P3317 HW from Lecture 15 and Recitation 8

Due Oct 23, 2018

Problem 1. Variational Energy of Helium Here we will estimate the ground state energy of Helium. Helium has two electrons circling around a nucleus with charge +2. We will treat the nucleus as stationary, and write down a wavefunction $\psi(\vec{r}_1, \vec{r}_2)$ for the two electrons. These are Fermions, but we will take them to have opposite spin, so the spatial wavefunction will be symmetric $\psi(\vec{r}_1, \vec{r}_2) = \psi(\vec{r}_2, \vec{r}_1)$. Given a normalized wavefunction, the energy is

$$\mathcal{E} = \int d^3r_1 \int d^3r_2 \left[\frac{\hbar^2}{2m} \left(|\nabla_{r_1}\psi|^2 + |\nabla_{r_2}\psi|^2 \right) - \frac{e^2}{4\pi\epsilon_0} \left(\frac{2}{r_1} + \frac{2}{r_2} - \frac{1}{|\vec{r}_1 - \vec{r}_2|} \right) |\psi|^2 \right]. \tag{1}$$

We can adimensionalize this equation by measuring energies in terms of E_0 and lengths in terms of r_0 to produce

$$E = \int d^3R_1 \int d^3R_2 \left[\frac{1}{2} \left(|\nabla_{R_1}\psi|^2 + |\nabla_{R_2}\psi|^2 \right) - \left(\frac{2}{R_1} + \frac{2}{R_2} - \frac{1}{|\vec{R}_1 - \vec{R}_2|} \right) |\psi|^2 \right]. \tag{2}$$

1.1. How is the dimensionless energy E related to the dimensionful energy $\mathcal{E}$? How is the dimensionless distance $\vec{R}_1$ related to the dimensionful distance $\vec{r}_1$

1.2. Experimentally the ground state energy of Helium is $\mathcal{E}_g = -78.975\text{eV}$. What value of E does this correspond to?

1.3. We will make the variational Ansatz

$$\psi(\vec{R}_1, \vec{R}_2) = A \exp\left(-\frac{|R_1|}{2d} \right) \exp\left(-\frac{|R_2|}{2d} \right). \tag{3}$$

Here d will be a variational parameter. Normalize this wavefunction by finding an expression for A in terms of d. You may find it useful to use

$$\int_0^\infty dR\, R^2 e^{-R/d} = 2d^3. \tag{4}$$

1.4. Since ψ only depends on the length $|R_1|$, the gradient is in the radial direction,

$$\nabla_{R_1}\psi = \hat{R}_1 \frac{\partial \psi}{\partial R_1}. \tag{5}$$

Calculate this gradient.

1.5. Calculate

$$T_1 = \int \int d^3R_1 \int d^3R_2 \, \frac{1}{2} |\nabla_{R_1}\psi|^2 \tag{6}$$

1.6. Calculate

$$V_1 = -2 \int \int d^3R_1 \int d^3R_2 \, \frac{1}{R_1} |\psi|^2. \tag{7}$$

You may find it useful to use

$$\int_0^\infty dR \, R \, e^{-R/d} = d^2. \tag{8}$$

1.7. The somewhat tricky part of the calculation is the expectation value of the coulomb repulsion between the electrons,

$$V_{12} = \int d^3R_1 \int d^3R_2 \, \frac{1}{|\vec{R}_1 - \vec{R}_2|} |\psi(R_1, R_2)|^2 \tag{9}$$

If we let θ be the angle between $\vec{R}_1$ and $\vec{R}_2$, this integral can be written

$$V_{12} = 8\pi \int_0^\infty dR_1 \, R_1^2 \int_0^\infty dR_2 \, R_2^2 \int_{-1}^{1} d(\cos\theta) \frac{1}{\sqrt{R_1^2 + R_2^2 - 2R_1R_2\cos(\theta)}} |\psi|^2. \tag{10}$$

The integral over $\cos(\theta)$ is of the form

$$\int_{-1}^{1} \frac{dx}{\sqrt{a - bx}} = \frac{-2}{b} \sqrt{a - bx} \Big|_{-1}^{1} = 2 \frac{\sqrt{a+b} - \sqrt{a-b}}{b}. \tag{11}$$

Use this identity to show that

$$\int_{-1}^{1} \frac{dx}{\sqrt{R_1^2 + R_2^2 - 2R_1R_2x}} = 2/s \tag{12}$$

where s is the larger of R_1 and R_2. Hint: Use $\sqrt{x^2} = |x|$.

