Problem Set #I, Due: Wednesday January 25 by 11:00am

PHY 362K - Quantum Mechanics II, UT Austin, Spring 2017 (Dated: February 8, 2017)

Some problems on: multiple particles, identical particles, and entanglement

I. VARIATIONAL METHOD – AN EXAMPLE

Consider a single particle in 1D in a quartic potential, i.e. with Hamiltonian:

$$H = \frac{\hat{p}^2}{2m} + V\hat{x}^4 \tag{1}$$

Consider a family of variational wavefunctions $\psi_b(x) = ae^{-bx^2}$.

1. Determine a in terms of b so that ψ is properly normalized.

Solution: In order for ψ_b to be properly normalized, we must have $\langle \psi_b | \psi_b \rangle = 1$, which in the position basis gives us

$$\int_{-\infty}^{\infty} \psi_b^* \psi_b dx = 1$$

but ψ_b is real, so this equation becomes

$$\int_{-\infty}^{\infty} \left(ae^{-bx^2} \right)^2 dx = a^2 \int_{-\infty}^{\infty} e^{-2bx^2} dx = 1$$
 (2)

This Gaussian integral has the well known solution $\int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}}$, using this in equation 2, we obtain

$$\langle \psi_b | \psi_b \rangle = a^2 \sqrt{\frac{\pi}{2b}} = 1 \implies \boxed{a = \left(\frac{2b}{\pi}\right)^{1/4}}$$
 (3)

2. After normalizing, there is only one free trial parameter, b. Varying with respect to b, what is the best variational estimate of the ground-state energy?

Solution: Consider the expected value of the energy of an arbitrary variational wavefunction

$$\langle E_b \rangle = \langle \psi_b | \hat{H} | \psi_b \rangle$$

if we expand $|\psi_b\rangle$ in the basis of energy eigenstates, $|\phi_n\rangle$ with energies E_n , as $|\psi_b\rangle = \sum_{n=0}^{\infty} a_n |\phi_n\rangle$, we obtain

$$\langle E_b \rangle = \left(\sum_{m=0}^{\infty} a_n^* \langle \phi_n | \right) \hat{H} \left(\sum_{n=0}^{\infty} a_n | \phi_n \rangle \right)$$
$$= \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} a_m^* a_n E_n \langle \phi_m | \phi_n \rangle$$
$$= \sum_{n=0}^{\infty} |a_n|^2 E_n \ge E_0 \sum_{n=0}^{\infty} |a_n|^2 = E_0$$

Therefore, the expected value of the energy for any one of our variational wavefunctions must be greater than the true ground state energy of the particle, E_0 . It follows that the best estimate of E_0 is the minimum value of $\langle E_b \rangle$ obtained by varying the free parameter b in the family of variational wavefunctions. We will now determine $\langle E_b \rangle$ using ψ_b .

$$\langle E_b \rangle = \int_{-\infty}^{\infty} \psi_b^* \hat{H} \psi_b^* dx = \int_{-\infty}^{\infty} a e^{-bx^2} \left(-\frac{\hat{p}}{2m} + V \hat{x}^4 \right) a e^{-bx^2} dx$$

$$= a^2 \int_{-\infty}^{\infty} e^{-bx^2} \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V x^4 \right) e^{-bx^2} dx$$

$$= a^2 \int_{-\infty}^{\infty} e^{-bx^2} \left[-\frac{\hbar^2}{2m} \left(4b^2 x^2 - 2b \right) e^{-bx^2} + V x^4 e^{-bx^2} \right] dx$$

$$= -a^2 \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \left[4b^2 x^2 - 2b - \frac{2m}{\hbar^2} V x^4 \right] e^{-2bx^2} dx$$

now if we apply the result

$$\int_{-\infty}^{\infty} x^{2n} e^{-\alpha x^2} dx = \frac{2(2n-1)!!}{\alpha^n 2^{n+1}} \sqrt{\frac{\pi}{\alpha}}$$

to the above integral, we find

$$\langle E_b \rangle = -a^2 \frac{\hbar^2}{2m} \left[4b^2 \left(\frac{2}{2b(2^2)} \sqrt{\frac{\pi}{2b}} \right) - 2b \sqrt{\frac{\pi}{2b}} - V \frac{2m}{\hbar^2} \left(\frac{2(3)!!}{(2b)^2 2^3} \sqrt{\frac{\pi}{2b}} \right) \right]$$

