

Physics 417: Problem Set 11 SOLUTIONS

Problem 1: Griffiths 5.7

For distinguishable particles, the 3-particle state is:

$$\psi = \psi_a(x_1)\psi_b(x_2)\psi_c(x_3) \quad (1)$$

For identical bosons, it must be symmetric under interchange of any pair of particles:

$$\begin{aligned} \psi &= \mathcal{N}(\psi_a(x_1)\psi_b(x_2)\psi_c(x_3) + (\text{all perms})) \\ &= \mathcal{N}(\psi_a(x_1)\psi_b(x_2)\psi_c(x_3) + \psi_a(x_1)\psi_b(x_3)\psi_c(x_2) + \psi_a(x_2)\psi_b(x_1)\psi_c(x_3) + \psi_a(x_2)\psi_b(x_3)\psi_c(x_1) \\ &\quad + \psi_a(x_3)\psi_b(x_1)\psi_c(x_2) + \psi_a(x_3)\psi_b(x_2)\psi_c(x_1)) \end{aligned} \quad (2)$$

There are six distinct orthonormal terms, so the normalization factor is $\mathcal{N} = 1/\sqrt{6}$.

For identical fermions, it must be anti-symmetric under interchange of any pair of particles:

$$\begin{aligned} \psi &= \mathcal{N}(\psi_a(x_1)\psi_b(x_2)\psi_c(x_3) \pm (\text{all perms})) \\ &= \mathcal{N}(\psi_a(x_1)\psi_b(x_2)\psi_c(x_3) - \psi_a(x_1)\psi_b(x_3)\psi_c(x_2) - \psi_a(x_2)\psi_b(x_1)\psi_c(x_3) + \psi_a(x_2)\psi_b(x_3)\psi_c(x_1) \\ &\quad + \psi_a(x_3)\psi_b(x_1)\psi_c(x_2) - \psi_a(x_3)\psi_b(x_2)\psi_c(x_1)) \end{aligned} \quad (3)$$

There are again six distinct orthonormal terms, so the normalization factor is again $\mathcal{N} = 1/\sqrt{6}$. Note that we could also get (3) from the *Slater determinant*:

$$\psi = \det \begin{pmatrix} \psi_a(x_1) & \psi_a(x_2) & \psi_a(x_3) \\ \psi_b(x_1) & \psi_b(x_2) & \psi_b(x_3) \\ \psi_c(x_1) & \psi_c(x_2) & \psi_c(x_3) \end{pmatrix} \quad (4)$$

Problem 2: Griffiths 5.11

(a) We want to compute $\langle 1/|\vec{r}_1 - \vec{r}_2| \rangle$ for the ground state of helium neglecting inter-electron interactions $\psi_0 = \psi_{100}(r_1)\psi_{100}(r_2)$. This is:

$$\begin{aligned} \left\langle \frac{1}{|\vec{r}_1 - \vec{r}_2|} \right\rangle &= \int d^3r_1 d^3r_2 |\psi_0(r_1, r_2)|^2 \frac{1}{|\vec{r}_1 - \vec{r}_2|} \\ &= \frac{64}{\pi^2 a^6} \int d^3r_1 d^3r_2 e^{-4(r_1+r_2)/a} \frac{1}{|\vec{r}_1 - \vec{r}_2|} \\ &= \frac{64}{\pi^2 a^6} \int d^3r_1 \int dr_2 d\theta_2 d\phi_2 r_2^2 \sin\theta_2 e^{-4(r_1+r_2)/a} \frac{1}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta_2}} \end{aligned} \quad (5)$$

The $d\phi_2$ integral just gives 2π trivially. The θ_2 integral can be done because it is a total derivative:

$$\int_0^\pi d\theta_2 \frac{\sin \theta_2}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos \theta_2}} = \frac{1}{r_1 r_2} \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos \theta_2} \Big|_0^\pi = \frac{1}{r_1 r_2} (r_1 + r_2 - |r_1 - r_2|) \quad (6)$$

Substituting this back into (5) yields

$$\left\langle \frac{1}{|\vec{r}_1 - \vec{r}_2|} \right\rangle = \frac{128}{\pi a^6} \int d^3 r_1 \int dr_2 r_2^2 e^{-4(r_1+r_2)/a} \frac{1}{r_1 r_2} (r_1 + r_2 - |r_1 - r_2|) \quad (7)$$

