

# An Exact Solution to a Correlated Two-Electron System With Positive Coulomb Interaction

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### **Abstract**

Even the simplest three-body problems with interactions between the particles are usually not exactly solvable, and thus approximations are required. We attempt to solve exactly the Schrödinger equation for two electrons orbiting a positive charge. This central charge can be replaced by a spherical ball of jellium substance with uniform positive charge density. In this case the electrons are bound to a common center by a simple harmonic oscillator potential. This system can then be separated into its center of mass ( $R$ ) and relative ( $r$ ) coordinates. The center of mass wavefunction can be solved simply by treating it as an independent harmonic oscillator. The relative coordinates wave function can be solved numerically. The results will be exact to numerical uncertainty and can be compared to existing theories.

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# 1 Introduction

Most problems examined in entry-level quantum mechanics courses are solvable one or two particle systems. However most real world problems are not so simple. Once there are more than two particles in the picture, things get complicated. Even the simplest three-body problems with interactions between the particles are usually not exactly solvable. Most actual problems involve  $N$  interacting particles where  $N$  is either very small as in the case of the Helium atom, or very large, as for a macroscopic object, where  $N$  is on the order of Avagadro's number,  $10^{23}$ . Because these problems are not exactly soluble, approximations are required.

Some of the first methods developed to deal with many electron systems were mean field theories. One example is the Hartree-Fock approximation [1], which forms its ground state wave function as a Slater determinant of single particle states. Simply put, this means that all the other particles are treated as exerting an average field on any one particle. This may be a good start, but it ignores the intricacies of the particle-particle interaction. It will be useful to have an exactly soluble model to test these approximations.

A more developed theory is Density Functional Theory [2, 4, 5], which was developed by P. Hohenberg, W. Kohn and L. J. Sham in 1964-65. This is based on a fundamental theorem, which states that an interacting  $N$ -body system can be solved for its exact electron density, in principle, by solving a set of  $N$  single particle Schrödinger Equations. Embedded in these equations is an exchange and correlation potential denoted by  $v_{xc}(n(r))$ , which is a functional of the electron density  $n(r)$ . For a given initial density, the Schrodinger equations may be solved yielding a set of  $N$  lowest energy single particle states and hence a density. Given a specific functional form for  $v_{xc}(n)$ , one iterates the equations to a self-consistent solution in which the initial and final densities are identical to within a numerical tolerance. This approximation

may be applied to isolated atoms, molecules and macroscopically large solids. It can also be generalized to spin polarized systems where the densities of up and down spin electrons are not equal.

## 1.1 The Model

The purpose of this project is to find an exact solution to a model correlated two-electron system with repulsive Coulomb interaction. In this sense the system we are dealing with is like a Helium atom. However, instead of using a point nucleus to bind the electrons, we use a spherical ball of jellium substance with uniform positive charge density. This massless jellium interacts with the system solely through charge interaction. In our case, this jellium ball is then spread throughout a surrounding space large enough that the electron density is totally enclosed within it. A uniform jellium density is the starting point for the construction of exchange and correlation potentials which are generally used in many electron problems. This uniform jellium density is a homogeneous system. Most theories then proceed by adding a homogeneous electron density as well. We are taking a different approach by looking at two electrons, making this a combination of homogeneous and inhomogeneous systems. In this case, non-interacting electrons are then bound to a common center by a simple harmonic oscillator potential. Gauss's Law states that an electron will only see that part of the jellium which is within the radius of its orbit. If it is perturbed slightly, the electron sees a total positive charge which varies like a harmonic oscillator. The potential seen by one electron is calculated as follows.

$$F = \frac{e'}{r^2} \int_V \frac{e}{\frac{4}{3}\pi(r_s a_0)^3} dV = \frac{e e'}{(r_s a_0)^3} r \quad (1)$$

$$U = - \int_0^R F = - \int_0^R \frac{e' e r}{(r_s a_0)^3} dr = - \frac{e' e}{2(r_s a_0)^3} R^2 = \frac{1}{2} k R^2 \quad (2)$$

Here,  $k$  is defined to be  $-\frac{ee'}{(r_s a_0)^3} = -\frac{4}{3}\pi e' \rho^+ = -\frac{e\rho^+}{3\epsilon_0}$ ,  $a_0$  is the Bohr radius,  $\rho^+ = \frac{e}{\frac{4}{3}\pi(r_s a_0)^3}$  is the positive jellium density, and  $R$  is distance from the center of the system to the electron. The system is slightly more complicated for two electrons because of the interaction between them.

$$U = \frac{1}{2}kr_1^2 + \frac{1}{2}kr_2^2 + \frac{e^2}{|\mathbf{r}_{12}|} \quad (3)$$

