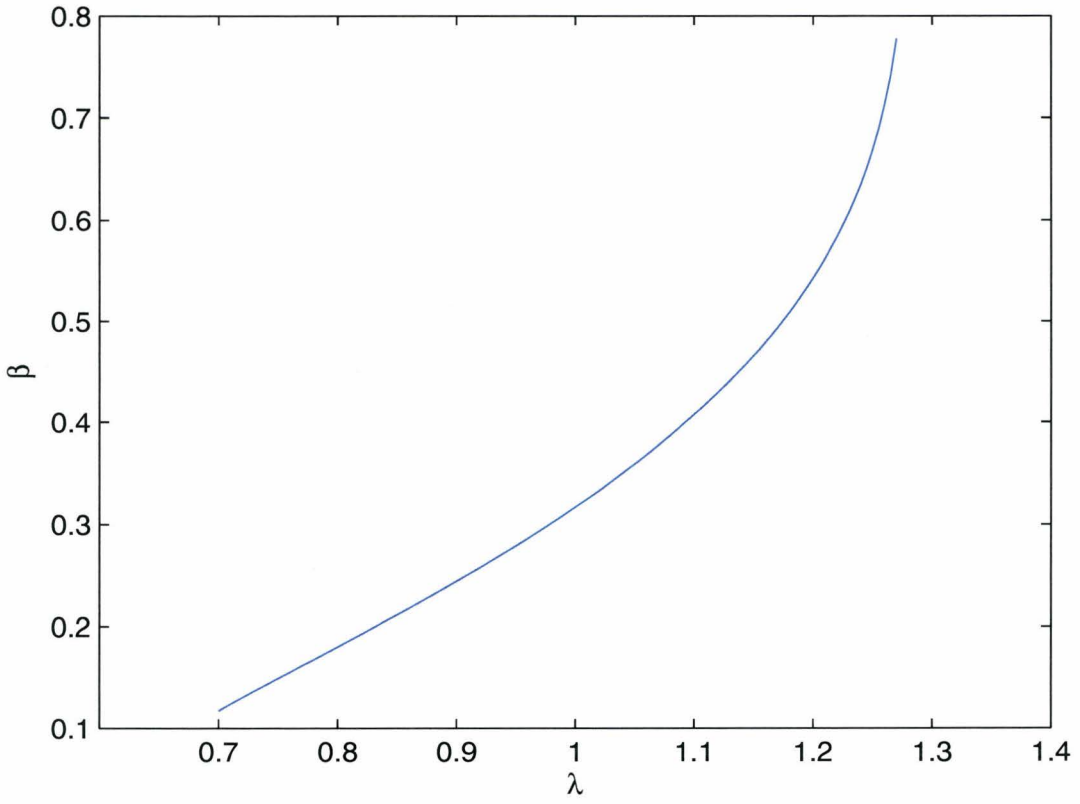

Figure 15: The variational parameter β vs. λ.

λ	I_{con}
1.25	-0.0160
1.26	-0.0109
1.27	-0.0055
1.28	-5.5289×10^{-14}
1.29	-6.1062×10^{-16}
1.30	-1.3877×10^{-16}

Table 7: I_{con} as defined by equation (3.59) and the corresponding λ

magnetic field (p_c) the minimum of the coefficient of the $\frac{1}{R^2}$ term becomes $-\frac{1}{4}$. We have checked the result numerically. In Figure 16 we plot the coefficient of the $\frac{1}{R^2}$ and the corresponding λ.

Figure 16 shows that for dipole moments stronger than the critical dipole moment, the minimum of the coefficient of $\frac{1}{R^2}$ in equation (3.45) is less than $-\frac{1}{4}$. However, as we have discussed above, to ensure the hermiticity of the Hamiltonian, we need the coefficient of $\frac{1}{R^2}$ in equation (3.45),

$$\frac{1}{I_1}\left(\frac{2m}{\hbar^2}pqI_d + I_3 - \frac{I_2}{2}\right),$$

to be greater than $-\frac{1}{4}$. This plays the role of a constraint while minimizing the energy E_0. In the following table (Table 7), we tabulate the numerical values of

$$I_{con} = -\frac{1}{4} - \frac{1}{I_1}(\frac{2m}{\hbar^2}pqI_d + I_3 - \frac{I_2}{2}), \tag{3.59}$$

and the corresponding λ. For $\lambda > \lambda_c$, the constraint plays an important role in obtaining the ground state energy.

We also note that, as $p \to 0$, in presence of the magnetic field $\vec{B}$ alone,

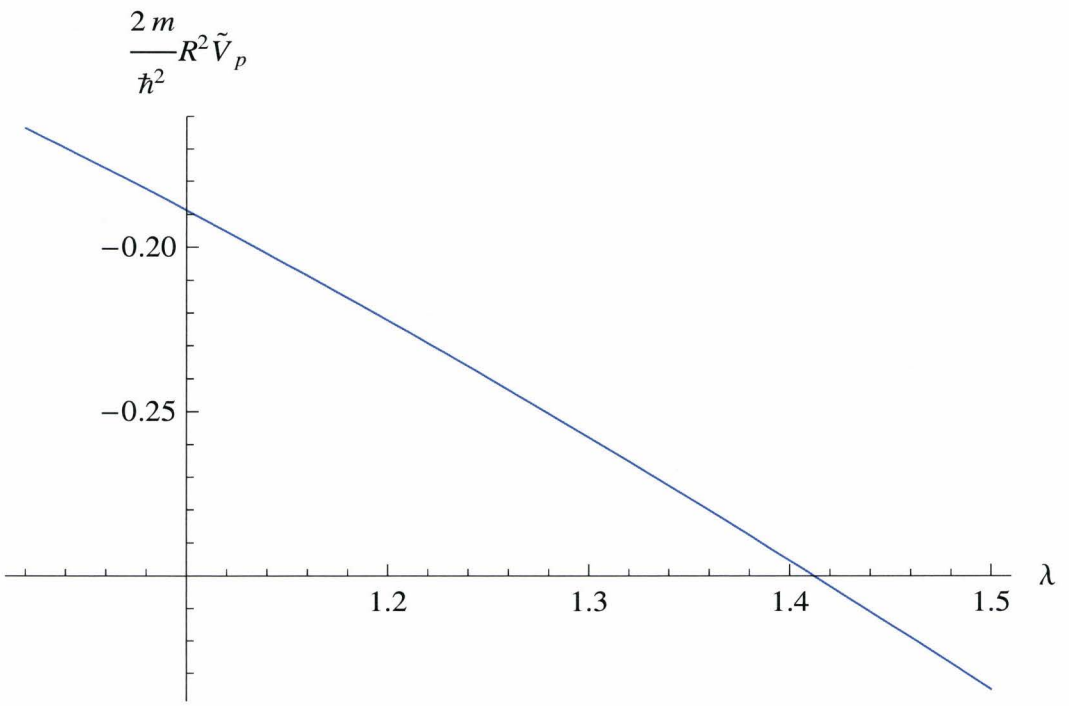

Figure 16: Minima of the coefficient of $\frac{1}{R^2}$ in equation (3.45) with respect to the variational parameters β, α_1 and α_2 vs. λ.

the minimum energy of the charged particle is given by,

$$E_0^B = \frac{\hbar^2}{m}\sqrt{\left(\frac{2m}{\hbar^2}\frac{q^2B^2}{8m}I_B I_1\right)}\left(1+\frac{1}{2}\sqrt{1+\frac{4}{I_1}\left(I_3-\frac{I_2}{2}\right)}\right). \tag{3.60}$$

However, in presence of the magnetic field $\vec{B}$ alone, as we know, a normalizable ground state wavefunction does not exist. So the expectation value, $\langle\Psi|\hat{H}-E_0|\Psi\rangle$ is not defined. Hence our method is not expected to work in such a situation. However, in presence of a point dipole, as we have mentioned, a bound state always exists. Therefore, in the limit $p \to 0$, one may expect that the minimum of E_0^B will give the minimum energy (say E_B) in presence of the magnetic field $\vec{B}$. We numerically minimized E_0^B to check this. We found,

$$E_{0\ min}^B = \frac{1}{2}\frac{\hbar q B}{m} \tag{3.61}$$

This is the same as obtained by analytical calculations. For an electron, in atomic units, we have $E_B = \frac{1}{2}$. The corresponding values of the variational parameters are given by, $\alpha_1 = -1.22 \times 10^{-20} \approx 0$, $\alpha_2 = 2.93 \times 10^{-21} \approx 0$, $\beta \approx 0$. This is expected because of the cylindrical symmetry of the potential in the presence of $\vec{B}$ alone. However, $\beta = 0$ also makes the relation, $z = \frac{R\cos\eta}{\sqrt{\beta}}$, undefined. This hints at the fact that our method is not applicable when only the magnetic field is present. Note that, E_0 approaches zero as $|\vec{B}| \to 0$.

3.3 The Finite Dipole and Magnetic Field

As mentioned earlier, the point electric dipole is an idealization. Any physical electric dipole is a finite dipole. Using our variational method we obtain the ground state energy of the charged particle in the presence of a finite electric dipole and a magnetic field. For simplicity we assume that the electric dipole is rigid, which means that the separation between the poles (2 d) remains constant. It is also assumed that the dipole is stationary. In cylindrical coordinates the dipole moment is given by $\vec{p} = p\hat{z}$. As shown in Figure 8, the magnetic field is given by $\vec{B} = B\hat{z}$. The potential $V_f(r, \theta)$, experienced by the charged particle in the presence of the finite dipole is given by equation (3.5)

The corresponding Hamiltonian is

$$\hat{H} = -\frac{\hbar^2}{2m}(\hat{p} - \frac{q}{2}\vec{B} \times \vec{r})^2 + \frac{Qq}{4\pi\epsilon_0}\left(\frac{1}{\sqrt{\rho^2 + (z-d)^2}} - \frac{1}{\sqrt{\rho^2 + (z+d)^2}}\right). \tag{3.62}$$

Because of the cylindrical symmetry, the azimuthal quantum number m_l is a good quantum number. We consider the ground state for $m_l = 0$. As before, we assume that the trial wavefunction for the ground state is given by,

$$\Psi(R, \eta) = \frac{1}{\sqrt{2\pi}}\Phi(R)\Theta(\eta), \tag{3.63}$$

where

$$\Theta(\eta) = N_1(1 + \alpha_1 P_1(\cos\eta)), \tag{3.64}$$

$$N_1 = \sqrt{\frac{15}{2}}\sqrt{\frac{1}{15 + 5\alpha_1^2}}, \tag{3.65}$$

For simplicity we keep only two variational parameters, β and α_1. α_1 is also assumed to be real. In terms of the coordinates (R, η), V_f may be expressed as,

$$V_f(R,\eta) = \frac{Qq}{4\pi\epsilon_0}\left(\frac{1}{\sqrt{R^2\sin^2\eta + (\frac{R^2\cos^2\eta}{\sqrt{\beta}} - d)^2}} - \frac{1}{\sqrt{R^2\sin^2\eta + (\frac{R^2\cos\eta}{\sqrt{\beta}} + d)^2}}\right). \tag{3.66}$$