To evaluate the remaining integral over r_2 , we have to split it into two parts, $r_2 < r_1$ and $r_2 > r_1$:

$$\begin{aligned} \left\langle \frac{1}{|\vec{r}_1 - \vec{r}_2|} \right\rangle &= \frac{128}{\pi a^6} \int d^3 r_1 \left(\int_0^{r_1} dr_2 r_2^2 e^{-4(r_1+r_2)/a} \frac{1}{r_1 r_2} (r_1 + r_2 - (r_1 - r_2)) \right. \\ &\quad \left. + \int_{r_1}^\infty dr_2 r_2^2 e^{-4(r_1+r_2)/a} \frac{1}{r_1 r_2} (r_1 + r_2 - (r_2 - r_1)) \right) \\ &= \frac{8}{\pi a^4} \int d^3 r_1 \frac{1}{r_1} e^{-8r_1/a} (a(-1 + e^{4r_1/a}) - 2r_1) \\ &= 4\pi \times \frac{8}{\pi a^4} \times \int dr_1 r_1^2 \times \frac{1}{r_1} e^{-8r_1/a} (a(-1 + e^{4r_1/a}) - 2r_1) \\ &= \frac{5}{4a} \end{aligned} \quad (8)$$

(b) The electron-electron interaction energy for Helium is just $e^2/|\vec{r}_1 - \vec{r}_2|$. So using first-order perturbation theory, we find the first order energy shift to the ground state energy to be:

$$E_0^{(1)} = e^2 \left\langle \frac{1}{|\vec{r}_1 - \vec{r}_2|} \right\rangle = \frac{5e^2}{4a} \quad (9)$$

Let's write this in terms of the ground state energy of hydrogen which is $-E_1 = \frac{e^2}{2a} = 13.6$ eV. Comparing with (9), we obtain

$$E_0^{(1)} = \frac{5}{2} \times 13.6 \text{ eV} = 34 \text{ eV} \quad (10)$$

Adding this to the zeroth order ground state energy of -109 eV, we get $E_0 \approx -75$ eV which is pretty close to the experimental value of -78.975 eV!

Problem 3: Griffiths 5.16

(a) The Fermi energy of a free electron gas according to [5.42] and [5.43] is

$$E_F = \frac{\hbar^2}{2m} \left(\frac{3Nq\pi^2}{V} \right)^{2/3} \quad (11)$$

If we model copper as a free electron gas then it should have $q = 1$ because its electron configuration is $[\text{Ar}]3d^104s^1$ so all shells are filled except the last one which contains a single electron with $\ell = 0$. Then to obtain E_F we need to know N/V . We are given the density and atomic weight of copper: 8.96 gm/cm^3 and 63.5 gm/mol respectively. So its N/V is

$$\frac{N}{V} = \frac{8.96 \text{ gm/cm}^3}{63.5 \text{ gm/mol}} \times 6.022 \times 10^{23} \text{ particles/mol} = 8.50 \times 10^{22} \text{ particles/cm}^3 \quad (12)$$

Plugging this into (11) with $m = 0.511 \text{ MeV } c^{-2}$ and $\hbar = 6.58 \times 10^{-16} \text{ eV s}$ we obtain

$$E_F \approx 7 \text{ eV} \quad (13)$$

(b) The corresponding electron velocity assuming nonrelativistic electrons would be $v_F = \sqrt{2E_F/m} = 0.005c$ so the electrons are reasonably nonrelativistic.

(c) The Fermi temperature is

$$T_F = E_F/k_B \approx 7 \text{ eV}/(8.61 \times 10^{-5} \text{ eV K}^{-1}) \approx 8 \times 10^4 \text{ K} \quad (14)$$

so copper below its melting point is always “cold”.

(d) The degeneracy pressure for copper in this model is (according to [5.46]):

$$P = \frac{(3\pi^2)^{2/3}\hbar^2}{5m} \left(\frac{N}{V} \right)^{5/3} = 3.8 \times 10^{10} \text{ Pa} \quad (15)$$

This is a very big number! By comparison, the atmospheric pressure on the surface of the Earth is only $\sim 10^5 \text{ Pa}$!

Problem 4: Fermions in a harmonic oscillator potential

Let's first consider a more general version of this problem, and then solve it in the two cases of interest. Suppose we have N spin 1/2 fermions in a potential well. Let the well have energy levels labelled by an integer $m \geq 0$. Let the energies be E_m and suppose that at each energy level, there is a total degeneracy d_m allowed by the Pauli exclusion

principle. This degeneracy, the total number of particles that we can put in this energy level, could result from a variety of things, e.g. spin, orbital angular momentum, etc.