This equation can then be rewritten in terms of the center-of-mass coordinates  $\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$  and the relative coordinates  $\mathbf{r} = 2(\mathbf{r}_1 - \mathbf{r}_2)$

$$U = \frac{1}{2}k[2(\mathbf{r}_1 + \mathbf{r}_2)^2 + (\mathbf{r}_1 - \mathbf{r}_2)^2] + \frac{e^2}{r} \quad (4)$$

$$U = \frac{1}{2}k[2R^2 + \frac{1}{2}r^2] + \frac{e^2}{r} \quad (5)$$

$$U = kR^2 + \frac{1}{4}kr^2 + \frac{e^2}{r} \quad (6)$$

The essential part of this approach is that the relative and center-of-mass coordinates of this system can then be separated and treated independently of one another. Since the electron-electron interaction can be written solely in terms of the relative coordinate, it enters only into the Schrödinger equation for that coordinate. This equation, involving both the attraction to the jellium center and the electron-electron repulsion can be further reduced to the numerical solution of a single ordinary differential equation. We will carry out this solution under a variety of circumstances. The solution to this problem depends first of all on the relative spin orientation of the two electrons.

We will first attempt to solve this atom-like system with electrons in antiparallel spin states [6]. These electrons can both be placed in the relative and center of mass ground states. We will be able to calculate numerically the exact energy ground state and the exact electron density as a function of  $r_s$ , a dimensionless jellium density parameter defined by: charge density  $\rho = \frac{1}{\frac{4}{3}\pi(r_s a_0)^3}$ , where  $a_0$  is the Bohr radius of

an atom. We will then attempt the same problem in the case of parallel spin states. This problem is different in that the electrons can no longer be in the same state. The system can still be put in the center-of-mass ground state, but must now be put in the first excited relative coordinates ground state.

The variable which is changed in the problem to vary the charge density is the dimensionless  $r_s$  parameter. In a perfectly homogeneous system, this  $r_s$  parameter times the Bohr radius would represent the spacing between the electrons. For elemental metals,  $r_s$  ranges from about 1.8 to 5.6.

## 2 The Solution

We first take the Hamiltonian for the two electron system:

$$H = \frac{-\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) + \frac{1}{2}k(r_1^2 + r_2^2) + \frac{e^2}{r_{12}} \quad (7)$$

and separate it into its center of mass and relative coordinates as follows:

$$H = \left(\frac{-\hbar^2}{2M}\nabla_R^2 + kR^2\right) + \left(\frac{-\hbar^2}{2\mu}\nabla_r^2 + \frac{1}{4}kr^2 + \frac{e^2}{r}\right) \quad (8)$$

This then needs to be scaled into a dimensionless form. The scaling used is  $\frac{\hbar^2}{2m} = 1$  and  $\frac{e^2}{4\pi\epsilon_0} = 2$ ,  $a_0 = 1$ . With this scaling,  $k = -\frac{e^2}{4\pi\epsilon_0(r_s a_0)^3} = \frac{2}{r_s^3}$ .

$$\frac{-\hbar^2}{2M}\nabla_R^2\psi + kR^2\psi = E_{CM}\psi \quad (9)$$

$$\frac{-\hbar^2}{2\mu}\nabla_r^2\phi + \frac{1}{4}kr^2\phi + \frac{e^2}{r}\phi = E_{rel}\phi \quad (10)$$

The next step is to multiply equations 9 and 10 by  $r_s^{\frac{3}{2}}$  and make the following substitutions.  $S = \frac{R}{r_s^{\frac{3}{4}}}$ ,  $s = \frac{r}{r_s^{\frac{3}{4}}}$ ,  $\epsilon_{CM} = r_s^{\frac{3}{2}}E_{CM}$ ,  $\epsilon_{rel} = r_s^{\frac{3}{2}}E_{rel}$

$$\frac{-\hbar^2}{2M}r_s^{\frac{3}{2}}\nabla_R^2\psi + r_s^{\frac{3}{2}}kR^2\psi = r_s^{\frac{3}{2}}E_{CM}\psi \quad (11)$$



$$-\frac{\hbar^2}{2\mu} r_s^{\frac{3}{2}} \nabla_r^2 \phi + \frac{1}{4} r_s^{\frac{3}{2}} k r^2 \phi + r_s^{\frac{3}{2}} \frac{e^2}{r} \phi = r_s^{\frac{3}{2}} E_{rel} \phi \quad (12)$$