Simplifying and substituting in $a = \left(\frac{2b}{\pi}\right)^{1/4}$, we obtain

$$\langle E_b \rangle = -\frac{\hbar^2}{2m} \sqrt{\frac{2b}{\pi}} \left[\sqrt{\frac{\pi b}{2}} - \sqrt{2\pi b} - V \frac{2m}{\hbar^2} \frac{45}{b^2} \sqrt{\frac{\pi}{2b}} \right]$$
$$= \frac{45V}{b^2} + \frac{\hbar^2}{2m} b$$

Now we must find the minimum value of $\langle E_b \rangle$, E_{\min} . We do this by differentiating the equation for $\langle E_b \rangle$ with respect to b, evaluating at the critical value b_{\min} , and setting equal to zero.

$$\frac{d\langle E_b \rangle}{db} \bigg|_{b=0} = -\frac{90V}{b^3} + \frac{\hbar^2}{2m} = 0 \implies b_{\text{crit}} = \left(90 \frac{2m}{\hbar^2} V\right)^{1/3}$$

Note that $\frac{d^2\langle E_b\rangle}{db^2} = \frac{270V}{b^4} > 0$ for all b, so $b_{\rm crit}$ does in fact give the minimum value of $\langle E_b\rangle$. This minimum value is

$$E_{\min} = \frac{45V}{\left(90\frac{2m}{\hbar^2}V\right)^{2/3}} + \frac{\hbar^2}{2m} \left(90\frac{2m}{\hbar^2}V\right)^{1/3}$$
$$E_{\min} = \left(\frac{\hbar^2}{2m}\right)^{2/3} \left(\frac{45}{90^{1/3}} + 90^{1/3}\right) V^{1/3}$$

So the best variational estimate of the ground state energy is

$$E_0 \approx E_{\min} = \left(\frac{\hbar^2}{2m}\right)^{2/3} \left(\frac{45}{90^{1/3}} + 90^{1/3}\right) V^{1/3}$$

II. NON-INTERACTING ELECTRON GAS

Consider N electrons moving in a 3D cube of length L in each direction and, with periodic boundary conditions. To make progress, let us ignore any interactions between the fermions. Each electron has two possible spin states, and let us assume that the Hamiltonian does not depend on the spin direction. Then the system is described by the Hamiltonian:

$$H = \sum_{i=1}^{N} \frac{\hat{\vec{p}}_i^2}{2m} \tag{4}$$

This is a simple model that describes the properties of metals (in fact, it does surprisingly well considering electrons are actually charged fermions with strong Coulomb interactions), and other systems of dense fermions.

1. What are the energies and wave-functions for just a single electron (N = 1)? Let's call the energy and momentum eigenvalues of these single particle eigenstates the "single particle" energies and momenta.

Solution: For a single electron in the position basis, the Hamiltonian becomes

$$\hat{H} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m} \nabla^2$$

We want to solve $\hat{H}|\psi\rangle = E|\psi\rangle$, which with this Hamiltonian becomes:

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi\tag{5}$$

If we assume that we can write $\psi(x, y, z)$ as $\psi(x, y, z) = X(x)(Y(y)Z(z))$, then we can solve this differential equation. Substituting this expression for ψ into equation 5 and denoting differentiation by primes $(X'' = \frac{d^2X}{dx^2})$, we obtain

$$-\frac{\hbar^2}{2m} \left[X''YZ + XY''Z + XYZ'' \right] = EXYZ$$

dividing through by $\psi = XYZ$ gives

$$\frac{X''}{X} + \frac{Y''}{Y} + \frac{Z''}{Z} = -\frac{2mE}{\hbar^2}$$

but $-\frac{2mE}{\hbar^2}$ is a constant, so each of the three terms on the right must be constants. Therefore we obtain the system of equations