We are interested in the ground state of this system. This is obtained by filling up the energy levels with electrons, each time picking the smallest possible m allowed by the exclusion principle. Once a given level is filled (i.e. once the number of particles in that level reaches d_m), we move on to the next higher level. This process ends when we run out of particles. Let's call the highest level we've reached $m = M$. Then the total number of particles N is given by

$$N = \sum_{m=0}^{M-1} d_m + \tilde{d} \quad (16)$$

where $1 \leq \tilde{d} \leq d_M$ is the number of particles in the highest level. We need to treat \tilde{d} separately since we need to account for the possibility of partially filled levels. This equation relates M to N , so we can view M as a function of N . Then the Fermi energy is E_M , and the ground state energy is

$$E_{gs} = \sum_{m=0}^{M-1} E_m d_m + E_M \tilde{d} \quad (17)$$

Now let's apply it to the 1D and the 2D harmonic oscillators.

(a) Consider N identical spin 1/2 particles in a 1D harmonic oscillator potential $V = \frac{1}{2}m\omega^2 x^2$. What are the ground state energy and the Fermi energy? (Your answers should be slightly different for N even and N odd!)

For a 1D harmonic oscillator, the energy levels are $E_m = (m + \frac{1}{2})\hbar\omega$ with $m \geq 0$, and the degeneracy is $d_m = 2$ for spin up and spin down. Thus (16) becomes

$$N = \sum_{m=0}^{M-1} 2 + \tilde{d} = 2M + \tilde{d} \quad (18)$$

Meanwhile (17) becomes

$$E_{gs} = \sum_{m=0}^{M-1} 2(m + \frac{1}{2})\hbar\omega + \tilde{d}(M + \frac{1}{2})\hbar\omega = (M^2 + \tilde{d}(M + \frac{1}{2}))\hbar\omega \quad (19)$$

Finally, $\tilde{d} = 2$ if N is even (the highest level is completely filled), and $\tilde{d} = 1$ if N is odd (the highest level is only half-filled). So for N even this gives $E_{gs} = (M + 1)^2\hbar\omega$ with $N = 2(M + 1)$, so

$$\begin{aligned} E_F &= (M + \frac{1}{2})\hbar\omega = \frac{1}{2}(N - 1)\hbar\omega \\ E_{gs} &= \frac{1}{4}N^2\hbar\omega \quad (N \text{ even}) \end{aligned} \quad (20)$$

For N odd this gives $E_{gs} = (M^2 + M + \frac{1}{2})\hbar\omega$ with $N = 2M + 1$, so

$$\begin{aligned} E_F &= (M + \frac{1}{2})\hbar\omega = \frac{1}{2}N\hbar\omega \\ E_{gs} &= \frac{1}{4}(N^2 + 1)\hbar\omega \end{aligned} \quad (N \text{ odd}) \quad (21)$$

(b) Repeat for a 2D isotropic harmonic oscillator $V = \frac{1}{2}m\omega^2(x^2 + y^2)$ in the limit of large N .

At large N we can ignore the partially filled levels and we can replace sums with integrals, so we set $\tilde{d} = d_M$, and (16) and (17) become

$$\begin{aligned} N &\approx \int^M d_m dm \\ E_{gs} &\approx \int^M E_m d_m dm \end{aligned} \quad (22)$$

For the 2D oscillator, the energies are just the sum of the energies of two decoupled oscillators, $E_{n_x n_y} = (n_x + n_y + 1)\hbar\omega$ with $n_{x,y} \geq 0$. So we identify the level $m = n_x + n_y \geq 0$. The degeneracy of each level is the number of ways we can sum $n_x + n_y = m$ keeping both n_x and n_y nonnegative. This is $(n_x, n_y) = (m, 0), (m-1, 1), \dots, (0, m)$ for a total of $m+1$ pairs. To summarize, $d_m = 2(m+1)$ (accounting for the spin) and $E_m = (m+1)\hbar\omega$. Substituting these into (22), we obtain:

$$\begin{aligned} N &\approx \int^M 2(m+1)dm \approx M^2 \\ E_{gs} &\approx \int^M 2(m+1)^2 \hbar\omega dm \approx \frac{2}{3}M^3 \end{aligned} \quad (23)$$

where we have dropped terms subleading in M . Therefore, in terms of N , the Fermi energy and the ground state energy are:

$$\begin{aligned} E_F &= E_M \approx M\hbar\omega \approx \sqrt{N}\hbar\omega \\ E_{gs} &\approx \frac{2}{3}M^3\hbar\omega \approx \frac{2}{3}N^{3/2}\hbar\omega \end{aligned} \quad (24)$$