In terms of the same variables the potential $V_B(R, \eta)$, experienced by the charged particle in its ground state, due to the magnetic field is given by equation (3.36). Therefore the total potential experienced by the charged particle in its ground state is

$$V_f^{(B)} = V_f + V_B. \tag{3.67}$$

The expectation value $< \Psi|\hat{H} - E_0|\Psi >$ now becomes,

$$\langle\Psi|\hat{H} - E_0|\Psi\rangle = \frac{2\pi}{\sqrt{\beta}}\int_0^\infty R^2 dR\left(\frac{\hbar^2}{2m}\{I_1\left(\frac{d}{dR}\Phi(R)\right)^2 + I_2\frac{\Phi}{R}\frac{d}{dR}\Phi(R) + I_3\frac{\Phi(R)^2}{R^2}\} + Qq\beta\frac{\Phi^2}{R}I_f + \frac{q^2B^2}{8m}I_B R^2\Phi(R)^2 - E_0\Phi(R)^2\right). \tag{3.68}$$

I_1, I_2, I_3, I_B may be obtained from equations (3.39), (3.40), (3.41), (3.42)

respectively by putting $\alpha_2 = 0$. Thus,

$$I_1 = \frac{1}{5}\frac{(10 + 2\alpha_1^2 + 5\beta + 3\beta\alpha_1^2)}{3 + \alpha_1^2}, \tag{3.69}$$

$$I_2 = \frac{4}{5}\left(\alpha_1^2\frac{(\beta - 1)}{3 + \alpha_1^2}\right), \tag{3.70}$$

$$I_3 = \frac{2}{5}\frac{(\alpha_1^2(1 + 4\beta))}{3 + \alpha_1^2}, \tag{3.71}$$

$$I_B = \frac{2}{7}\frac{(7\alpha_1^2 + 35)}{(5\alpha_1^2 + 15)}. \tag{3.72}$$

I_f is given by,

$$I_f = \frac{1}{R(1-\beta)^{3/2}}\left(\frac{-6\alpha_1}{3 + {\alpha_1}^2}\left(2\sqrt{\beta(1-\beta)} + \frac{d\beta}{R}\log\left(\frac{\left(\frac{d^2\beta}{R^2} - (1-\beta)\right)}{\left(\frac{d\sqrt{\beta}}{R} + \sqrt{1-\beta}\right)^2}\right)\right)\right) \tag{3.73}$$

for $R < d\sqrt{\beta}$ and

$$I_f = \left(\frac{1}{R(1-\beta)^{3/2}}\left(\frac{-6\alpha_1}{3 + {\alpha_1}^2}\left(\frac{2d\beta\sqrt{1-\beta}}{R} + \frac{d\beta}{R}\log\left(\frac{\beta}{\left(1 + \sqrt{1-\beta}\right)^2}\right)\right)\right)\right), \tag{3.74}$$

for $R > d\sqrt{\beta}$. Performing variation with respect to $\Phi(R)$, using the Euler-Lagrange equation, we obtain,

$$\frac{d^2}{dR^2}\Phi(R) + \frac{2}{R}\frac{d}{dR}\Phi(R) - \frac{2m}{\hbar^2 I_1}(\tilde{V}_f^{(B)}(R) - E_0)\Phi(R) = 0, \tag{3.75}$$

where $\tilde{V}_f^{(B)}$ denotes the effective potential. As before, with $\Phi(R) = \frac{u(R)}{R}$,

we get,

$$-\frac{d^2}{dR^2}u(R) + \frac{2m}{\hbar^2 I_1}\tilde{V}_f^{(B)}(R)u(R) = \frac{2m}{\hbar^2 I_1}E_0 u(R). \tag{3.76}$$

The effective potential, $\tilde{V}^{(f)}(R)$, is given by,

$$\tilde{V}_f^{(B)}(R) = \tilde{V}_k(R) + \tilde{V}_f(R) + \tilde{V}_B(R). \tag{3.77}$$

The contribution from the kinetic term to the effective potential ($\tilde{V}_k$) is given by,

$$\tilde{V}_k(R) = \frac{\hbar^2}{2m}\left(I_3 - \frac{I_2}{2}\right). \tag{3.78}$$

The contribution from the magnetic field to the effective potential ($\tilde{V}_B$) is given by,

$$\tilde{V}_B(R) = \frac{q^2B^2}{8m}\frac{2}{7}\frac{(7\alpha_1^2+35)}{(5\alpha_1^2+15)}R^2. \tag{3.79}$$

The contribution from the finite dipole to the effective potential ($\tilde{V}_f$) is given by,

$$\tilde{V}_f(R) = QqI_f, \tag{3.80}$$

where I_f is given by equations (3.73) and (3.74). In spite of having different forms for $R > \sqrt{\beta}d$ and $R < \sqrt{\beta}d$, $\tilde{V}_f(R)$ is continuous at $R = d\sqrt{\beta}$. $\tilde{V}_f(d\sqrt{\beta})$ it is given by,

$$\tilde{V}_f(d\sqrt{\beta}) = Qq\left(\frac{1}{d\sqrt{\beta}(1-\beta)^{3/2}}\left(\frac{-6\alpha_1}{3+\alpha_1^2}\left(2\sqrt{\beta(1-\beta)}\right.\right.\right.$$
$$\left.\left.\left.+\sqrt{\beta}\log\left[\frac{\beta}{\left(1+\sqrt{1-\beta}\right)^2}\right]\right)\right)\right). \tag{3.81}$$

Evidently, the effective potential $\tilde{V}_f^{(B)}$ is also continuous at $R = d\sqrt{\beta}$.

Unlike the case of a point dipole, the effective potential is well behaved at short range ($R \to 0$). As $r \to 0$, the contribution of the finite dipole to the actual potential $V_f^{(B)}(r,\theta)$ approaches 0. As may be expected, as $R \to 0$, $\tilde{V}_f(R)$ also approaches 0. To show this, we note that as $R \to 0$, $R\frac{\sqrt{1-\beta}}{d\sqrt{\beta}} \ll 1$. Therefore, ignoring the higher powers of $R\frac{\sqrt{1-\beta}}{d\sqrt{\beta}}$,

$$\log\left(\frac{\left(\frac{d^2\beta}{R^2}-(1-\beta)\right)}{\left(\frac{d\sqrt{\beta}}{R}+\sqrt{1-\beta}\right)^2}\right) = \log\left(\frac{\left(1-R\frac{\sqrt{1-\beta}}{d\sqrt{\beta}}\right)}{\left(1+R\frac{\sqrt{1-\beta}}{d\sqrt{\beta}}\right)}\right) \approx -2R\frac{\sqrt{1-\beta}}{d\sqrt{\beta}}. \tag{3.82}$$

Substituting this in equation (3.80), it is straightforward to show that $\tilde{V}_f(R)$ vanishes at $R = 0$. As $r \to \infty$, in V_f the $\frac{1}{r^2}$ term dominates. Correspondingly, as $R \to \infty$, $\tilde{V}_f \sim \frac{1}{R^2}$. Like the Schrodinger equation with the Hamiltonian given by equation (3.62), equation (3.76) is also not solvable analytically. However, before we proceed to numerical solutions, we make the following observation. As a function of $\tilde{R} = \frac{R}{d}$, the effective potential $\tilde{V}_f^{(B)}(\tilde{R})$ may be written as,

$$\tilde{V}_f^{(B)}(\tilde{R}) = \frac{h^2}{2m}\left(I_3-\frac{I_2}{2}\right)\frac{1}{d^2\tilde{R}^2}+\frac{\lambda}{2d^2}\left(\frac{1}{\tilde{R}(1-\beta)^{3/2}}\left(\frac{-6\alpha_1}{3+\alpha_1^2}\left(2\sqrt{\beta(1-\beta)}+\frac{\beta}{\tilde{R}}\log\left(\frac{\left(\frac{\beta}{\tilde{R}^2}-(1-\beta)\right)}{\left(\frac{\sqrt{\beta}}{\tilde{R}}+\sqrt{1-\beta}\right)^2}\right)\right)\right)\right)+\frac{q^2B^2}{8m}\frac{2}{7}\frac{(7{\alpha_1}^2+35)}{(5\alpha_1^2+15)}d^2\tilde{R}^2, \tag{3.83}$$

for $\tilde{R} \leq \sqrt{\beta}$ and

$$\tilde{V}_f^{(B)}(\tilde{R}) = \frac{h^2}{2m}\left(I_3 - \frac{I_2}{2}\right)\frac{1}{d^2\tilde{R}^2} + \frac{\lambda}{2d^2}\left(\frac{1}{\tilde{R}(1-\beta)^{3/2}}\left(\frac{-6\alpha_1}{3+\alpha_1^2}\left(\frac{2\beta\sqrt{1-\beta}}{\tilde{R}}\right.\right.\right.$$
$$\left.\left.\left. + \frac{\beta}{\tilde{R}}\log\left(\frac{\beta}{\left(1+\sqrt{1-\beta}\right)^2}\right)\right)\right)\right) + \frac{q^2B^2}{8m}\frac{2}{7}\frac{(7{\alpha_1}^2+35)}{(5{\alpha_1}^2+15)}d^2\tilde{R}^2, \tag{3.84}$$

for $\tilde{R} \geq \sqrt{\beta}$.

In terms of $\tilde{R}$ equation (3.76) may be written as,

$$-\frac{1}{d^2}\frac{d^2}{d\tilde{R}^2}u(\tilde{R}) + \frac{2m}{\hbar^2 I_1}\tilde{V}_f^{(B)}(\tilde{R})u(\tilde{R}) = \frac{2m}{\hbar^2 I_1}E_0 u(\tilde{R}). \tag{3.85}$$

Multiplying both sides by d^2, this equation gives,

$$-\frac{d^2}{d\tilde{R}^2}u(\tilde{R}) + \frac{2m}{\hbar^2 I_1}d^2\tilde{V}_f^{(B)}(\tilde{R})u(\tilde{R}) = \frac{2m}{\hbar^2 I_1}d^2E_0 u(\tilde{R}). \tag{3.86}$$

From the above equation it is evident that if we keep the products, $mqQd$ and qBd^2, unchanged, then md^2E_0 also remains unchanged. For a given test particle, therefore, fixing λ and d^2B (say $d^2B = b$) implies that E_0 may be expressed as $\frac{f(\lambda,b)}{d^2}$. Rewriting the Hamiltonian (equation 3.62) in terms of $\tilde{r}$, where $\tilde{r} = \frac{r}{d}$, also makes this evident.