$$\frac{X''}{X} = C_x$$

$$\frac{Y''}{Y} = C_y$$

$$\frac{Z''}{Z} = C_z$$

$$C_x + C_y + C_z = -\frac{2mE}{\hbar^2}$$

Now consider the X equation, $\frac{X''}{X} = C_x$. We recognize that this differential equation has either exponential or sinusoidal solutions. However, in this problem we are enforcing periodic

boundary conditions and so we must have a sinusoidal solution. Therefore we can write $C_x = -k_x^2$, where K_x is a real constant. Then the solution to this equation is

$$X(x) = Ae^{ik_x x}$$

where A is a complex constant. Now, enforcing the periodic boundary condition (namely, X(0) = X(L)) produces

$$A = Ae^{ik_xL} \implies 1 = \cos(k_xL) + i\sin(k_xL) \implies \cos(k_xL) = 1 \implies k_x = \frac{2n_x\pi}{L}$$

where n_x is a positive integer. Therefore the solution to the X equation is $X(x) = Ae^{(2\pi n_x i/L)x}$

A similar argument shows that the solutions for the Y and Z equations are $Y(y) = Be^{ik_yy}$ and $Z(z) = Ce^{ik_zz}$. Therefore, the wavefunction for the single electron is

$$\psi(x, y, z) = ABCe^{ik_x x}e^{ik_y}e^{ik_z}$$
$$= De^{i\frac{2\pi}{L}(n_x x + n_y y + n_z z)}$$

where D = ABC. If we define $\vec{n} = n_x \hat{x} + n_y \hat{y} + n_z \hat{z}$, then we can write

$$\boxed{\psi_{\vec{n}}(\vec{r}) = De^{i\frac{2\pi}{L}\vec{n}\cdot\vec{r}}}$$
(6)

Now, the condition $C_x + C_y + C_z = -\frac{2mE}{\hbar^2}$ along with the definition $C_{x,y,z} = -k_{x,y,z}^2$, gives

$$-\frac{4\pi^2}{L^2}(n_x^2 + n_y^2 + n_z^2) = -\frac{2mE_{\vec{n}}}{\hbar^2}$$

solving for $E_{\vec{n}}$, we find

$$E_{\vec{n}} = \frac{2\pi^2 \hbar^2}{mL^2} |\vec{n}|^2 \tag{7}$$

2. We will next consider the ground-state for very large N, which we will obtain by filling up the single particle orbitals with electrons accounting for Pauli exclusion, which forbids us from putting two electrons of the same spin in the same single-particle orbital. To compute various properties this let's take the limit of $L \to \infty$, and write: $N = \rho L^3$ where ρ is the density of electrons. Then, you can replace discrete sums over momentum eigenvalues $\vec{p} = \frac{2\pi\vec{n}}{\hbar}$ by continuous integrals:

$$\sum_{p} = L^{3} \sum_{p} \frac{(\Delta p)^{3}}{(2\pi\hbar)^{3}} \underset{(L\to\infty)}{\approx} L^{3} \int \frac{d^{3}p}{(2\pi\hbar)^{3}}$$
 (8)

where $\Delta p = \frac{2\pi\hbar}{L}$ is the spacing between the discrete values of p.

(a) What is the largest single-particle momentum, p_F , and energy, ε_F , state that we need to occupy to fit a density ρ of fermions and satisfy Pauli exclusion principle (don't forget to account for spin!). These are called the Fermi momentum (p_F) and Fermi energy ε_F respectively.

Solution: Since electrons are spin-1/2 fermions, we can only put two electrons in each state. We showed in problem 1 that the states are given by $\psi_{\vec{n}} = De^{i\frac{2\pi}{L}\vec{n}\cdot\vec{r}}$.