By then expanding the kinetic energy term, the final radial equations can be written as

center of mass radial equation:

$$-\frac{1}{2} \left[ \frac{d^2}{dS^2} + \frac{2}{S} \frac{d}{dS} - \frac{L(L+1)}{S^2} \right] \psi + 2S^2 \psi = \epsilon_{CM} \psi \quad (13)$$

relative radial equation:

$$-2 \left[ \frac{d^2}{ds^2} + \frac{2}{s} \frac{d}{ds} - \frac{l(l+1)}{s^2} \right] \phi + \frac{s^2}{2} \phi + \frac{2r_s^{\frac{3}{2}}}{s} \phi = \epsilon_{rel} \phi \quad (14)$$

Here,  $\epsilon_{CM}$  and  $\epsilon_{rel}$  are the scaled energies of the center-of-mass and relative coordinates wave equations. As can be easily seen, the center of mass radial equation is simply a harmonic oscillator which can be exactly solved. However, the relative radial equation has an extra perturbative term due to the repulsion between the two electrons. In order to solve this exactly, we must use the numerical methods outlined in the next section.

The density  $n(\mathbf{x})$  is calculated using:

$$n(\mathbf{x}) = \langle \Psi(\mathbf{r}_1, \mathbf{r}_2) | (\delta(\mathbf{x} - \mathbf{r}_1) + \delta(\mathbf{x} - \mathbf{r}_2)) | \Psi(\mathbf{r}_1, \mathbf{r}_2) \rangle \quad (15)$$

$$n(\mathbf{x}) = \int d^3 r_1 \int d^3 r_2 | \Psi(\mathbf{r}_1, \mathbf{r}_2) |^2 (\delta(\mathbf{x} - \mathbf{r}_1) + \delta(\mathbf{x} - \mathbf{r}_2)) \quad (16)$$

where  $\mathbf{x}$  is the position vector and  $\mathbf{r}_1$  and  $\mathbf{r}_2$  are the position vectors of the two electrons.  $\mathbf{r}_1 = \mathbf{R} + \mathbf{r}/2$  and  $\mathbf{r}_2 = \mathbf{R} - \mathbf{r}/2$ , and  $\Psi(\mathbf{r}_1, \mathbf{r}_2)$  is the total wavefunction including both the center-of-mass and the relative coordinates wave functions.

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \psi(\mathbf{R}) \phi(\mathbf{r}) \chi(1, 2) \quad (17)$$

Since the radial equation separates into center of mass and relative coordinates we can rewrite Equation 16 as

$$n(\mathbf{x}) = \int d^3 \mathbf{R} \int d^3 \mathbf{r} | \psi_L(\mathbf{R}) |^2 | \phi_l(\mathbf{r}) |^2 (\delta(\mathbf{R} + \frac{\mathbf{r}}{2} - \mathbf{x}) + \delta(\mathbf{R} - \frac{\mathbf{r}}{2} - \mathbf{x})) \quad (18)$$

$$n(\mathbf{x}) = \int R^2 dR \int r^2 dr \int d\Omega_R \int d\Omega_r |\psi_L(R)|^2 |Y_L^M(\Omega)|^2 |\phi_l(r)|^2 |Y_l^m(\Omega)|^2 \quad (19)$$

$$(\delta(\mathbf{R} + \frac{\mathbf{r}}{2} - \mathbf{x}) + \delta(\mathbf{R} - \frac{\mathbf{r}}{2} - \mathbf{x})) \quad (20)$$

where  $R$  is the center-of-mass coordinate and  $r$  is the relative coordinate.  $\psi_L(\mathbf{R})$  is the center-of-mass wave function and  $\psi_L(R)$  is the center of mass radial function.  $\phi_l(\mathbf{r})$  is the relative wave function,  $\phi_l(r)$  is the numerical relative radial function which was calculated using MAPLE V. The  $Y_L^M(\Omega)$  is the angular part of the center-of-mass wave function, and the  $Y_l^m(\Omega)$  is the angular part of the relative wave function. For the case of antiparallel spin states in the ground state wave equation, both  $\psi(R)$  and  $\phi(r)$  can have angular momentum  $L, l = 0$ .  $L$  represents the angular momentum of the center-of-mass wave function, and  $l$  represents the angular momentum of the relative wave function. For parallel spin states in the ground state wave equation this is no longer the case. The Pauli Exclusion Principle states that two electrons with identical spins cannot occupy the same angular momentum state. Therefore, in the ground state of the system, one electron will occupy the  $l = 0$  state and the other will occupy the  $l = 1$  state. The center-of-mass equation treats the electrons as independent of each other, so this does not apply, and the wave equation can remain in the  $L=0$  state. Thus the angular component of this function is simply  $\frac{1}{\sqrt{4\pi}}$ . The Pauli Exclusion Principle does however affect the relative radial equation, and so it must be in the  $l = 1$  state. For the  $L = 0$  state of the center-of-mass equation, the solution is that of a harmonic oscillator and the density equation becomes:

$$n(\mathbf{x}) = \int R^2 dR \int r^2 dr \int d\Omega_r e^{-\beta^2 R^2} |\phi_l(r)|^2 |Y_l^m(\Omega)|^2 \quad (21)$$

$$(\delta(\mathbf{R} + \frac{\mathbf{r}}{2} - \mathbf{x}) + \delta(\mathbf{R} - \frac{\mathbf{r}}{2} - \mathbf{x})) \quad (22)$$

where  $\beta = \sqrt{\frac{m\omega}{\hbar}}$ . Scaled, this becomes  $\beta = 2^{\frac{1}{4}} r_s^{-\frac{3}{4}}$

$$n(\mathbf{x}) = \int r^2 dr \int d\Omega_r [e^{-\beta^2(\mathbf{x}-\mathbf{r}/2)^2} + e^{-\beta^2(\mathbf{x}+\mathbf{r}/2)^2}] |\phi_l(r)|^2 |Y_l^m(\Omega)|^2 \quad (23)$$

$$n(\mathbf{x}) = \int r^2 dr \int d\Omega_r [e^{-\beta^2(x^2+(\frac{r}{2})^2-\mathbf{x}\cdot\mathbf{r})} + e^{-\beta^2(x^2+(\frac{r}{2})^2+\mathbf{x}\cdot\mathbf{r})}] |\phi_l(r)|^2 |Y_l^m(\Omega)|^2 \quad (24)$$

$$n(\mathbf{x}) = \int r^2 dr \int d\Omega_r e^{-\beta^2(x^2+\frac{r^2}{4})} (e^{\beta^2\mathbf{x}\cdot\mathbf{r}} + e^{-\beta^2\mathbf{x}\cdot\mathbf{r}}) |\phi_l(r)|^2 |Y_l^m(\Omega)|^2 \quad (25)$$

This equation is symmetric when switching the parity so it can be simplified to:

$$n(\mathbf{x}) = 2 \int r^2 dr \int d\Omega_r e^{-\beta^2 x^2} e^{-\beta^2 \frac{r^2}{4}} e^{\beta^2 \mathbf{x}\cdot\mathbf{r}} |\phi_l(r)|^2 |Y_l^m(\Omega)|^2 \quad (26)$$

For the  $l = 0$  state this is relatively simple because  $Y_l^m(\Omega)$  is just  $\frac{1}{\sqrt{4\pi}}$ , and so for the  $l = 0$  state, Equation 26 becomes:

$$n(\mathbf{x}) = 2 \int r^2 dr \int d\Omega_r e^{-\beta^2 x^2} e^{-\beta^2 \frac{r^2}{4}} e^{\beta^2 \mathbf{x}\cdot\mathbf{r}} |\phi_0(r)|^2 \frac{1}{4\pi} \quad (27)$$

$$n(\mathbf{x}) = 2 \int r^2 dr e^{-\beta^2 x^2} e^{-\beta^2 \frac{r^2}{4}} e^{\beta^2 \mathbf{x}\cdot\mathbf{r}} |\phi_0(r)|^2 \quad (28)$$

Equation 26 contains an  $e^{\beta^2 \mathbf{x}\cdot\mathbf{r}}$  term. This dot product can be rewritten as  $xr \cos \theta_{xr}$  where  $\theta_{xr}$  is the angle between  $\mathbf{x}$  and  $\mathbf{r}$  (see Figure 1). This would be fine, except that  $|Y_l^0|^2 = \frac{3}{4\pi} \cos^2 \theta$  and  $|Y_l^1|^2 = |Y_l^{-1}|^2 = \frac{3}{8\pi} \sin^2 \theta$ . Each of these terms contains either a  $\cos \theta$  or a  $\sin \theta$ , but  $\theta \neq \theta_{xr}$ . It was therefore necessary to write  $\cos \theta$  in terms of  $\theta_{xr}$ . It was not necessary to also calculate  $\sin \theta$  as well because  $\cos^2 \theta = 1 - \sin^2 \theta$ . In spherical coordinates, the unit vectors  $\hat{x}$ ,  $\hat{r}$ , and  $\hat{z}$  can be expressed in terms of the angles  $\theta$  and  $\phi$ .