1.8. The result in Eq. (12) allows us to write

$$V_{12} = 16\pi \int_0^\infty dR_1 \, R_1 \int_0^{R_1} dR_2 \, R_2^2 \, |\psi|^2 + 16\pi \int_0^\infty dR_1 \, R_1^2 \int_{R_1}^\infty dR_2 \, R_2 \, |\psi|^2 \tag{13}$$

Carry out the integrals. [By symmetry they should be equal to one-another.]

1.9. One can combine these results to write

$$E = \frac{\alpha}{d^2} - \frac{\beta}{d}. \tag{14}$$

Find α and β.

1.10. In terms of α and β, what is your best variational estimate of the energy? [Do not substitute in your expressions.]

1.11. Substitute in your expressions to calculate an upper bound for E. How close is it to the experimental value of the ground state energy?

Problem 2. An electron in one dimension has a wavefunction $\psi(x,\sigma)$, with

$$\begin{aligned} \psi(x,\uparrow) &= Ae^{-(x-a)^2/d^2} \\ \psi(x,\downarrow) &= Ae^{-(x+a)^2/d^2}, \end{aligned} \tag{15}$$

where a, d, A are constants, with $d \ll a$. These can be combined into a vector as

$$\vec{\psi}(x) = \begin{pmatrix} \psi(x,\uparrow) \\ \psi(x,\downarrow) \end{pmatrix}. \tag{16}$$

2.1. You measure the location of the electron. What is the probability that you find it near a? [This is an easy problem. An electron with $x = a + \delta$ is "near" if δ is small compared to a. Since $d \ll a$ you don't even need to do an integral. You should be able to instantly state the answer (which is a number – independent of a or d – as long as $d \ll a$.]

2.2. Suppose you find the electron near a, what will it's spin projection along the $\hat{z}$ axis be?

2.3. We will define spin angular momentum operators S_z, S_x, S_y. There are a few different notations for these operators, but they all mean the same thing. The most intuitive comes from representing your wavefunction as a vector, whence

$$S_z \begin{pmatrix} \psi(x,\uparrow) \\ \psi(x,\downarrow) \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \psi(x,\uparrow) \\ \psi(x,\downarrow) \end{pmatrix}. \tag{17}$$

An equivalent way to think about it is that ψ is a function of two variables: x and σ. If I act on ψ with the S_z operator, I get a new function $\phi = S_z\psi$. The function ϕ is also a function of two variables: x and σ. Clearly $\phi(x,\uparrow) = \psi(x,\uparrow)$ and $\phi(x,\downarrow) = -\psi(x,\downarrow)$. We can write this as

$$(S_z\psi)(x,\uparrow) = (\hbar/2)\psi(x,\uparrow) \tag{18}$$

$$(S_z\psi)(x,\downarrow) = -(\hbar/2)\psi(x,\downarrow) \tag{19}$$

Similarly, with S_x and S_y obey

$$(S_x\psi)(x,\uparrow) = (\hbar/2)\psi(x,\downarrow) \tag{20}$$

$$(S_x\psi)(x,\downarrow) = (\hbar/2)\psi(x,\uparrow) \tag{21}$$

$$(S_y\psi)(x,\uparrow) = -i(\hbar/2)\psi(x,\downarrow) \tag{22}$$

$$(S_y\psi)(x,\downarrow) = i(\hbar/2)\psi(x,\uparrow). \tag{23}$$

Is the wavefunction in Eq. (15) an eigenstate of any of these operators?

2.4. Write down a wavefunction $\psi(x,\sigma)$ which is an eigenstate of S_x with eigenvalue $\hbar/2$. [It may be easier to use the vector form.]