Therefore each state can be represented by a point in n-space. Since points can only exist at integer values in n-space, there are 8 possible states in a unit cube of n-space. 2 electrons can be placed in each state, so a unit volume of n-space can support 16 electrons. Now, as the number of electrons, N, grows large, the states required begin to fill out an octant of a sphere in n-space. Since we have N total electrons, we need the volume of this sphere to be equal to N/16 in order to fit all the electrons. If we let the radius of the sphere in n-space be n_r , then we have

$$\left(\frac{1}{8}\right)\left(\frac{4}{3}\pi n_r^3\right) = \frac{N}{16}\tag{9}$$

However, n_r corresponds to the maximum magnitude of allowed \vec{n} in n-space, so the maximum allowed energy, known as the Fermi energy E_F , is given by the expression found in problem 1 to be $E_F = \frac{2\pi^2\hbar^2}{mL^2}n_r^2 \implies n_r = \frac{L}{\pi\hbar}\sqrt{\frac{mE_F}{2}}$. Substituting into equation 9, we find

$$\frac{4}{3}\pi \left(\frac{L^3}{\pi^3 * \hbar^3}\right) \left(\frac{mE_F}{2}\right)^{3/2} = \frac{N}{2}$$

solving for E_F , we find

$$E_F = \frac{2\pi^2 \hbar^2}{mL^2} \left(\frac{3}{8\pi}\right)^{2/3} N^{2/3}$$
 (10)

If we consider an electron with the maximum allowed energy, E_F , in the state $|\psi_F\rangle$, and apply the time independent Schrodinger equation with the Hamiltonian for a single electron $\hat{H} = \frac{\hat{p}^2}{2M}$, then we find

$$\hat{H}|\psi_F\rangle = E_F|\psi_F\rangle \implies \hat{p}^2|\psi_F\rangle = 2mE_F|\psi_F\rangle$$

Now, the maximum energy, E_F , must correspond to the maximum momentum, p_F , since the electrons are non-interacting. From this observation and the previous equation it follows that

$$p_F^2 = 2mE_F \implies p_F = \sqrt{2mE_F} \implies p_F = \frac{2\pi\hbar}{L} \left(\frac{3}{8\pi}\right)^{1/3} N^{1/3}$$

(b) What is the total energy per unit volume of the ground-state of a density of ρ fermions? **Solution:** A density of ρ fermions corresponds to $N = \rho L^3$ fermions. As discussed in part (a), the states of these fermions fill an octant of a sphere in n-space, with a radius that is given by $n_r = \frac{L}{\pi\hbar} \sqrt{\frac{mE_F}{2}}$. Substituting the expression for the Fermi energy given in equation 10 we find $n_r = \left(\frac{3}{8\pi}\right)^{1/3} N^{1/3} = \left(\frac{3}{8\pi}\right)^{1/3} L \rho^{1/3}$. To find the total energy of these electrons, E_T , we would have to sum over all of the states inside the octant of the sphere in n-space, however, if we assume N is large, then we can approximate this sum with a volume integral over the octant of the sphere, O.

$$E_T \approx 2 \iiint_{Q} E_{\vec{n}} d^3 n = 2 \iiint_{Q} \frac{2\pi^2 \hbar^2}{mL^2} |\vec{n}|^2 d^3 n$$

we see that the integrand only depends on the magnitude of \vec{n} , so we can transform to spherical coordinates to evaluate the integral.

$$E_T \approx 2 \int_0^{\pi/2} \int_0^{\pi/2} \int_0^{n_r} \frac{2\pi^2 \hbar^2}{mL^2} r^2 (r^2 \sin \theta) dr d\theta d\phi$$

$$\approx 2 \frac{2\pi^2 \hbar^2}{mL^2} \left(\frac{\pi}{2}\right) \int_0^{n_r} r^4 dr$$

$$\approx \frac{2\pi^3 \hbar^2}{5mL^2} n_r^5$$

substituting $n_r = \left(\frac{3}{8\pi}\right)^{1/3} L \rho^{1/3}$, we find

$$E_T \approx \frac{2\pi^3 \hbar^2}{5m} \left(\frac{3}{8\pi}\right)^{5/3} L^3 \rho^{5/3} \tag{11}$$

So the total energy per unit volume is

$$\left| \frac{E_T}{L^3} \approx \frac{2\pi^3 \hbar^2}{5m} \left(\frac{3}{8\pi} \right)^{5/3} \rho^{5/3} \right| \tag{12}$$

III. FERMION DEGENERACY PRESSURE: WHITE DWARFS

Background comments: A white dwarf is a remnant of a star which has burned off most of its hydrogen that was driving the nuclear fusion reaction. Once this fusion reaction stops the remaining elements (mostly helium and carbon) get compressed by gravity into a very dense state, where the electrons are not bound to nuclei but rather roam freely (similar to a metal). We can approximate this gas by the non-interacting electron gas whose properties you worked out in the previous problem.