We note that, in the presence of $\vec{B}$, similar to the case of the point dipole, a finite electric dipole of any strength binds a charged particle. This is evident from the long range part of the above equation. As $R \to \infty$, which requires $r \to \infty$, in the effective potential, the contribution from the magnetic field, $\tilde{V}_B$, dominates. Such a potential, analogous to the harmonic

potential, always supports bound states. Using a different method the same conclusion was made by Herman and Wallis [14]. However, as we will see, for molecular dipoles ($\sim$ 1 a.u.) in presence of laboratory scale uniform magnetic fields ($\sim$ 10T) the binding energies are very small. For weaker magnetic fields, therefore, obtaining the bound states numerically may be difficult. The short range part of $\tilde{V}_f^{(B)}$ includes contributions from the kinetic term, $\frac{2I_3 - I_2}{2I_1R^2}$, and also from the finite electric dipole. Therefore, one may expect that, for the same magnetic field $\vec{B}$, different values of the parameter λ will support ground states with different energies. Unlike a point dipole, sufficiently strong λ's are expected to support negative energy bound states. As before, we consider an electron as the test particle. With $m = 1$ and $q = -1$, we tabulate our results below, which clearly reflect this. We assume that $p < 0$. For a given $\gamma = 1$, $B = 2.35\gamma \times 10^5$ T. As before, considering the spin (say $\vec{S}$) of the electron, the ground state energy (say E_0^s) of the electron is given by,

$$E_0^s = E_0 - \vec{\mu}.\vec{B}, \tag{3.87}$$

where the magnetic moment of the electron $\vec{\mu} \approx -\vec{S}$ in a.u. Therefore the actual ground state energy of an electron, with $S_z = \frac{1}{2}$, is given by $(E_0 + .5)$. For $S_z = -\frac{1}{2}$, the actual ground state energy is $(E_0 - .5)$. The corresponding binding energy (say E_b^s), as before, is given by,

$$E_b^s = E_b + \vec{\mu}.\vec{B},$$

where, $E_b = \frac{\gamma}{2} - E_0$, as stated before. For very strong magnetic fields, when

r_c	d	β	α_1	E_0	E_b
0.4472	.05	$.1 \times 10^{-3}$	-.005	2.4994	$.6 \times 10^{-3}$ ($.1565 \times 10^{-3}$)
0.4472	0.5	.22	-.873	2.2023	.2977 (.3744)

Table 8: Energies E_0 and E_b for different values of (2 d) and γ and the corresponding variational parameters β and α_1. γ denotes the strength of the magnetic field in atomic unit. r_c is the corresponding cyclotron radius. 2 d is the separation between the poles of the finite dipole. The binding energies (rounded off to appropriate decimal places) obtained in [13] appear in parentheses.

the cyclotron radius corresponding to $\vec{B}$ ($\sqrt{\frac{\hbar}{eB}}$) is less than the dipole length (2d), the method described in [13] produces better results than ours. In such a situation the electron stays close to the z axis and the energy is minimum when it is close to the positive pole. In reference [13] the variational method was constructed keeping the positive pole at the origin. The wavefunction also explicitly accounts for the strong magnetic field. However, for a cyclotron radius greater than the dipole length, when the electron is not strongly centered around the positive pole, our method gives higher binding energy. Table 8 compares the binding energies obtained by our method with those obtained in [13]. In reference [13] energies for magnetic fields less than 1.175×10^6T are not calculated. Therefore we compare the binding energies for $\gamma = 5$, $d = .05$ a.u. and $d = .5$ a.u. The corresponding cyclotron radius (r_c)is 0.4472 a.u. The binding energies (rounded off to appropriate decimal places) obtained in [13] appear in parentheses.

The strongest uniform magnetic field available in a laboratory is 45 T (Source: www.magnet.fsu.edu). The pulsed fields are even higher. For example the highest field for a long-pulsed magnet is 60T. The corresponding γ is 1.915×10^{-4}. The corresponding cyclotron radius is 72.265 a. u. A typical

molecular dipole moment is about 1 a. u. Also, recall that the critical value $p_c \approx .639$ a.u. Therefore our method is expected to work well in a laboratory set up. In Table 9 we tabulate the binding energies corresponding to $d = .5$ a.u. (dipole moment = 1a.u.), in the presence of magnetic fields of the order of 10 T to 1000 T. We use large γ to avoid numerical errors. R_{max} denotes R corresponding to the maximum value of $\Phi(R)$ and R_{apprx} denotes the approximate range where $\Phi(R)$ is appreciable. The R_{apprx} is noted from the plot of the wavefunction by eye estimation. These very roughly indicate the size of the system. As expected, with weaker magnetic fields the binding becomes weaker. Hence both R_{max} and R_{apprx} increase as B decreases. In Figure 17 we plot $\Phi(R)$ as a function of R for $\gamma = .001$ and $d = 0.5$ a.u. The corresponding value of R_{apprx} is approximately 90 a.u.

γ	r_c	β	α_1	E_0	E_b	R_{max}	R_{apprx}
0	-	.77	-.779	-3.501(-4)	3.501(-4)	10.60	120
1(-4)	100.00	.77	-.779	-3.563(-4)	4.063(-4)	10.60	120
0.5(-3)	44.72	.77	-.779	-3.319(-4)	5.819(-4)	10.48	110
1(-3)	31.62	.77	-.779	-2.950(-4)	7.950(-4)	10.40	90
7.5(-3)	11.55	.70	-.797	8.425(-4)	2.832(-3)	7.50	40
1(-2)	10.00	.70	-.802	1.517(-3)	3.483(-3)	7.20	35
2(-2)	7.07	.66	-.802	4.227(-3)	5.773(-3)	6.20	25
3.5(-2)	5.35	.64	-.802	8.702(-3)	8.798(-3)	5.10	20
5(-2)	4.47	.60	-.825	1.347(-2)	1.153(-2)	4.36	15
1	1.00	.36	-.873	3.932(-1)	1.068(-1)	1.29	4

Table 9: Energies E_0 and E_b for d = .5 a.u. in presence of various magnetic fields and the corresponding variational parameters β and α_1. γ denotes the strength of the magnetic field in atomic unit. r_c is the corresponding cyclotron radius. 2 d is the separation between the poles of the finite dipole.The numbers in parentheses are powers of 10 with which the corresponding entries are to be multiplied.

We also tabulate (Table 10) E_0 and the corresponding E_b for $d = 1$ (dipole

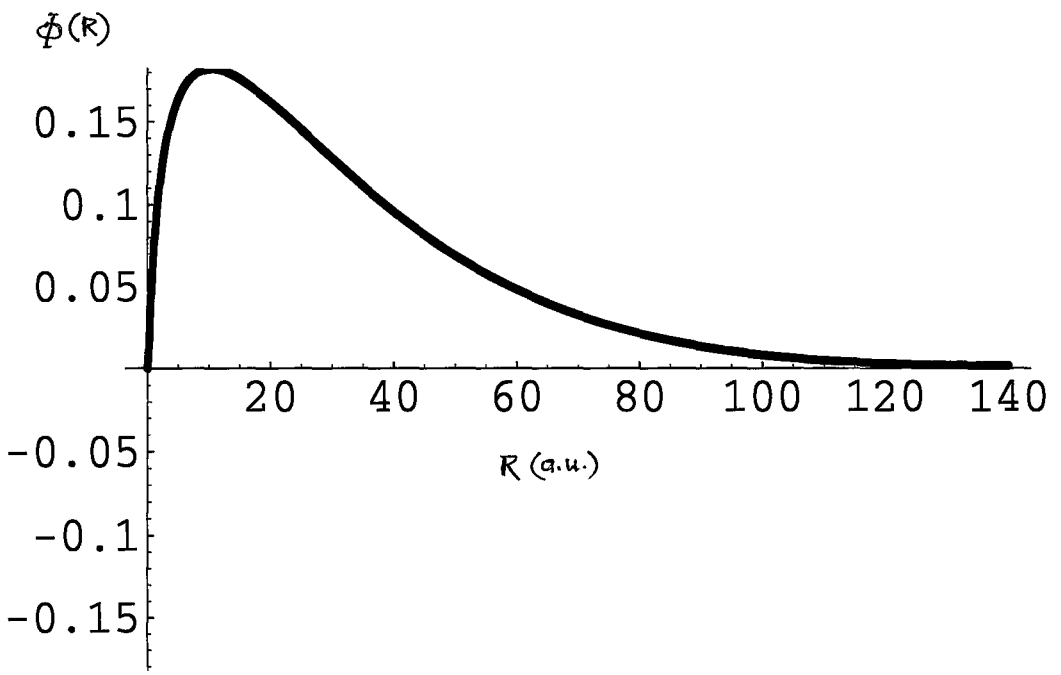

Figure 17: Normalized $\Phi(R)$ vs. R corresponding to $\gamma = .001$ for a finite dipole with $Q = 1$ and $d = .5$ a.u. γ denotes the strength of the magnetic field in atomic unit. 2 d is the separation between the poles of the finite dipole.

moment p =2 a. u.) with different B's.

In Figures 18 and 20 we plot E_b and the corresponding B for $d = 0.5$ a.u. and $d = 1$ a.u. respectively. In Figures 19 and 21 E_0 and the corresponding B have been plotted for the cases mentioned above.

Note that α_1 is always negative. Since the positive pole of the electric dipole is located at $z = -d$, therefore, for a fixed ρ, the probability density of the electron is expected to be greater along the negative z axis. In our trial wavefunction, $\Phi(R)$ is independent of the sign of z, but $\Theta(\eta)$ is not. As shown in Figure 22, a negative α_1 makes $\Theta(\eta)$ larger along the negative z

γ	r_c	β	α_1	E_0	E_b	R_{max}	R_{apprx}
.01	10.00	.56	-1.083	-.0466	.0516	1.92	10
.146	2.62	.53	-1.111	-.0307	.1037	1.76	9
1	1.00	.36	-1.141	.2287	.2713	1.20	4
1.46	0.83	.30	-1.171	.4137	.3163	1.08	3
2	0.70	.26	-1.200	.6291	.3709	0.96	2.5
3	0.58	.21	-1.202	1.0559	.4441	0.83	2
4	0.50	.18	-1.233	1.5088	.4912	0.75	1.8
5	0.45	.16	-1.233	1.9734	.5266	0.67	1.6

Table 10: Energies E_0 and E_b for d = 1 a.u. in presence of various magnetic fields and the corresponding variational parameters β and α_1. γ denotes the strength of the magnetic field in atomic unit. r_c is the corresponding cyclotron radius. 2 d is the separation between the poles of the finite dipole.

d	β	α_1	E_0	E_b
0.5	.68	-0.83	.001	.004
1.0	.56	-1.08	-.047	.052
1.5	.44	-1.23	-.100	.105
2.0	.36	-1.33	-.131	.136
3.0	.27	-1.44	-.153	.158

Table 11: Energies E_0 and E_b corresponding to $\gamma = .01$ ($r_c = 10$ a.u.) and various charge separations (2 d) and the corresponding variational parameters β and α_1.

axis. Thus the asymmetry along the z axis is taken care of. Figure 23, a 3D plot of $\Theta(\eta)$ also reflects the asymmetry along the z axis. The ellipsoid shape hints at the absence of any spherical symmetry.

Stronger magnetic fields evidently give rise to larger values of E_0. In Figure 24, β and the corresponding B have been plotted. As expected, since β decreases as γ increases. Recall that $\beta \rightarrow 0$ for only B.

We also tabulate (Table 11) E_0 and the corresponding E_b for various dipole moments with $Q = 1$ and $\gamma = .01$. The corresponding cyclotron radius is 10 a.u. The separation 2 d is varied to obtain different dipole moments. In

Figure 25 we plot E_b and the corresponding d. Evidently the binding becomes stronger as d increases. This may be because of the fact that as the negative pole moves away, the electron will be strongly bound by the positive pole. In reference [13] the authors obtained similar result. For larger dipole moments α_1 increases. Considering that α_1 strengthens the coupling between the odd and the even Legendre polynomials, such a behavior is expected. Note that β decreases with increasing d, hinting towards the domination of the magnetic field over the dipole. This also may be attributed to the fact that for large dipole length the electron will be bound mainly by the positive pole. The dipole effects may not dominate.