Problem 3. Classical dipole in a uniform field

3.1. What is the energy of a classical dipole of dipole moment $\tilde{\mu}$ in a magnetic field $\tilde{\mathbf{B}}$. Hint: The units of a dipole moment is current times area – and you can think about it as a small current loop of area A with current I. The dipole moment is $\tilde{\mu} = IA\hat{\mathbf{n}}$. The exact geometry is irrelevant as long as the loop is sufficiently small. For the following problems imagining it to be a square loop may help. Hint 2: Both $\tilde{\mu}$ and $\tilde{\mathbf{B}}$ are vectors, but the energy is a scalar. Hint 3: As a last resort, you can look it up in your electricity + magnetism text.

3.2. Does this uniform magnetic field exert a net force on the dipole? For simplicity, imagine the dipole is formed from currents in a square shaped loop. Think about the force on each segment. If there is a net force, write an expression for it in terms of μ and $\mathbf{B}$. [An alternative logic is to think about how the energy varies as you move the dipole. The gradient of the energy is a force.]

3.3. Does this uniform magnetic field exert a net torque on the dipole? Think about the force on each segment. If there is a net torque, write an expression for it in terms of $\tilde{\mu}$ and $\tilde{\mathbf{B}}$. [An alternative logic is to think about how the energy varies as you rotate the dipole.]

3.4. Our picture of an electron's spin is that it is a spinning charged particle. Thus we have an angular momentum aligned with $\tilde{\mu}$. We define the ratio of the magnetic moment to the angular momentum to be the "gyromagnetic ratio":

$$\tilde{\mathbf{L}} = \frac{1}{\gamma}\tilde{\mu} \tag{24}$$

Given that $\partial_t\tilde{\mathbf{L}} = \tilde{\tau}$, you should be able to see that the dipole will precess. What will the precession frequency be? [This is known as the Larmour precession frequency.]

Hint: You should have in your mechanics class seen differential equations of the form:

$$\partial_t\tilde{\mathbf{A}} = \nu\hat{\mathbf{n}} \times \tilde{\mathbf{A}}. \tag{25}$$

The solution to this equation is that $\mathbf{A}$ precesses about the unit vector $\hat{\mathbf{n}}$ with frequency ν.

Problem 4. Quantum dipole in a uniform field The quantum mechanical, Hamiltonian for a spin-1/2 particle in a uniform magnetic field $\tilde{\mathbf{B}} = B\hat{\mathbf{z}}$ is

$$H = -\gamma B S_z. \tag{26}$$

4.1. What should the energy of an electron in the $|S = 1/2, m_s = \pm 1/2\rangle$ state be in terms of the gyromagentic ratio γ and B. How does the energy between these levels compare with the Larmour precession frequency?

This splitting between the levels is known as the "Zeeman effect." The fact that you can relate energy spacings to dynamics should not be surprising. [Think of the energy splitting in Ammonia, and the rate of tunneling.]

Problem 5. Stern-Gerlach Effect

In this problem we will use *semiclassical* reasoning. We will treat the position of an electron classically, and spin quantum mechanically. The problem can be done entirely with Quantum Mechanics (and it is not too hard) but semiclassical arguments are very powerful, and it is useful to get practice with them.

5.1. Suppose that a magnetic field points in the $\hat{z}$ direction everywhere, but its strength varies – ie. $\tilde{\mathbf{B}} = B(\mathbf{r})\hat{\mathbf{z}}$. How will the energy $E(\mathbf{r})$ of an electron in the $|S = 1/2, m_s = 1/2\rangle$ state vary with position?

5.2. Given that the gradient of the energy is a force – what is the force on the electron?

Clearly an electron in the state $|S = 1/2, m_s = -1/2\rangle$ feels an opposite force. If an electron is in a superposition $|S = 1/2, m_s = 1/2\rangle + |S = 1/2, m_s = -1/2\rangle$, then it is not an energy eigenstate in the magnetic field, and this semiclassical argument is not applicable. Instead, the $|S = 1/2, m_s = 1/2\rangle$ component feels a force in one direction and the $|S = 1/2, m_s = -1/2\rangle$ feels a force in the other direction. The electrons wavepacket will separate into two spatially separated bits – each with their spin aligned in the $\pm\hat{z}$ direction. This is the Stern-Gerlach effect. Eq. (15) is an example of what the wavefunction might look like after the packet is pulled apart.