$$\hat{x} = (0, 0, 1) \quad (29)$$

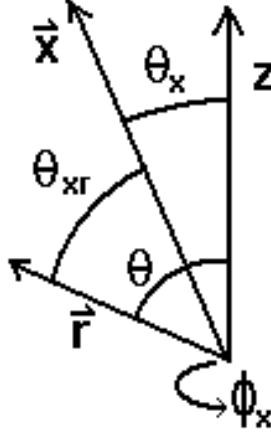


Figure 1: This is a representation of the x and r position vectors with respect to the z axis

$$\hat{r} = (\sin(\theta_{xr}) \cos(\phi_{xr}), \sin(\theta_{xr}) \sin(\phi_{xr}), \cos(\theta_{xr})) \quad (30)$$

$$\hat{z} = (\sin(\theta_x) \cos(\phi_x), \sin(\theta_x) \sin(\phi_x), \cos(\theta_x)) \quad (31)$$

$\cos \theta$  is the angle between the  $\mathbf{r}$  and  $\mathbf{z}$  vectors. Therefore  $\hat{r} \cdot \hat{z} = \cos \theta$ .  $\cos \theta$  can then be rewritten as:

$$\cos(\theta) = \sin(\theta_x) \sin(\theta_{xr}) [\cos(\phi_x) \cos(\phi_{xr}) + \sin(\phi_x) \sin(\phi_{xr})] + \cos(\theta_x) \cos(\theta_{xr}) \quad (32)$$

$$\cos(\theta) = \sin(\theta_x) \sin(\theta_{xr}) \cos(\phi_x - \phi_{xr}) + \cos(\theta_x) \cos(\theta_{xr}) \quad (33)$$

Since the wave function is spherically symmetric over  $\phi$ ,  $(\phi_x - \phi_{xr})$  can be replaced by an arbitrary  $\phi$ . This greatly simplifies later integrations. This equation for  $\cos(\theta)$  is then inserted into the equation for the density. The integral is then taken over  $\Omega$ , which is the same as integrating over  $\phi$  from 0 to  $2\pi$  and over  $\sin \theta_{xr} d\theta_{xr}$  from 0 to  $\pi$ . Once the angular integral is taken, the density equation becomes much more complex.

The density equation involving  $Y_1^0$  is:

$$n(\mathbf{x}) = \int r^2 dr e^{-\beta^2 x^2} e^{-\beta^2 \frac{r^2}{4}} J_{1,0} |\phi_l(r)|^2 \quad (34)$$

where  $J_{1,0}$  is defined as:

$$J_{1,0} = \frac{3 \sin^2(\theta_x) [e^{-\beta^2 x r} (\beta^2 x r + 1) + e^{\beta^2 x r} (\beta^2 x r - 1)]}{\beta^6 x^3 r^3} \quad (35)$$

$$- \frac{3 \cos^2(\theta_x) [e^{-\beta^2 x r} (\beta^4 x^2 r^2 + 2\beta^2 x r + 2) - e^{\beta^2 x r} (\beta^4 x^2 r^2 - 2\beta^2 x r + 2)]}{\beta^6 x^3 r^3} \quad (36)$$

and the density equation involving  $Y_1^{1,-1}$  is:

$$n(\mathbf{x}) = \int r^2 dr 2e^{-\beta^2 x^2} e^{-\beta^2 \frac{r^2}{4}} J_{1,[1,-1]} | \phi_l(r) |^2 \quad (37)$$

where  $J_{1,[1,-1]}$  is defined as:

$$J_{1,[1,-1]} = \frac{3 \sin^2(\theta_x) [-e^{-\beta^2 x r} (\beta^2 x r + 1) - e^{\beta^2 x r} (\beta^2 x r - 1)]}{\beta^6 x^3 r^3} \quad (38)$$

$$+ \frac{3 \cos^2(\theta_x) [e^{-\beta^2 x r} (\beta^4 x^2 r^2 + 2\beta^2 x r + 2) - e^{\beta^2 x r} (\beta^4 x^2 r^2 - 2\beta^2 x r + 2)]}{\beta^6 x^3 r^3} \quad (39)$$

$$+ \frac{3 e^{\beta^2 x r} - e^{-\beta^2 x r}}{\beta^2 x r} \quad (40)$$

However, these equations turned out to be too difficult for the  $l = 1$  state. Instead of separately calculating  $Y_1^0$ ,  $Y_1^1$ , and  $Y_1^{-1}$ , it is much simpler to calculate the sum of the probabilities. The average is then obtained by dividing by 3.

$$\sum_{m=-l}^l | Y_l^m |^2 = \frac{2l+1}{4\pi} \quad (41)$$

$$n(\mathbf{x}) = \int r^2 dr \int d\Omega_r 2e^{-\beta^2 x^2} e^{-\beta^2 \frac{r^2}{4}} e^{\beta^2 x r \cos \theta_{xr}} \frac{2l+1}{3 \cdot 4\pi} | \phi_1(r) |^2 \quad (42)$$

$$n(\mathbf{x}) = \int r^2 dr \frac{2e^{-\frac{1}{4}\beta^2(4x^2+r^2)}}{\beta^2 x r} \sinh(\beta^2 x r) | \phi_1(r) |^2 \quad (43)$$