As is expected, when the cyclotron radius is much smaller than the dipole length, a finite dipole may be approximated by a point dipole. In Table 12 we compare the binding energies corresponding to $\gamma = .001$ and $p \in \{.8, 1, 1.2\} a.u.$ The corresponding cyclotron radius is 31.623 a.u. The numbers in the square braces are the corresponding entries for the point dipole. The last three rows of the Table indicate that the approximation, as mentioned above, holds good even when the charge separation in the dipole (2 d) is increased keeping the dipole moment unaltered. Also the data indicates that, the smaller the separation is, the better the approximation holds. To demonstrate this, however, we have assumed fractional charges at the poles. The binding energies increase with the dipole moment as expected. The binding energies corresponding to the point dipoles are slightly higher than the binding energies corresponding to the finite dipoles of the same moment. This may be because of the fact that at short range ($r \to 0$) the point dipole potential is stronger than that of the finite dipole. The use of

p	d	β	α_1	E_0	E_b
0.4	0.20	0.17 [.180]	-.486 [-.493]	4.957(-4) [4.933(-4)]	4.30(-6)[6.70(-6)]
0.6	0.30	0.42 [.542]	-.647 [-.626]	4.491(-4) [4.378(-4)]	5.09(-5)[6.22(-5)]
0.5	0.25	0.29 [.317]	-.585 [-.589]	4.762(-4) [4.746(-4)]	2.16(-5)[2.54(-5)]
0.5	0.50	0.27 [.317]	-.585 [-.589]	4.767(-4) [4.746(-4)]	2.12(-5)[2.54(-5)]
0.5	1.00	0.27 [.317]	-.585 [-.589]	4.775(-4) [4.746(-4)]	2.04(-5)[2.54(-5)]

Table 12: E_b corresponding to $\gamma = .001$ ($r_c = 31.623$ a.u.)for point and finite dipoles with various dipole moments and the corresponding variational parameters β, α_1. The numbers in square brackets are the corresponding values for point dipoles. The numbers in parentheses are powers of 10 with which the corresponding entries are to be multiplied.

one more variational parameter (α_2) may also cause the difference. However, such a comparison is meaningful only for $p < p_c$, where p_c denotes the critical dipole moment in absence of the magnetic field. As we have already discussed, for $p > p_c$ the point dipole potential is anomalous. However, for $p > p_c$ finite dipoles have negative energy bound states. Therefore, in presence of a sufficiently weak magnetic field, a finite dipole may have negative energy (E_0) bound states. The results in Tables 9, 10 and 11 reflect this. On the contrary, for a point dipole with $p > p_c$, equation (3.55) with the constraint imposed by equation (3.50) assures the non-negativity of the ground state energy E_0 for any magnetic field. This has stopped us from tabulating the binding energies for the point dipoles with $p > p_c$.

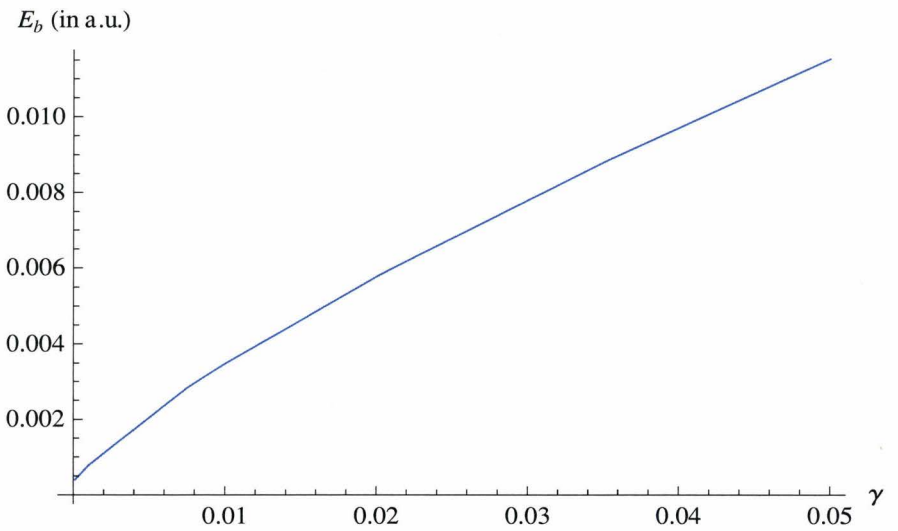

Figure 18: Binding energy (E_b) vs. the corresponding γ for a finite dipole with $Q = 1$ and $d = .5$ a.u. γ denotes the strength of the magnetic field in atomic unit. 2 d is the separation between the poles of the finite dipole.

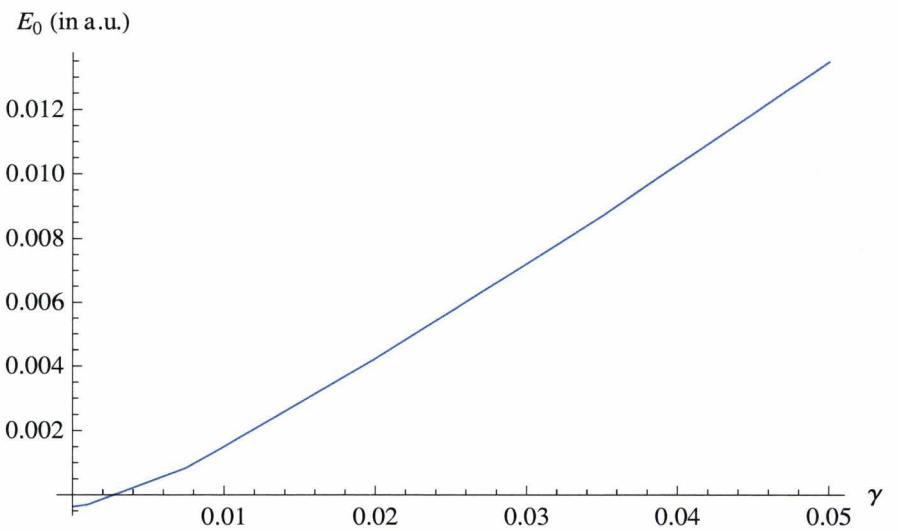

Figure 19: Ground state energy E_0 vs. the corresponding γ for a finite dipole with $Q = 1$ and $d = .5$ a.u.

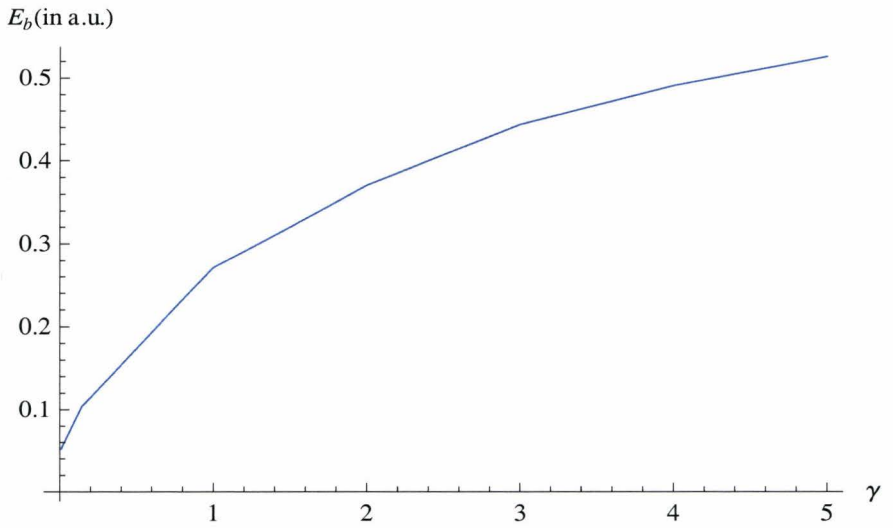

Figure 20: Binding energy (E_b) vs. the corresponding γ for a finite dipole with $Q = 1$ and $d = 1$ a.u.

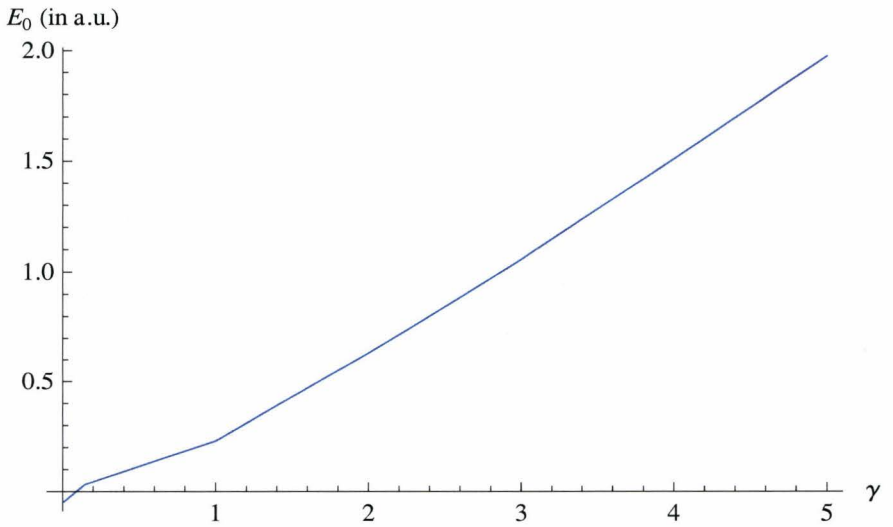

Figure 21: Ground state energy E_0 vs. the corresponding γ with $Q = 1$ and $d = 1$ a.u.

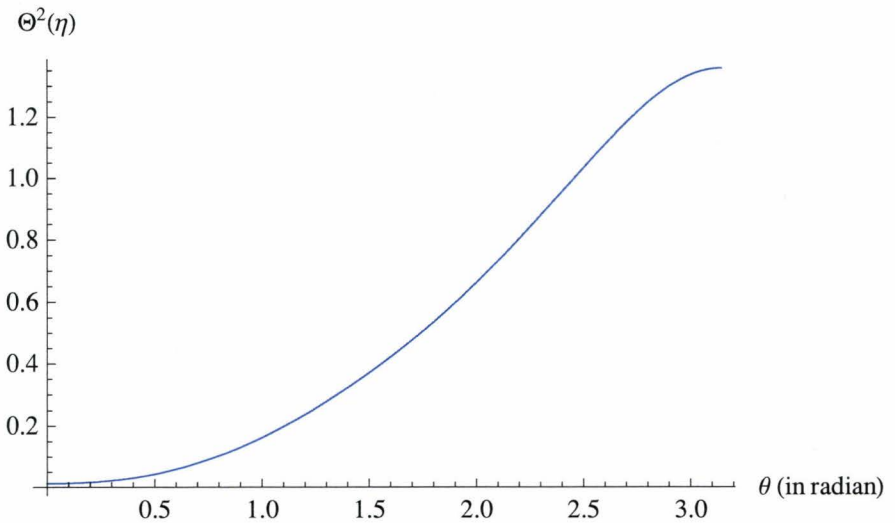

Figure 22: $\Theta^2(\eta)$ (equation (3.65)) corresponding to $\lambda = 1$ and $\gamma = .05$ vs. θ.