Some simplifying approximations: Let's approximate the white dwarf as having a perfectly spherical shape of radius R. In principle you would need to solve the previous problem again for a spherical system. However, since the energy is mostly determined by mostly by the volume, so for a large object we can ignore the difference between a sphere and a cube, and just replace L in the previous problem by equating the volume of the sphere and the cube: $L^d = \frac{4\pi}{3}R^3$. Real white dwarfs contain many different elements and isotopes (mostly He and C), but predominately contains He⁴ whose nucleus contains 2 protons with mass and two neutrons with mass. For simplicity, let's ignore the relatively less abundant other elements and isotopes, and consider the star to be made completely of He⁴, and denote the mass of a He⁴ atom by: $m_{\rm He}$.

1. In the previous problem, you calculated the energy of the ground-state of electrons at density ρ coming purely from kinetic energy and Pauli exclusion – this is called the "degeneracy energy". Re-express this degeneracy energy in terms of the total mass, $M = \frac{4\pi}{3}R^3\rho$, and radius R of the star, and the mass of a helium atom: m_{He} . Note that the energy decreases with increasing R, which acts as an effective outward pressure trying to push the star apart. This pressure is usually referred to as "degeneracy pressure".

Solution: In the previous problem, we found that an electron gas taking up a volume L^3 with a density ρ has an energy

$$E_d \approx \frac{2\pi^3\hbar^2}{5m} \left(\frac{3}{8\pi}\right)^{5/3} L^3 \rho^{5/3}$$

in the ground state. Now, if we have a star of mass M that we assume to be made up entirely of He⁴, then the number of atoms in the star is $N_A = M/m_{\rm He} = \frac{4\pi}{3m_{\rm He}}R^3\rho_m$, where ρ_m is the mass density of the star. Each helium atom has two electrons, so the number of electrons, N_e , is $N_e = 2N_A = \frac{8\pi}{3m_{\rm He}}R^3\rho_m$. It follows that the number density of electrons, ρ , is

$$\rho = N_e \left(\frac{4\pi}{3}R^3\right)^{-1} = \frac{2\rho_m}{m_{\rm He}}$$

But we can write the mass density in terms of the total mass of the star as $\rho_m = \frac{3M}{4\pi R^3}$. Substituting this into the expression for the number density of electrons we find

$$\rho = \frac{3M}{2\pi m_{\rm He} R^3}$$

Now, substituting this expression into the expression for the total energy and using $L^3 = \frac{4\pi}{3}R^3$, we find the total energy in terms of M, R and m_{He} to be

$$E_d = \frac{8\pi^4 \hbar^2}{15m} \left(\frac{9M}{16\pi^2 m_{\text{He}}} \right)^{5/3} \frac{1}{R^2}$$
 (13)

which decreases with increasing R, as expected.

2. The size of the star is determined by the balance against the degeneracy pressure and the gravitational forces trying to pull all the matter into the center of the star. Compute the gravitational energy of the white dwarf, assuming it forms a uniform density sphere of radius R and total mass M. (Remember back to Freshman physics that the gravitational field satisfies Gauss' law: $\nabla \cdot \vec{g}(\vec{r}) = -4\pi G \rho_M(\vec{r})$, where $\rho_M(\vec{r})$ is the mass density at point \vec{r} , and G is Newton's constant, and that the gravitational force on a particle of mass m at position \vec{r} is $\vec{F}_g = m\vec{g}$. Then, you can compute the gravitational energy for the sphere by computing the work to bring in infinitesimally thick shells of thickness dr, and integrate this process up to the total radius R.)