## 2.1 A Classical Approximation of the Potential

The Coulomb potential which the electrons see is dependent on the two forces it feels. One from the positive jellium encompassed by its orbit, and the other from the

second electron. The potential from the positive jellium goes as  $r^2$ . The force due to the other electron is proportional to  $\frac{1}{r}$ . The combination of these two forces results in a potential similar to the one shown in Figure 2. The minimum point  $r_0$  can be calculated as follows:

$$U = \frac{e^2}{r} + \frac{1}{4}kr^2 \quad (44)$$

Where  $U$  is the potential seen by the electron,  $r$  is the radial coordinate, and  $k$  the “spring constant”. We must first scale this equation using the methods of the previous section so that this result can be compared to our numerical results.

$$u = \frac{2r_s^{\frac{3}{4}}}{s} + \frac{1}{2}s^2 \quad (45)$$

By taking the derivative of this and setting the result equal to zero, we are solving for the point at which the potential is at a minimum, or the force is zero.

$$\frac{du}{ds} = \frac{-2r_s^{\frac{3}{4}}}{s^2} + s_0 = 0 \quad (46)$$

$$s_0^3 = 2r_s^{\frac{3}{4}} \quad (47)$$

$$s_0 = 2^{\frac{1}{3}}r_s^{\frac{1}{4}} \quad (48)$$

This is the equilibrium point about which simple harmonic oscillation occurs. This is the classical approximation and is shown for two reasons. The first is that it provides a visual representation of the system. The second is that it should match the results fairly closely and can therefore provide a guide which would show any glaring discrepancies with the data.

### Classical Approximation of the Potential

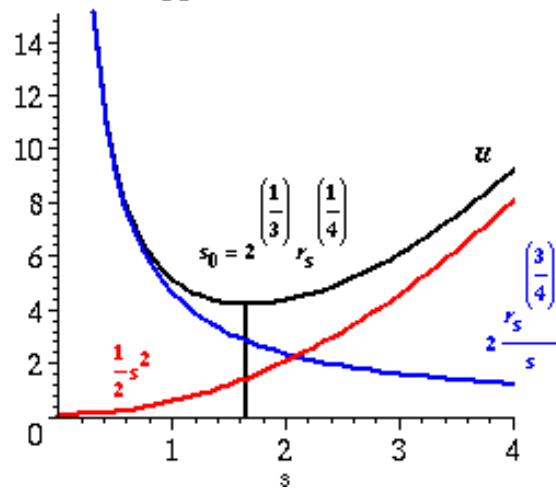


Figure 2: This is the classical approximation of the potential for  $r_s = 3.0$ .  $s_0 = 1.6581$

### 3 Numerical Methods

#### 3.1 Obtaining the Energy: The Shooting Method

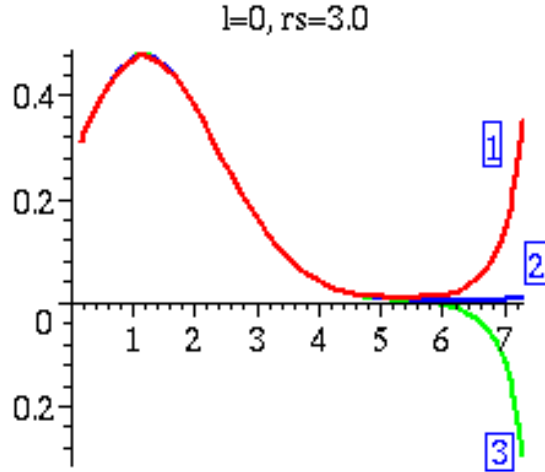


Figure 3: The solution for the relative radial equation for  $l = 0, r_s = 3.0$ . Solution 1 has an energy equal to 6.036, Solution 2 has an energy equal to 6.03759, and Solution 3 has an energy equal to 6.039

In order to solve the ordinary differential equation (ODE) for various  $r_s$  values, we needed the corresponding energies. This was done using the shooting method [8] in MAPLE V. We knew that the general shape of solution to the ODE would resemble a gaussian curve and that it would intersect the y-axis at a non-zero point. However, only the correct energy would allow the wave function to correctly die away to zero at infinity. If the energy was too large then the graph of the solution would start off correctly but then blow up in the positive y-direction as the function moved away from the origin. If the energy was too low, the function would blow up in the negative y-direction (see Figure 3). The starting point was a scaled energy equal to 3.0 because this would be the energy of the system with an  $r_s$  parameter of 0. I tried this value for the solution of  $r_s = 0.1$ . This value was too small as I had expected. I therefore



increased it little by little until the graph of the function dipped below the x-axis. I then decreased the value of the energy by a smaller amount. Using this method, I gradually zeroed in on the correct energy. I then repeated this process using the other  $r_s$  values for  $l = 0, 1$ .