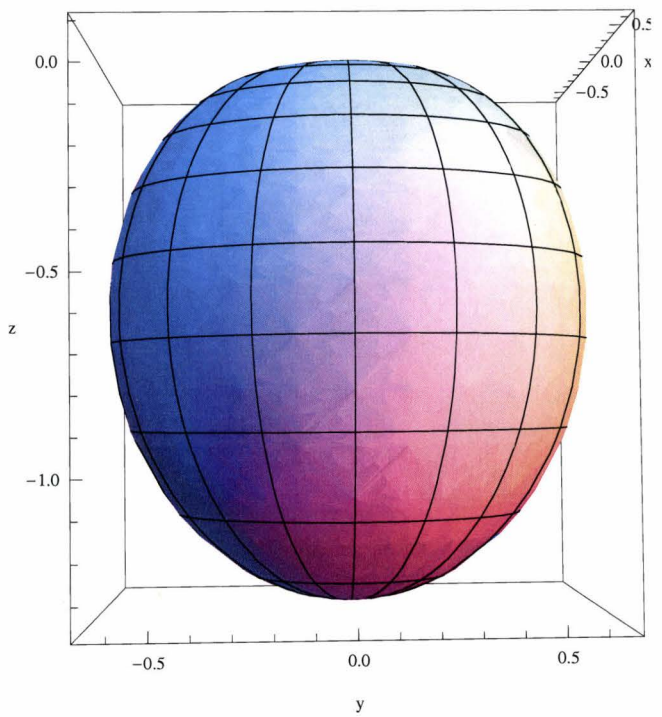

Figure 23: A 3D plot of $\Theta^2(\eta)$ (equation (3.65)) corresponding to $\lambda = 1$ and $\gamma = .05$.

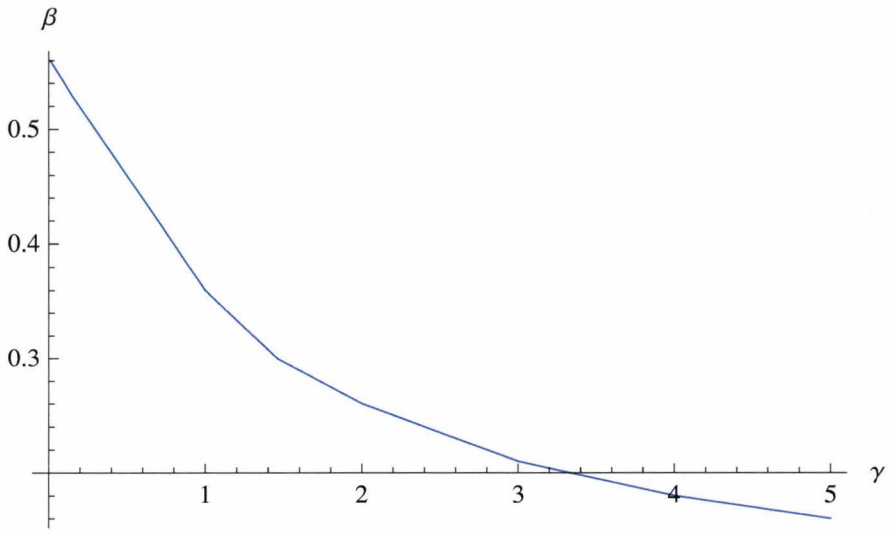

Figure 24: The variational parameter β for a finite dipole with $Q = 1$ and $d = 1$ a.u. vs. γ

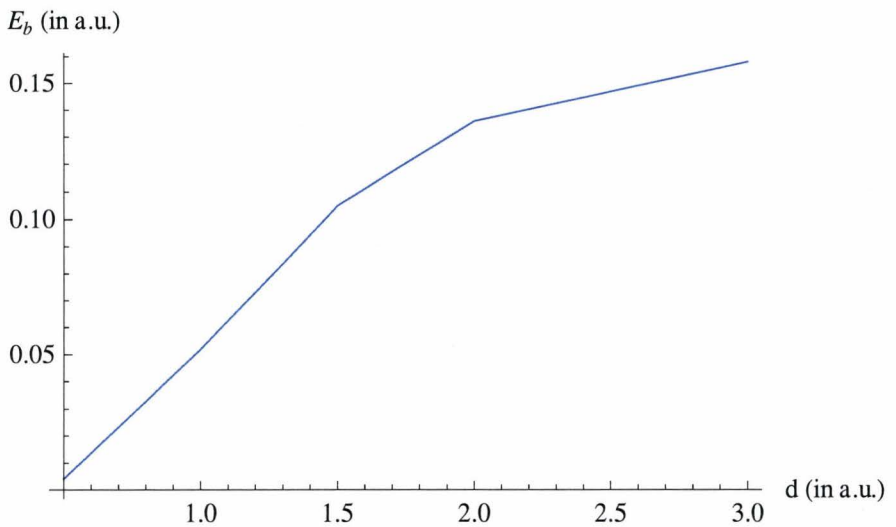

Figure 25: The binding energy E_b for the magnetic field given by $\gamma = .01$ vs. d.

Comment :

A sign change in λ and the parity transformation evidently transform the Hamiltonians in equations (3.29) and (3.62) in the same way. Hence, following our argument in comment (b) of the previous section, $\lambda \rightarrow -\lambda$ implies $\alpha_1 \rightarrow -\alpha_1$. However, β and E_0 will remain the same. Considering the spin part, we note that $\vec{S}.\vec{B}$ remains unchanged under parity transformation. However, the sign of the term $\vec{\mu}.\vec{B}$ depends on the sign of the charge q. Therefore if q changes sign then the actual ground state energy with $m_l = 0$ will also change accordingly.

4 Conclusion

In conclusion, in the presence of a magnetic field along the dipole moment, the binding energy of a rigid and stationary dipole binding a charged particle increases. We considered (Table 9)a dipole with dipole moment 2.54 D (2 d = 1 a.u.) binding an electron. In the absence of a magnetic field the binding energy is found to be 9.5 meV. Though we assumed the dipole to be stationary and rigid, this still turned out to be in good agreement with the binding energy of an electron in presence of a water dimar ($\sim$ 2.6 D) [8, 23]. In the laboratory, as we mentioned, very high magnetic fields are in the range 10-100 T. In the presence of such magnetic fields, the binding energy is found to increase by 15 % - 66 %. The values of the binding energies are listed in Table 9. The thermal energy corresponding to 1 K is 8.62×10^{-5} eV, at room temperature (300 K) this becomes 2.59×10^{-2} eV. Thus, even in the presence of very strong magnetic field, the binding energy is still much less than the thermal energy at room temperature. However, since the binding energy increases significantly, so it may be easier to detect such bound states. Also the mobility of eletrons in a polar medium will be affected. At lower temperatures, of course, the effect of such bound states will be stronger.

We have also shown that in the presence of a magnetic field along the dipole moment, a point dipole of any dipole moment binds a charged particle. The point dipole potential is anomalous for $p > p_c$, where p_c denotes the critical dipole moment in absence of a magnetic field. Hence the cases with $p > p_c$, are not considered. For weak magnetic fields (the cyclotron radius

$r_c \gg 2d$), the point dipole is a good approximation to the finite dipole. As expected, the approximation becomes even better as the charge separation in the finite dipole decreases. However, such an approximation is valid only for $p > p_c$. The finite dipoles, with dipole moments less than p_c, also bind a charged particle in presence of a magnetic field.

This variational method may also be applied to obtain the excited states with $m_l = 0$. The excited states with other values of m_l's may also be obtained by suitably choosing $\Theta(\eta)$. The implicit dependence of our variables (R, η) on (r, θ) measured from the center of the dipole, however, restrict the validity of our approach to large dipole length and to very strong magnetic fields. As we already discussed, our method will still be useful to determine the energy levels of the electron when the cyclotron radius of $\vec{B}$ is greater than the dipole separation.

A Appendix

The two lowest moments of a point electric dipole supporting zero energy bound states with the azimuthal quantum number $m_l = 0$.

We obtain a few of the dipole moments which are greater than the critical dipole moment but also support zero energy bound state with azimuthal quantum number $m_l = 0$. We assume that the wavefunction is given by,

$$\Psi(r,\theta,\phi) = \frac{1}{\sqrt{2\pi}}\Phi(r)\Theta(\theta), \Theta(\theta) = N_n(1 + \Sigma_{i=1}^{n}\alpha_i P_i(\cos\theta)), \tag{A.1}$$

where N_n is the corresponding normalization constant. To keep calculations simple we assume that $n = 5$. We consider $\langle\Psi|\hat{H} - E_0|\Psi\rangle$. We do variation with respect to the radial part of the wavefunction, $\Phi(r)$,

$$\delta\langle\Psi|\hat{H} - E_0|\Psi\rangle = 0.$$

As before, with $u(r) = \dfrac{\Phi(r)}{r}$, the Euler-Lagrange equation gives,

$$-\frac{d}{dr^2}u(r) + \frac{(2310\alpha_1^2 + 4158\alpha_2^2 + 5940\alpha_3^2 + 7700\alpha_4^2 + 9450\alpha_5^2)}{1155\alpha_1^2 + 693\alpha_2^2 + 5\,(693 + 99\alpha_3^2 + 77\alpha_4^2 + 63\alpha_5^2)}\frac{u(r)}{r^2}$$
$$+\frac{(462\alpha_1(5 + 2\alpha_2) + 594\alpha_2\alpha_3 + 440\alpha_3\alpha_4 + 350\alpha_4\alpha_5)\lambda}{1155\alpha_1^2 + 693\alpha_2^2 + 5\,(693 + 99\alpha_3^2 + 77\alpha_4^2 + 63\alpha_5^2)}\frac{u(r)}{r^2} = \frac{2m}{\hbar^2}E_0 u(r). \tag{A.2}$$

For a zero energy bound state $E_0 = 0$, we demand that the coefficient of $\frac{1}{r^2}$ to be equal to $-\frac{1}{4}$ [15, 16]. Therefore,

$$\frac{(2310\alpha_1^2 + 4158\alpha_2^2 + 5940\alpha_3^2 + 7700\alpha_4^2 + 9450\alpha_5^2)}{1155\alpha_1^2 + 693\alpha_2^2 + 5\,(693 + 99\alpha_3^2 + 77\alpha_4^2 + 63\alpha_5^2)} + \frac{(462\alpha_1(5 + 2\alpha_2) + 594\alpha_2\alpha_3 + 440\alpha_3\alpha_4 + 350\alpha_4\alpha_5)\lambda}{1155\alpha_1^2 + 693\alpha_2^2 + 5\,(693 + 99\alpha_3^2 + 77\alpha_4^2 + 63\alpha_5^2)} = -\frac{1}{4}. \tag{A.3}$$

Now we claim that for non-degenerate zero energy bound states the variational parameters must be unique. Solving for the variational parameter α_1 from the above equation we get the following,

$$\alpha_1 = \frac{1}{20790}\left(-9240\lambda - 3696\alpha_2\lambda \pm \sqrt{D_1}\right). \tag{A.4}$$

where,

$$D_1 = (9240\lambda + 3696\alpha_2\lambda)^2 - 41580\left(3465 + 17325\alpha_2^2 + 24255\alpha_3^2 + 31185\alpha_4^2 + 38115\alpha_5^2 + 2376\alpha_2\alpha_3\lambda + 1760\alpha_3\alpha_4\lambda + 1400\alpha_4\alpha_5\lambda\right). \tag{A.5}$$

For unique α_1 we demand that the discriminant of the above equation D_1 vanishes. Therefore,

$$\alpha_1 = \frac{1}{20790}\left(-9240\lambda - 3696\alpha_2\lambda\right). \tag{A.6}$$

Also this gives us the following equation.

$$\alpha_2^2\left(-720373500+13660416\lambda^2\right)+\alpha_2\left(-98794080\alpha_3\lambda+68302080\lambda^2\right)-144074700$$
$$-1008522900\alpha_3^2-1296672300\alpha_4^2-1584821700\alpha_5^2-73180800\alpha_3\alpha_4\lambda$$
$$-58212000\alpha_4\alpha_5\lambda+85377600\lambda^2=0. \tag{A.7}$$