Solution: Consider an infinitesimally thin shell of the star of thickness dr with a radius r. This shell has mass $dm = 4\pi \rho_m r^2 dr$. Now, if we imagine the gravity of the portion of the star that lies inside the shell bringing this shell in from infinity to its location at r in the star, we can calculate the work done in this process by

$$dW = \int_{-\infty}^{r} d\vec{F}_g \cdot d\vec{l}$$

where $d\vec{F}_g = -\frac{G(4\pi r^3/3)\rho_m dm}{l^2}\hat{l}$ is the infinitesimal force on the shell from gravity, and \vec{l} is the radial displacement vector from the center of the star to the location of the shell. Substituting these quanities and evaluating the integral, we find

$$dW = \int_{\infty}^{r} \frac{G\left(\frac{4\pi}{3}r^{3}\rho_{m}\right)dm}{l^{2}}dl$$

$$= -\frac{G\left(\frac{4\pi}{3}r^{3}\rho_{m}\right)dm}{r} = -\frac{16\pi^{2}}{3}Gr^{4}\rho_{m}^{2}dr$$

$$= -\frac{16\pi^{2}}{3}Gr^{4}\left(\frac{3M}{4\pi R^{3}}\right)^{2}dr$$

$$= -\frac{3GM^{2}}{R^{6}}r^{4}dr$$
(14)

Now, to find the total gravitational energy, E_g , of the star, we can integrate this infinitesimal work element from r = 0 to r = R

$$E_g = \int_0^R dW = -\int_0^R \frac{3GM^2}{R^6} r^4 dr$$

$$E_g = -\frac{3GM^2}{5R} \tag{15}$$

3. For a given total mass M, find the radius, R, that minimizes the total energy ("degeneracy energy" + "gravitational energy"). Does increasing the total mass, M, make a white dwarf larger or smaller?

Solution: The total energy of the star is

$$E_T = E_d + E_g = \frac{8\pi^4 \hbar^2}{15m} \left(\frac{9M}{16\pi^2 m_{\text{He}}}\right)^{5/3} \frac{1}{R^2} - \frac{3GM^2}{5R}$$
 (16)

we can find the value of R that minimizes the total energy by differentiating this expression with respect to R and setting the result equal to zero.

$$0 = \frac{dE_T}{dR} = -2\frac{8\pi^4\hbar^2}{15m} \left(\frac{9M}{16\pi^2 m_{\text{He}}}\right)^{5/3} \frac{1}{R^3} + \frac{3GM^2}{5R^2}$$

solving for R, we find

$$R = \frac{2}{3GM^2} \frac{8\pi^4 \hbar^2}{3m} \left(\frac{9M}{16\pi^2 m_{\rm He}}\right)^{5/3}$$

which can be simplified to

$$R = \frac{16\pi^4\hbar^2}{9Gm} \left(\frac{9}{16\pi^2 m_{\text{He}}}\right)^{5/3} \frac{1}{M^{1/3}}$$
 (17)

It follows that increasing the mass of the star decreases the radius of the star.

4. What is the mass-density of matter (electrons plus nuclei) in a white dwarf star whose mass is equal to the mass of the sun? (please give an actual number with units). How much would a teaspoon ($\approx 10^{-5} m^3$) of matter from a white dwarf weigh (in kg)?

Solution: For a white dwarf star with mass equal to the mass of the sun $(M = 2 \times 10^{30} \text{ kg})$, we can use equation 17 to calculate the radius of this white dwarf. Using equation 17 with $m = 9 \times 10^{-31} \text{ kg}$, $m_{\text{He}} = 4 \text{ Da} = 4(1.66 \times 10^{-27} \text{ kg})$, $M = 2 \times 10^{30} \text{ kg}$, and the values of all the constants in SI units, we find:

$$R \approx 9.1 \times 10^5 \text{ m}$$

It follows that the volume of this white dwarf is:

$$V = \frac{4\pi}{3}R^3 \approx 3.1 \times 10^{18} \text{ m}^3$$

Therefore, the mass density of the white dwarf is:

$$\rho_m = \frac{M}{V} \approx 6.4 \times 10^{11} \text{ kg/m}^3$$
 (18)

A teaspoon ($\approx 10^{-5} \text{ m}^3$) of the white dwarf matter would weigh

$$(6.4 \times 10^{11} \text{ kg/m}^3) (10^{-5} \text{ m}^3) \approx 6.4 \times 10^6 \text{ kg}$$
 (19)