Problem 6. Fermi pressure: Consider a gas of N spin-polarized fermionic lithium atoms trapped in a magnetic trap. As far as we are concerned these are spinless point particles. As we pointed out in class, you can find the many-body state of the atoms by filling up the N lowest energy states. This is analogous to how we found the electronic state of an atom by filling up the hydrogenic levels.

This procedure makes the cloud pretty big – from a phenomenological point of view it looks like there is a force supporting the atoms. We call this “Fermi pressure.” One can think of the stability of atoms, and in fact of all matter, as being a consequence of this “pressure.” In this problem you will calculate this mysterious force.

The simplest way to measure the pressure of a gas is to put it in a box, with a piston, then try pushing on the piston. The pressure is the force per unit area on the piston at equilibrium.

We can use energetics to calculate the pressure. If we compress the fluid we do work. The work done is the force times the distance – which is just the pressure times the change in volume. Thus

$$P = -\left(\frac{\partial E}{\partial V}\right)_N . \tag{27}$$

As you probably recall from your introductory courses, there are some subtleties about if we let the gas heat up during the compression, but for a zero temperature calculation is fine. We should carry it out at fixed number of particles.

6.1. Suppose we put fermions in a box of size $L_x \times L_y \times L_z$. Lets fill all states with energy less than ϵ_F. How many particles will there be? (Assume ϵ_F is large, so all of the sums can be approximated by integrals, and you don't have to worry about rounding. Also, as we already said, ignore spin.) This gives $N(\epsilon_F)$. We call ϵ_F the "Fermi Energy."

[Hint: You can do this with either hard wall or periodic boundary conditions – you get the same answer either way. The eigenstates are labeled by three quantum numbers k_x, k_y, k_z, and $E = \hbar^2(k_x^2 + k_y^2 + k_z^2)/2m$. You need to first figure out what the allowed values of k_x, k_y, k_z are. You then need to figure out which of these yield energies less than ϵ_F. Finally, add them up (replacing the sums with integrals). You should find the result only depends L_x, L_y and L_z through their product $V = L_x \times L_y \times L_z$.]

Hint: Here is how I would make this argument. Lets use hard wall boundary conditions. In that case the allowed values of k_x, k_y, k_z are $k_x = \pi n_x/L_x$, $k_y = \pi n_y/L_y$ and $k_z = \pi n_z/L_z$ where n_x, n_y, n_z are positive integers. The total number of particles will be

$$N = \sum_{n_x,n_y,n_z} 1 \tag{28}$$

with the constraint that the n's are positive and

$$\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} < \frac{2m\epsilon_F}{\pi^2\hbar^2}. \tag{29}$$

As was stated in the question, the easiest way to do this sum is to convert it into an integral

$$N = \iiint_{\substack{\frac{n_x^2}{\alpha_x^2} + \frac{n_y^2}{\alpha_y^2} + \frac{n_z^2}{\alpha_z^2} < 1 \\ n_x > 0, n_y > 0, n_z > 0}} d^3n. \tag{30}$$

where

$$\alpha_x = \frac{L_x\sqrt{2m\epsilon_F}}{\pi\hbar}, \tag{31}$$

with α_y and α_z given by identical expressions with just $x \to y, z$.
The integral in Eq. (34) is straightforward. You can do it in Cartesian coordinates, but it is easier to first rescale axes, and use spherical coordinates. Define

$$s_x = n_x/\alpha_x \tag{32}$$

$$ds_x = \frac{dn_x}{\alpha_x}, \tag{33}$$

and equivalent scalings for the other directions. This gives an integral

$$N = \alpha_x\alpha_y\alpha_z \iiint_{\substack{s_x^2 + s_y^2 + s_z^2 < 1 \\ s_x > 0, s_y > 0, s_z > 0}} d^3s. \tag{34}$$

The last integral is now trivial in spherical coordinates – or you can recognize it as 1/8'th the volume of the unit sphere.