Solving for α_2 we get,

$$\alpha_2=\frac{35640\alpha_3\lambda-24640\lambda^2\pm\sqrt{D_2}}{2\left(-259875+4928\lambda^2\right)}. \tag{A.8}$$

where,

$$D_2=\left(-35640\alpha_3\lambda+24640\lambda^2\right)^2-4\left(-259875+4928\lambda^2\right)\left(-51975-363825\alpha_3^2\right.$$
$$\left.-467775\alpha_4^2-571725\alpha_5^2-26400\alpha_3\alpha_4\lambda-21000\alpha_4\alpha_5\lambda+30800\lambda^2\right). \tag{A.9}$$

For unique α_2 the discriminant of the above equation, D_2 must vanish. Therefore,

$$\alpha_2=\frac{35640\alpha_3\lambda-24640\lambda^2}{2\left(-259875+4928\lambda^2\right)} \tag{A.10}$$

Also this leads to the equation,

$$\begin{aligned}
&\alpha_3^2\left(1270209600\lambda^2+1455300\left(-259875+4928\lambda^2\right)\right)\\
&+\alpha_3\left(-1756339200\lambda^3+105600\alpha_4\lambda\left(-259875+4928\lambda^2\right)\right)\\
&+607129600\lambda^4+207900\left(-259875+4928\lambda^2\right)+1871100\alpha_4^2\left(-259875+4928\lambda^2\right)\\
&+2286900\alpha_5^2\left(-259875+4928\lambda^2\right)+84000\alpha_4\alpha_5\lambda\left(-259875\right.\\
&\left.+4928\lambda^2-123200\lambda^2\left(-259875+4928\lambda^2\right)=0.\right.
\end{aligned} \tag{A.11}$$

Solving for α_3 we get,

$$\alpha_3=\frac{8316000\alpha_4\lambda+532224\lambda^3-157696\alpha_4\lambda^3\pm\sqrt{D_3}}{2\left(-114604875+2558160\lambda^2\right)}. \tag{A.12}$$

where,

$$\begin{aligned}
D_3=&\left(-8316000\alpha_4\lambda-532224\lambda^3+157696\alpha_4\lambda^3\right)^2-4\left(-114604875+2558160\lambda^2\right)\\
&\left(-16372125-147349125\alpha_4^2-180093375\alpha_5^2-6615000\alpha_4\alpha_5\lambda+10012464\lambda^2\right.\\
&\left.+2794176\alpha_4^2\lambda^2+3415104\alpha_5^2\lambda^2+125440\alpha_4\alpha_5\lambda^3\right).
\end{aligned} \tag{A.13}$$

For unique α_3, claiming that the discriminant of the above equation D_3 must vanish, we obtain,

$$\alpha_3=\frac{8316000\alpha_4\lambda+532224\lambda^3-157696\alpha_4\lambda^3}{2\left(-114604875+2558160\lambda^2\right)}. \tag{A.14}$$

Also,

$$\begin{aligned}
&\alpha_4^2(69155856000000\lambda^2 - 2622799872000\lambda^4 \\
&+24868028416\lambda^6 + 589396500\left(-114604875 + 2558160\lambda^2\right) \\
&-11176704\lambda^2\left(-114604875 + 2558160\lambda^2\right)) \\
&+\alpha_4\left(8851949568000\lambda^4 - 167859191808\lambda^6\right. \\
&+26460000\alpha_5\lambda\left(-114604875 + 2558160\lambda^2\right) \\
&-501760\alpha_5\lambda^3\left(-114604875 + 2558160\lambda^2\right) = 0.
\end{aligned} \tag{A.15}$$

Solving for α_4,

$$\alpha_4 = \frac{9(-23152500\alpha_5\lambda + 516800\alpha_5\lambda^3 + 67584\lambda^4 \pm \sqrt{15}\sqrt{D_4})}{11\left(843908625 - 19701360\lambda^2 + 16384\lambda^4\right)}. \tag{A.16}$$

For unique α_4 claiming the discriminant of the above equation to be zero we get,

$$\alpha_4 = \frac{9(-23152500\alpha_5\lambda + 516800\alpha_5\lambda^3 + 67584\lambda^4)}{11\left(843908625 - 19701360\lambda^2 + 16384\lambda^4\right)}. \tag{A.17}$$

Also,

$$\begin{aligned}
&\alpha_5^2\left(-86686230666853125 + 3994430311746000\lambda^2 - 48450969020160\lambda^4\right. \\
&+55371853824\lambda^6) + \alpha_5\left(-208631808000\lambda^5 + 465698\right) \\
&-7880566424259375 + 5029846600086000\lambda^2 - 128966221359360\lambda^4 \\
&+460241408000\lambda^6 = 0.
\end{aligned} \tag{A.18}$$

Solving for α_5,

$$\alpha_5 = \frac{11\left(-40960\lambda^5 \pm \sqrt{D_5}\right)}{21\left(17829244125 - 423580320\lambda^2 + 510208\lambda^4\right)}. \tag{A.19}$$

where,

$$D_5 = 5\left(-21064754052045309375 + 1347503003547472800 0\lambda^2 - 363961674836282880\lambda^4 \right.$$
$$\left. +1680656736632832\lambda^6 - 1577154969600\lambda^8 + 335544320\lambda^{10}\right). \tag{A.20}$$

Obviously it is required that the denominators in the expressions obtained for the variational parameters are non-zero. For unique α_5 as before claiming that the discriminant of the above equation, D_5 to be zero we get the following solutions for λ,

$$\lambda = \pm 57.167, \pm 34.0293, \pm 15.1034, \pm 6.66936, \pm 1.27863. \tag{A.21}$$

However among these values $\pm 34.0293, \pm 6.66936$ are the roots of the following equation which appears in the denominator of α_4,

$$843908625 - 19701360\lambda^2 + 16384\lambda^4 = 0. \tag{A.22}$$

Thus these correspond to the singularities of the coefficient α_4. Eliminating these values from the list we obtain the first three values of λ which support a zero energy bound state,

$$\lambda = \pm 57.167, \pm 15.1034, \pm 1.27863 \tag{A.23}$$

As may be evident, these values of λ can also be obtained by substituting the expressions for α_1,α_2,α_3,α_4,α_5 in equation(24), assuming the corresponding discriminants to be zero. Assuming the denominators to be non zero as before, a straight forward simplification gives,

$$\frac{-\left(8\lambda^2\left(9157093096633453125-237839965834274496\lambda^2+1202365414801920\lambda^4\right)\right)}{D} \\ \frac{-\left(8\lambda^2\left(-1403318190080\lambda^6+331939840\lambda^8\right)\right)}{D}=-\frac{1}{4}, \tag{A.24}$$

where,

$$D=44503472449638582187 5+815677050011531400 0\lambda^2+195706209785522688\lambda^4 \\ -82098239545344\lambda^6+317594992640\lambda^8+173015040\lambda^{10}, \tag{A.25}$$

or,

$$-24960941775+15384681648\lambda^2-71635200\lambda^4+20480\lambda^6=0, \tag{A.26}$$

Therefore,

$$\lambda=\pm 57.167, \pm 15.1034, \pm 1.27863.$$

B Appendix

The two lowest moments of a point electric dipole supporting zero energy bound states with the azimuthal quantum number $m_l = 1$.

We obtain the lowest two dipole moments which are greater than the critical dipole moment but also support zero energy bound state with the azimuthal quantum number (m_l) 1. We assume that the wavefunction is given by,

$$\Psi(r, \theta, \phi) = \frac{1}{\sqrt{2\pi}} \Phi(r) \Theta(\theta) e^{i\phi}, \tag{B.1}$$

$$\Theta(\theta) = N_5 (P_1^1(\cos\theta) + \Sigma_{i=2}^{6} \alpha_i P_i^1(\cos\theta)), \tag{B.2}$$

where N_5 is the corresponding normalization constant.

We perform variation of $\langle \Psi | \hat{H} - E_0 | \Psi \rangle$ with respect to the radial part of the wavefunction, $\Phi(r)$,

$$\delta \langle \Psi | \hat{H} - E_0 | \Psi \rangle = 0.$$

As before, with $u(r) = \frac{\Phi(r)}{r}$, the Euler-Lagrange equation gives,

$$-u''(r) + \frac{2\left(15015 + 81081\alpha_1^2 + 231660\alpha_2^2 + 500500\alpha_3^2 + 921375\alpha_4^2 + 1528065\alpha_5^2\right)}{\left(27027\alpha_1^2 + 5\left(7722\alpha_2^2 + 7\left(429 + 1430\alpha_3^2 + 1755\alpha_4^2 + 2079\alpha_5^2\right)\right)\right)r^2}u(r)$$
$$+\frac{2(1287\alpha_1(7 + 12\alpha_2) + 21450\alpha_2\alpha_3 + 27300\alpha_3\alpha_4 + 33075\alpha_4\alpha_5)\lambda}{\left(27027\alpha_1^2 + 5\left(7722\alpha_2^2 + 7\left(429 + 1430\alpha_3^2 + 1755\alpha_4^2 + 2079\alpha_5^2\right)\right)\right)r^2}u(r) = \frac{2m}{\hbar^2}E_0 u(r), \tag{B.3}$$

where as usual $u''(r) = \frac{d^2}{dr^2}u(r)$. For a zero energy bound state $E_0 = 0$, we demand that the coefficient of $\frac{1}{r^2}$ to be equal to $-\frac{1}{4}$ [15, 16]. Therefore,

$$\frac{2\left(15015 + 81081\alpha_1^2 + 231660\alpha_2^2 + 500500\alpha_3^2 + 921375\alpha_4^2 + 1528065\alpha_5^2\right)}{\left(27027\alpha_1^2 + 5\left(7722\alpha_2^2 + 7\left(429 + 1430\alpha_3^2 + 1755\alpha_4^2 + 2079\alpha_5^2\right)\right)\right)}$$
$$+\frac{2(1287\alpha_1(7 + 12\alpha_2) + 21450\alpha_2\alpha_3 + 27300\alpha_3\alpha_4 + 33075\alpha_4\alpha_5)\lambda}{\left(27027\alpha_1^2 + 5\left(7722\alpha_2^2 + 7\left(429 + 1430\alpha_3^2 + 1755\alpha_4^2 + 2079\alpha_5^2\right)\right)\right)} = -\frac{1}{4}. \tag{B.4}$$

For single zero energy bound states the variational parameters must be unique. Solving for the variational parameter α_1 from the above equation we get the following,

$$\alpha_1 = \frac{1}{450450}(-24024\lambda - 41184\alpha_2\lambda \pm \sqrt{D_1}). \tag{B.5}$$

where,

$$D_1 = ((24024\lambda + 41184\alpha_2\lambda)^2 - 900900(45045 + 630630\alpha_2^2 + 1351350\alpha_3^2 + 2477475\alpha_4^2 + 4099095\alpha_5^2 + 57200\alpha_2\alpha_3\lambda + 72800\alpha_3\alpha_4\lambda + 88200\alpha_4\alpha_5\lambda)). \tag{B.6}$$

For unique α_1 we demand that the discriminant of the above equation D_1 vanishes. Therefore,

$$\alpha_1 = \frac{(-24024\lambda - 41184\alpha_2\lambda)}{450450}. \tag{B.7}$$

Solving $D_1 = 0$ for α_2 we get,

$$\alpha_2 = \frac{10010000\alpha_3\lambda - 384384\lambda^2 \pm \sqrt{D_2}}{2\,(-110360250 + 329472\lambda^2)}, \tag{B.8}$$

where,

$$D_2 = (-4(-7882875 - 236486250\alpha_3^2 - 433558125\alpha_4^2 - 717341625\alpha_5^2 - 12740000\alpha_3\alpha_4\lambda - 15435000\alpha_4\alpha_5\lambda + 112112\lambda^2)(-110360250 + 329472\lambda^2) + (-10010000\alpha_3\lambda + 384384\lambda^2)^2). \tag{B.9}$$