The scaled energies obtained for various  $r_s$  values are shown in Table 1 below.

Table 1: The scaled energy values for the relative coordinates wave equation. The unscaled energy

$E$  is equal to  $\frac{\epsilon}{r_s^{\frac{3}{2}}}$

$r_s$	$\epsilon (l = 0)$	$\epsilon (l = 1)$
0	3.0	5.0
0.1	3.27897	5.18806
0.3	3.62270	5.42551
1.0	4.46024	6.03015
3.0	6.03759	7.26158
10.0	9.34893	10.13582

### 3.2 Normalizing the Relative Radial Equation

MAPLE can solve this ODE, but I had trouble normalizing it and thus needed to use a slightly indirect approach. In order to normalize the radial wave function, I decided to solve for  $s\phi(s)$  as well as just  $\phi(s)$  because I could not get MAPLE to calculate the integral of the product of a numerical function ( $\psi(s)$ ) and a symbolic function ( $s$ ). Using the transformation  $F(s) = s\phi(s)$ , the relative radial equation becomes:

$$-2\left[\frac{d^2}{ds^2} - \frac{l(l+1)}{s^2}\right]F(s) + \frac{s^2}{2}F(s) + \frac{2r_s^{\frac{3}{4}}}{s}F(s) = \epsilon_{rel}F(s) \quad (49)$$

MAPLE can then solve these equations for  $F(s)$  which only involves a numeric calculation and integrate the square of the solution to obtain the normalization factor

(N).

$$\int_0^\infty F(s)^2 ds = \int_0^\infty \phi(s)^2 s^2 ds = N^2 \quad (50)$$

### 3.3 Calculating the Electron Densities

The calculation of the densities is moderately straightforward. I had the relative radial, center of mass radial, and angular components of the wave equation. I just had to integrate over space. The angular integral was the easiest and could be done analytically using MAPLE V. The integration of the rest of the function required that I calculate the product of the relative and center of mass wave equations at a mesh of points ranging from 0 to about 8 (depending on the particular equation). The density of this mesh depended on the shape of each particular density function. I then used a very crude method to integrate over  $s$ . I calculated the height of the function at each point on the mesh, multiplied each calculation by the resolution of the mesh, and then summed the results to obtain a rough integration. Time constraints unfortunately limited the accuracy of this calculation. The function 'pointplot()' was then used to display the results. There is a normalization coefficient missing, but I do not know what it is or where I have left it out of the calculations. The electron densities were all multiplied by  $\beta^3$ , which is proportional to  $r_s^{-9/4}$ , in order that the densities were normalized correctly relative to each other. This was needed because I had multiplied a nonscaled center-of-mass function by a scaled relative function when calculating the electron densities.

### 3.4 Summary of Numerical Work

MAPLE V was used to perform all calculations. Because of the complexity and singular nature of the equations around the origin, indirect methods were sometimes needed to calculate the solution. The solutions of the  $Y_l^m$ 's of the wave functions had

to be separated into four equations because the sum of these four components was beyond MAPLE's ability to calculate in one command. It crashed repeatedly in the attempt. In order to normalize the radial wave function, it was necessary to solve for  $s\psi(s)$  as well as just  $\psi(s)$  because I did not at that point realize that MAPLE could calculate the integral of the product of a numerical function and a symbolic function. Dverk78, a 7th-8th order continuous Runge-Kutta method was used in the dsolve routine in order to obtain the desired precision. All numerical answers are correct to five significant figures. For the center of mass radial equation, calculations have been completed for angular momentum values of  $l = 0, 1$ . For the relative radial equation, calculations have been completed for angular momentum values of  $l = 0, 1$  with  $r_s$  values of 0, 0.1, 0.3, 1.0, 3.0, and 10.0. The cases with  $r_s = 0$  were calculated in order to provide a reference to what the relative radial equation would look like without the  $r_s$  parameter. The densities for the ground state with anti-parallel spin electrons has been calculated but not correctly normalized. The average electron density has been calculated for the case of parallel spin electrons, but has also not been correctly normalized.