6.2. Add the energies of all these particles to get how the total energy as a function of the Fermi energy, $E(\epsilon_F)$.

6.3. You have one expression which gives $N(\epsilon_F)$, and a second which gives $E(\epsilon_F)$. Combine these expressions to eliminate ϵ_F, and yield $E(N)$.

6.4. Calculate the pressure by taking the derivative with respect to volume.

6.5. This argument applies to any fermions – not just lithium atoms. In a typical metal (say copper) the electron density is about $10^{29}/\text{m}^3$. Estimate the Fermi pressure of the electrons (in

Pascals). Do not worry about spin – it does not change the answer much. To understand if this number is big or small, you can compare it to the yield strength of copper (70MPa)?

Problem 7. In deriving the Hartree approximation, we used the following result

$$\frac{\delta}{\delta\phi_j^*(r)}\int dr_1 dr_2 \frac{\rho(r_1)\rho(r_2)}{|r_1-r_2|} = 2\phi_i(r)\int dr_2 \frac{\rho(r_2)}{|r-r_2|} \tag{35}$$

where

$$\rho(r) = \sum_i |\phi_i(r)|^2. \tag{36}$$

Here you will prove this by discretizing space. To keep life simple, we will work with an analog 1D integral

$$U = \int dx dx' V(|x-x'|)\rho(x)\rho(x'), \tag{37}$$

where

$$\rho(x) = \sum_i |\phi_i(x)|^2. \tag{38}$$

7.1. Suppose we discretize space, defining ρ only on a set of discrete points $x_1, x_2, \cdots$ where the x_j are separated by a distance δ. Define $\rho_n = \rho(x_n)$. The integral (37) can be approximated by a sum

$$U = \sum_{nm} A_{nm}\rho_n\rho_m. \tag{39}$$

Find A_{nm}. [Don't forget the measure – your answer should involve δ.]

7.2. In terms of entries in the matrix A, what is

$$\frac{\partial U}{\partial \rho_\ell}? \tag{40}$$

Do not substitute your expression for A_{nm} *into this.*

7.3. We define $\phi_{im} = \phi_i(r_m)$. What is

$$\frac{\partial \rho_n}{\partial \phi_{im}^*}? \tag{41}$$

7.4. Using chain rule, find

$$\frac{\partial U}{\partial \phi_{i\ell}^*} \tag{42}$$

in terms of A_{nm}.

7.5. If $x = x_m$, we define

$$\frac{\delta U}{\delta \phi_j^*(x)} = \frac{1}{\delta}\frac{\partial U}{\partial \phi_{im}^*}. \tag{43}$$

Use your answers to the previous subproblems to write

$$\frac{\delta U}{\delta \phi_j^*(x)} \tag{44}$$

in terms of a sum over ρ_m's.

7.6. Interpret your result as a Riemann integral to express

$$\frac{\delta U}{\delta \phi_j^*(x)} \tag{45}$$

in terms of an integral over $\rho(x)$.

Problem 8. Consider the adimensionalized time independent Schrodinger equation for a a particle in a double well potential

$$E\psi(x) = -\frac{1}{2}\partial_x^2\psi(x) + V_0(x^2-1)^2\psi(x). \tag{46}$$

8.1. Plot the potential.

8.2. Numerically calculate the energies of the lowest 6 eigenstates as a function of V_0. Make a plot of E vs V_0 showing these six eigenvalues, with V_0 running from 1 to 50. [Plot them all on one graph.]

When the barrier becomes large, you should see the lowest two levels separate from the others, and become nearly degenerate. These are the two-levels we used when we modeled Ammonia as a two-level system. For that modeling to be sound, there must be a separation of energy scales: The separation between the two levels must be much smaller than their offset from the rest of the spectrum.

8.3. Looking at your graph, how big do you think V_0 needs to be before one can treat this as a two-level system [at least in a low energy experiment]?

Problem 9. Feedback

9.1. How long did this homework take?

9.2. Which of the following words come to mind when you think about this homework (feel free to add your own words if you have something better): frustrating, fun, tedious, insightful, hard, easy, useful, useless, fair, unfair