For unique α_2 the discriminant of the above equation, D_2 must vanish. Therefore,

$$\alpha_2 = \frac{10010000\alpha_3\lambda - 384384\lambda^2 \pm \sqrt{D_2}}{2\,(-110360250 + 329472\lambda^2)}. \tag{B.10}$$

Solving $D_2 = 0$ for α_3 we get,

$$\alpha_3 = \frac{802620000\alpha_4\lambda + 1098240\lambda^3 - 2396160\alpha_4\lambda^3 \pm \sqrt{D_3}}{2\left(-14898633750 + 58778720\lambda^2\right)}, \tag{B.11}$$

where,

$$\begin{aligned} D_3 = ((-802620000\alpha_4\lambda - 1098240\lambda^3 + 2396160\alpha_4\lambda^3)^2 - 4(-14898633750 + 58778720\lambda^2) \\ (-496621125 - 27314161875\alpha_4^2 - 45192522375\alpha_5^2 - 972405000\alpha_4\alpha_5\lambda \\ +8545680\lambda^2 + 81544320\alpha_4^2\lambda^2 + 134918784\alpha_5^2\lambda^2 + 2903040\alpha_4\alpha_5\lambda^3)). \end{aligned} \tag{B.12}$$

For unique α_3, claiming that the discriminant of the above equation D_3 must vanish, we obtain,

$$\alpha_3 = \frac{802620000\alpha_4\lambda + 1098240\lambda^3 - 2396160\alpha_4\lambda^3}{2\left(-14898633750 + 58778720\lambda^2\right)}. \tag{B.13}$$

Solving $D_3 = 0$ for α_4,

$$\alpha_4 = \frac{11\left(-4375822500\alpha_5\lambda + 17263680\alpha_5\lambda^3 + 133120\lambda^4\right)}{\left(195\left(13867189875 - 60197424\lambda^2 + 16384\lambda^4\right)\right)}, \tag{B.14}$$

where,

$$D_4 = 77\sqrt{15}((-1494895202316140625 - 1360354634107687968750\alpha_5^2 + 336477905241660000\lambda^2 + 1153273806221922000\alpha_5^2\lambda^2 - 140067438600960\lambda^4 - 2696065598677248\alpha_5^2\lambda^4 - 1585059840000\alpha_5\lambda^5 + 120671948800\lambda^6 + 1039588651008\alpha_5^2\lambda^6 + 6253445120\alpha_5\lambda^7)). \tag{B.15}$$

For unique α_4 claiming the discriminant of the above equation to be zero we get,

$$\alpha_4 = \frac{11\,(-4375822500\alpha_5\lambda + 17263680\alpha_5\lambda^3 + 133120\lambda^4)}{(195\,(13867189875 - 60197424\lambda^2 + 16384\lambda^4))}. \tag{B.16}$$

Solving $D_4 = 0$ for α_5,

$$\alpha_5 = \frac{13\left(-40960\lambda^5 \pm \sqrt{D_5}\right)}{(9\,(10155405385125 - 46029390176\lambda^2 + 19671296\lambda^4))}. \tag{B.17}$$

where,

$$D_5 = \sqrt{5}(-10863792107983996118437 5 + 2509071041245016001600\lambda^2 - 1157380727736331929 6\lambda^4 + 1398125650688409 6\lambda^6 - 4305653268480\lambda^8 + 335544320\lambda^{10}). \tag{B.18}$$

Obviously it is assumed that the denominators in the expressions obtained for the variational parameters are non-zero. For unique α_5 as before claiming

that the discriminant of the above equation, D_5 to be zero we get the following solutions for λ,

$$\lambda = \pm 91.0975, \pm 58.5423, \pm 28.3094, \pm 15.715, \pm 7.58394. \tag{B.19}$$

However among these values $\pm 58.5423, \pm 15.715$ are the roots of the following equation which appears in the denominator of α_4,

$$13867189875 - 60197424\lambda^2 + 16384\lambda^4 = 0. \tag{B.20}$$

Thus these correspond to the singularities of the coefficient α_4. Among the rest, the lowest two values are the first two values of λ which support zero energy bound states with $m_l = 1$,

$$\lambda = \{\pm 28.3094, \pm 7.58394\} \tag{B.21}$$

C Appendix

The two lowest moments of a point electric dipole supporting zero energy bound states with the azimuthal quantum number $m_l = 2$.

We obtain the lowest two dipole moments which are greater than the critical dipole moment but also support zero energy bound state with the azimuthal quantum number (m_l) 2. We assume that the wavefunction is given by,

$$\Psi(r,\theta,\phi) = \frac{1}{\sqrt{2\pi}}\Phi(r)\Theta(\theta)e^{i2\phi}, \tag{C.1}$$

$$\Theta(\theta) = N_5(P_2^2(\cos\theta) + \Sigma_{i=3}^{7}\ \alpha_i P_i^2(\cos\theta)), \tag{C.2}$$

where N_5 is the corresponding normalization constant. We perform variation of $\langle\Psi|\hat{H} - E_0|\Psi\rangle$ with respect to the radial part of the wavefunction, $\Phi(r)$,

$$\delta\langle\Psi|\hat{H} - E_0|\Psi\rangle = 0.$$

As before, with $u(r) = \dfrac{\Phi(r)}{r}$, the Euler-Lagrange equation gives,

$$-u''(r) + \frac{2\left(9009 + 64350\alpha_1^2 + 250250\alpha_2^2 + 716625\alpha_3^2 + 1697850\alpha_4^2 + 3531528\alpha_5^2\right)}{10725\alpha_1^2 + 7\left(429 + 3575\alpha_2^2 + 6825\alpha_3^2 + 11550\alpha_4^2 + 18018\alpha_5^2\right)}\frac{u(r)}{r^2}$$
$$+\frac{2(715\alpha_1(3 + 10\alpha_2) + 15925\alpha_2\alpha_3 + 29400\alpha_3\alpha_4 + 48510\alpha_4\alpha_5)\lambda}{10725\alpha_1^2 + 7\left(429 + 3575\alpha_2^2 + 6825\alpha_3^2 + 11550\alpha_4^2 + 18018\alpha_5^2\right)}\frac{u(r)}{r^2} = \frac{2m}{\hbar^2}E_0 u(r), \tag{C.3}$$

where as usual $u''(r) = \frac{d^2}{dr^2}u(r)$. For a zero energy bound state $E_0 = 0$, we demand that the coefficient of $\frac{1}{r^2}$ to be equal to $-\frac{1}{4}$ [15, 16]. Therefore,

$$\frac{2(9009 + 64350\alpha_1^2 + 250250\alpha_2^2 + 716625\alpha_3^2 + 1697850\alpha_4^2 + 3531528\alpha_5^2)}{10725\alpha_1^2 + 7(429 + 3575\alpha_2^2 + 6825\alpha_3^2 + 11550\alpha_4^2 + 18018\alpha_5^2)} + \frac{2(715\alpha_1(3 + 10\alpha_2) + 15925\alpha_2\alpha_3 + 29400\alpha_3\alpha_4 + 48510\alpha_4\alpha_5)\lambda}{10725\alpha_1^2 + 7(429 + 3575\alpha_2^2 + 6825\alpha_3^2 + 11550\alpha_4^2 + 18018\alpha_5^2)} = -\frac{1}{4}. \tag{C.4}$$

Now we claim that for single zero energy bound states the variational parameters must be unique. Solving for the variational parameter α_1 from the above equation we get the following,

$$\alpha_1 = \frac{1}{210210}(-3432\lambda - 11440\alpha_2\lambda \pm \sqrt{D_1}). \tag{C.5}$$

where,

$$\begin{aligned} D_1 = ((3432\lambda + 11440\alpha_2\lambda)^2 - 420420(15015 + 405405\alpha_2^2 + 1156155\alpha_3^2 \\ +2732730\alpha_4^2 + 5675670\alpha_5^2 + 25480\alpha_2\alpha_3\lambda \\ +47040\alpha_3\alpha_4\lambda + 77616\alpha_4\alpha_5\lambda)). \end{aligned} \tag{C.6}$$

For unique α_1 we demand that the discriminant of the above equation D_1 vanishes. Therefore,

$$\alpha_1 = \frac{1}{210210}(-3432\lambda - 11440\alpha_2\lambda). \tag{C.7}$$

Solving $D_1 = 0$ for α_2 we get,

$$\alpha_2 = \frac{18727800\alpha_3\lambda - 137280\lambda^2 \pm \sqrt{D_2}}{2(-297972675 + 228800\lambda^2)}, \tag{C.8}$$

where,

$$D_2 = (-18727800\alpha_3\lambda + 137280\lambda^2)^2 - 4(-11036025 - 849773925\alpha_3^2 \\ -2008556550\alpha_4^2 - 4171617450\alpha_5^2 - 34574400\alpha_3\alpha_4\lambda - 57047760\alpha_4\alpha_5\lambda \\ +20592\lambda^2)(-297972675 + 228800\lambda^2)). \tag{C.9}$$

For unique α_2 the discriminant of the above equation, D_2 must vanish. Therefore,

$$\alpha_2 = \frac{18727800\alpha_3\lambda - 137280\lambda^2}{2(-297972675 + 228800\lambda^2)} \tag{C.10}$$

Solving $D_2 = 0$ for α_3 we get,

$$\alpha_3 = \frac{1466942400\alpha_4\lambda + 183040\lambda^3 - 1126400\alpha_4\lambda^3 \pm \sqrt{D_3}}{2(-36054693675 + 40170000\lambda^2)}, \tag{C.11}$$

where,

$$D_3 = ((-1466942400\alpha_4\lambda - 183040\lambda^3 + 1126400\alpha_4\lambda^3)^2 \\ -4(-36054693675 + 40170000\lambda^2)(-468242775 - 85220185050\alpha_4^2 \\ -176995768950\alpha_5^2 - 2420454960\alpha_4\alpha_5\lambda + 1233232\lambda^2 + 65436800\alpha_4^2\lambda^2 \\ +135907200\alpha_5^2\lambda^2 + 1858560\alpha_4\alpha_5\lambda^3))). \tag{C.12}$$

For unique α_3, claiming that the discriminant of the above equation D_3 must vanish, we obtain,

$$\alpha_3 = \frac{1466942400\alpha_4\lambda + 183040\lambda^3 - 1126400\alpha_4\lambda^3}{2(-36054693675 + 40170000\lambda^2)}. \tag{C.13}$$

Solving $D_3 = 0$ for α_4,

$$\alpha_4 = \frac{13(-2662500456\alpha_5\lambda + 2966400\alpha_5\lambda^3 + 4096\lambda^4 \pm \sqrt{D_4})}{10(243729729243 - 314223888\lambda^2 + 32768\lambda^4)}, \tag{C.14}$$

where,

$$\begin{aligned} D_4 = 18(&-10729671217761971475 - 4055815720314025217550\alpha_5^2 \\ &+45807763925146608\lambda^2 + 10141460221853312352\alpha_5^2\lambda^2 - 49598119056640\lambda^4 \\ &-7248551127206400\alpha_5^2\lambda^4 - 1211733540864\alpha_5\lambda^5 + 13236736000\lambda^6 \\ &+1096381440000\alpha_5^2\lambda^6 + 1350041600\alpha_5\lambda^7)). \end{aligned} \tag{C.15}$$