## 4 The Results

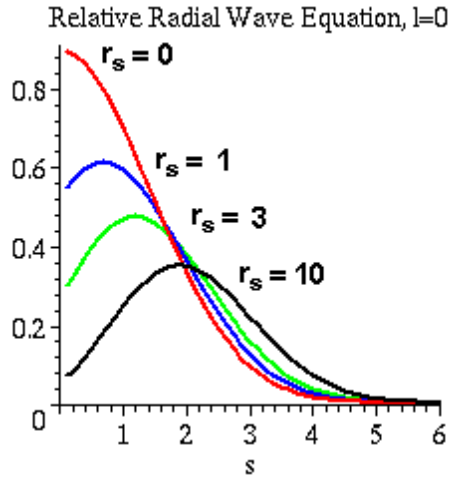


Figure 4: These are the relative coordinates wave functions for the  $l=0$  state.

The function for  $r_s = 3.0$  appears to peak at about  $s = 1.17$ . This is not very close to the classically estimated value of  $s_0 = 1.6581$ . I believe there may be an error in the scaling of the  $s$  parameter by a factor of two in the relative radial equation.

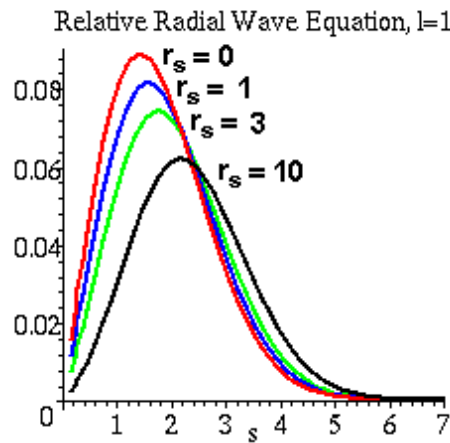


Figure 5: These are the relative coordinates wave functions for the  $l=1$  state.

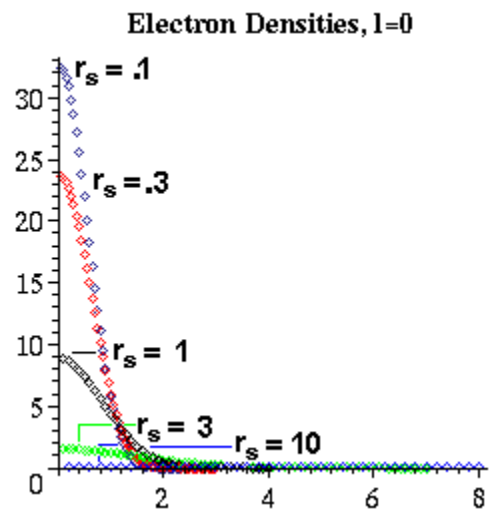


Figure 6: These are the non-normalized electron densities for the  $l = 0$  state.

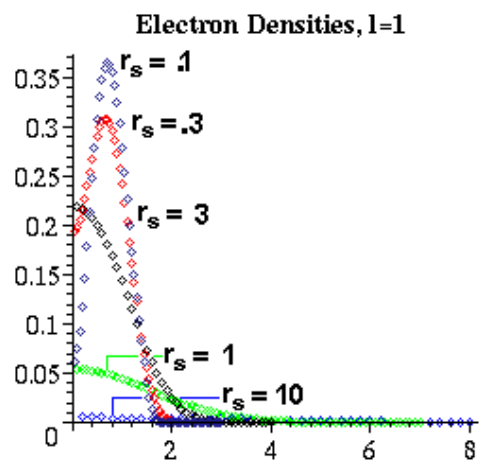


Figure 7: These are the average non-normalized electron densities for the  $l = 1$  state.

## 5 Conclusions

Due to unforeseen and frequent problems with MAPLE, I have unfortunately not reached the stage at which I had hoped I would be at this point. While I have learned a great deal about MAPLE, it has been less than cooperative in many things. At this point I have calculated the normalized center of mass radial equation for  $l = 0, 1$ , and the normalized relative radial equation for  $l = 0, 1$  with  $r_s = 0, 0.1, 0.3, 1, 3, 10$ . I have also calculated the non-normalized electron density for the ground state of the anti-parallel spin state system and the average electron density for the ground state of the parallel spin state system. We should be able to extend the calculations to solve for the excited states of the system as well as for the ground state. In principle, we can numerically calculate the entire energy spectrum and electron densities of the system for the singlet or triplet spin states and for variable jellium densities. Since our system is exactly soluble, in the future, it would be possible to compare its energies and densities with approximations using various density functional exchange and correlation potentials. These  $v_{xc}(n)$  are developed via perturbation theory applied to a homogeneous electron gas with a positive jelly background. Both sets of results should closely match. It should thus be possible to assess which potentials yield the best results.

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