For unique α_4 claiming the discriminant of the above equation to be zero we get,

$$\alpha_4 = \frac{13(-2662500456\alpha_5\lambda + 2966400\alpha_5\lambda^3 + 4096\lambda^4)}{10(243729729243 - 314223888\lambda^2 + 32768\lambda^4)}. \tag{C.16}$$

Solving $D_4 = 0$ for α_5,

$$\alpha_5 = \frac{-16384\lambda^5 \pm \sqrt{D_5}}{594\,(184643734275 - 255977696\lambda^2 + 44800\lambda^4)} \tag{C.17}$$

where,

$$D_5 = 2(-15911834174160559648138125 + 722628476529045598512 00\lambda^2 \\ -9107852363097923635 2\lambda^4 + 36606338229288960\lambda^6 \\ -4274823168000\lambda^8 + 134217728\lambda^{10}). \tag{C.18}$$

Obviously it is assumed that the denominators in the expressions obtained for the variational parameters are non-zero. For unique α_5 as before claiming that the discriminant of the above equation, D_5 to be zero we get the following solutions for λ,

$$\lambda = \pm 140.235, \pm 93.478, \pm 47.2378, \pm 29.1756, \pm 19.0581. \tag{C.19}$$

However among these values ± 93.478, ± 29.1756 are the roots of the following equation which appears in the denominator of α_4,

$$(243729729243 - 314223888\lambda^2 + 32768\lambda^4) = 0. \tag{C.20}$$

Thus these correspond to the singularities of the coefficient α_4. Among the rest, the lowest two values are the first two values of λ which supports zero energy bound states with $m_l = 2$,

$$\lambda = \pm 47.2378, \pm 19.0581. \tag{C.21}$$

D Appendix

Addendum to Section 3.2

The trail wavefunction for the electron is given by,

$$\Psi(R,\eta) = \frac{1}{\sqrt{2\pi}}\Phi(R)\Theta(\eta), \tag{D.1}$$

$$\Theta(\eta) = N_2(1+\alpha_1 P_1(\cos\theta)+\alpha_2 P_2(\cos\theta)), \tag{D.2}$$

where

$$N_2 = \sqrt{\frac{15}{2}}\sqrt{\frac{1}{15+5\alpha_1^2+3\alpha_2^2}}, \tag{D.3}$$

$$R = \sqrt{\rho^2+\beta z^2}, \tag{D.4}$$

$$\eta = \arctan\left(\frac{\rho}{\sqrt{\beta}z}\right). \tag{D.5}$$

Also,

$$\rho = R\sin\eta, \tag{D.6}$$

$$\sqrt{\beta}z = R\cos\eta. \tag{D.7}$$

In terms of (R,η,ϕ),

$$\rho\, d\rho\, dz = \frac{1}{\sqrt{\beta}}R^2\ \sin\eta\, dR\, d\eta. \tag{D.8}$$

We evaluate the quantity $\langle\Psi|\hat{p}^2|\Psi\rangle$.

$$
\begin{aligned}
&\frac{\sqrt{\beta}}{\hbar^2}\langle\Psi|\hat{p}^2|\Psi\rangle \\
&= 2\pi\sqrt{\beta}\int_0^\infty\int_0^\infty \rho\, d\rho\, dz \left(\left(\frac{\partial\Psi}{\partial\rho}\right)^2 + \left(\frac{\partial\Psi}{\partial z}\right)^2\right) \\
&= 2\pi\sqrt{\beta}\int \left(\left(\frac{\partial R}{\partial\rho}\frac{\partial\Psi}{\partial R} + \frac{\partial\eta}{\partial\rho}\frac{\partial\Psi}{\partial\eta}\right)^2 + \left(\frac{\partial R}{\partial z}\frac{\partial\Psi}{\partial R} + \frac{\partial\eta}{\partial z}\frac{\partial\Psi}{\partial\eta}\right)^2\right)\rho\, d\rho\, dz \\
&= \int_0^\infty\int_0^\pi R^2\sin\eta\, dR\, d\eta \left(\left(\left(\sin^2\eta + \beta\cos^2\eta\right)\left(\frac{\partial\Phi}{\partial R}\right)^2\Theta^2\right)\right. \\
&\left. + \left(2\frac{(1-\beta)}{R}\sin\eta\cos\eta\ \Phi\ \theta\frac{\partial\Phi}{\partial R}\frac{\partial\Theta}{\partial\eta}\right) + \left(\frac{\beta}{R^4}\left(\sin^2\eta + \frac{\cos^2\eta}{\beta}\right)\Phi^2\left(\frac{\partial\Theta}{\partial\eta}\right)^2\right)\right) \\
&= \int_0^\infty R^2\, dR \left(\frac{\partial\Phi}{\partial R}\right)^2 \frac{14\alpha_1^2 + 21\beta\alpha_1^2 + 10\alpha_2^2 + 11\beta\alpha_2^2 - 28\alpha_2 + 28\beta\alpha_2 + 35\beta + 70}{7(15 + 5\alpha_1^2 + 3\alpha_2^2)} \\
&+ \int_0^\infty R\, dR\, \Phi\frac{\partial\Phi}{\partial R}\frac{4(-1+\beta)(7\alpha_1^2 + 3\alpha_2^2 + 21\alpha_2)}{7(15 + 5\alpha_1^2 + 3\alpha_2^2)} \\
&+ \int_0^\infty dR\, \Phi^2\, \frac{2(7\alpha_1^2 + 28\beta\alpha_1^2 + 27\alpha_2^2 + 36\beta\alpha_2^2)}{7(15 + 5\alpha_1^2 + 3\alpha_2^2)}.
\end{aligned}
\tag{D.9}
$$

Maple and Mathematica were used to evaluate the integrals.

E Appendix

Atomic Units

We have used the atomic units in the thesis. We tabulate (Table 13) the values of a few useful physical quantities in the atomic units and the corresponding values in the SI unit. We also note that 1 Hartree energy $\approx$ 27.2114

physical quantity	name	in atomic unit	in SI unit
mass	electron mass	1	$9.10938215(45) \times 10^{-31}$ kg
length	Bohr radius	1	$5.2917720859(36) \times 10^{-11}$ m
charge	proton charge	1	$1.602176487(40) \times 10^{-19}$ C
energy	Hartree energy	1	$4.35974394(22) \times 10^{-18}$ J
angular momentum	$\hbar$	1	$1.054571628(53) \times 10^{-34}$ Js
electric constant	ϵ_0	$\frac{1}{4\pi}$	$8.854187817 \times 10^{-12}$ F m^{-1}

Table 13: Relation between atomic unit and SI unit. The numbers in parentheses are the corresponding standard uncertainties. Source: http://physics.nist.gov/cuu/Constants

eV. The square of the ratio (say γ) of the Bohr radius ($a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_q q^2}$) and the cyclotron radius ($r_c = \sqrt{\frac{\hbar}{|q|B}}$) has been used as a measure of the magnetic field strength. This ratio is evidently dimensionless. For electrons, in atomic units, we have, $a_0 = 1$ and $r_c = \sqrt{\frac{1}{B}}$. Therefore,

$$\gamma = \left(\frac{a_0}{r_c}\right)^2 = B. \tag{E.1}$$

In SI units, $\gamma = 1$ implies $|\vec{B}| = 2.35052 \times 10^5 \approx 2.35 \times 10^5$ Tesla. For dipole moments, 1 a.u. = 2.541765 D $\approx$ 2.54 D, where D denotes Debye. 1 D $\approx 3.33564 \times 10^{-30}$ coulomb meter.

References

[1] J. E. Turner. Minimum dipole moment required to bind an electron-molecular theorists rediscover phenomenon mentioned in Fermi- Teller paper 20 years earlier. *American Journal of Physics*, 45:758–766, 1977.

[2] E. Fermi and E. Teller. The capture of negative mesotrons in matter. *Physical Review*, 72:399–408, 1947.

[3] A. S. Wightman. Moderation of negative meson in Hydrogen I: Moderation from high energies to capture by an H_2 molecule. *Physical Review*, 77:521–528, 1949.

[4] M. H. Mittleman and V. P. Myerscough. Minimum moment required to bind a charged particle to an extended dipole. *Physics Letters*, 23:545–546, 1966.

[5] J. E. Turner and K. Fox. Minimum dipole moment required to bind an electron to a finite dipole. *Physics Letters*, 23:547–549, 1966.

[6] R. F. Wallis, R. Herman, and H.W. Milnes. *Journal of Molecular Spectroscopy*, 4:51–74, 1960.

[7] W. R. Garrett. *Journal of Chemical Physics*, 73:5721, 1980.

[8] Th. Klahn and P. Krebs. Electron and anion mobility in low density hydrogen cyanide gas. I. Dipole-bound electron ground states. *Journal of Chemical Physics*, 109:531–542, 1998.

[9] M. Gutowski, P. Skurski, K.D. Jordan, and J. Simons. Energies of dipole-bound anionic states. *International Journal of Quantum Chemistry*, 64:183–191, 1998.

[10] P.W. Fry et al. . *Physical Review Letters*, 84:733–736, 2000.

[11] R. J. Warburton et al. Giant permanent dipole moments of excitons in semiconductor nanostructures. *Physical Review B*, 65:113303–1–4, 2002.

[12] O. H. Crawford. Bound states of a charged particle in a dipole field. *Proceedings of the Royal Society, London*, 91:279–284, 1967.

[13] R. Herman and R. F. Wallis. Energy levels of an electron in the field of a finite electric dipole in a magnetic field. *Physical Review B*, 23:4902–4912, 1981.

[14] R. Herman and R. F. Wallis. Binding of an electron to an electric dipole in a high magnetic field. *Physical Review B*, 25:7398 – 7402, 1982.

[15] Andrew M. Essin and David J. Griffiths. Quantum mechanics of the $\frac{1}{x^2}$ potential. *American Journal of Physics*, 74:109–117, 2006.

[16] S. A. Coon and B. R. Holstein. Anomalies in quantum mechanics: The $\frac{1}{r^2}$ potential. *American Journal of Physics*, 70:513–519, 2002.

[17] H. E. Camblong et al. Quantum anomaly in molecular physics. *Physical Review Letters*, 87:220402–1–4, 2001.

[18] Kevin Connoly and David J. Griffiths. Critical dipoles in one, two and three dimensions. *American Journal of Physics*, 75:524–531, 2007.

[19] A. D. Alhaidari and H. Bahlouli. Electron in the Field of a Molecule with an Electric Dipole Moment. *Physical Review Letters*, 100:110401–1–4, 2008.

[20] R.K. Bhaduri, Y. Nogami, and C.S. Warke. Hydrogen atom and Hydrogen molecule ion in homogeneous magnetic fields of arbitrary strength. *The Astrophysical Journal*, 217:324–329, 1977.

[21] George B. Arfken and Hans J. Weber. *Mathematical Methods for Physicists.* Academic Press, 2005.

[22] S. Flugge. *Practical Quantum Mechanics.* Springer Verlag, 1974.

[23] C. Desfrancois, B. Baillon, J.P. Schermann, S.T. Arnold, J.H. Hendricks, and K.H. Bowen. Prediction and Observation of a New, Ground State, Dipole-Bound Dimer Anion: The Mixed Water/ Ammonia System. . *Physical Review Letters*, 72:48–51, 1994.