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PH 253 / LeClair

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Problem Set 10: Solutions

1. For a one-dimensional infinite square well of length l the allowed energies for noninteracting particles of mass m were found to be $E_n = n^2 E_o$, where n is a positive integer and $E_o = h^2/8ml^2$. The generalization to a three-dimensional infinite well of side l is

$$\mathsf{E} = \left(\mathfrak{n}_{x}^{2} + \mathfrak{n}_{y}^{2} + \mathfrak{n}_{z}^{2}\right)\mathsf{E}_{o} \qquad \mathsf{E}_{o} = \frac{\mathfrak{h}^{2}}{8\mathfrak{m}\mathfrak{l}^{2}} \tag{1}$$

where n_x , n_y , and n_z are positive integers. It is seen that a number of different states (n_x, n_y, n_z) may have the same energy, a situation called degeneracy. For the first 6 energy levels, list the energy of the level and the order of degeneracy, i.e., the number of states having the given energy.

Solution: The quantum numbers n_x , n_y , and n_z can take on integer values of 1 and higher. In order to find the lowest 6 energy levels, we need to find the permutations which give the lowest 6 values of $n_x^2 + n_y^2 + n_z^2$. The *degeneracy* of a given energy means how many different ways a given energy can be obtained from combinations of $n_x^2 + n_y^2 + n_z^2$. That is, for a given energy, how many (n_x, n_y, n_z) states have the same energy – for example, $(n_x, n_y, n_z) = (100), (010), (001)$ all give the same energy, viz., $3E_o$. Running through the permutations (trial and error possibly involved):

| Energy | Equal-energy states (n_x,n_y,n_z) | Degeneracy |
|------------------|-------------------------------------|------------|
| 3Eo | (111) | 1 |
| 6Eo | (211), (121), (112) | 3 |
| $9E_o$ | (221), (212), (122) | 3 |
| 11E ₀ | (311), (131), (113) | 3 |
| $12E_{o}$ | (222) | 1 |
| $14E_{o}$ | (123), (132), (213) | 6 |
| | (231), (312), (321) | |

2. For electrons in a metal or gas molecules in a container, the value of l in the previous problem is so large that the energy levels can be regarded as forming a continuous spectrum. For this case determine the number of states (n_x, n_y, n_z) with energies in the interval between E and E+dE.

Solution: If the electrons are non-interacting, we may treat a collection of N electrons as particles in a square box, with the energy levels given according to the previous problem. Since we know

that different combinations of (n_x, n_y, n_z) may give the same energy, it is convenient to define a variable

$$n^2 = n_x^2 + n_y^2 + n_z^2$$
(2)

which will uniquely determine the energy. If you like, think of this as the "energy level." Think of this n as a vector to a point n_x, n_y, n_z in a three-dimensional space. In this space, every integer set (n_x, n_y, n_z) specifies one state of energy $n^2 E_o$. Thus, in the space with coordinate axes (n_x, n_y, n_z) , each unit cube contains one state. If the number of states is very large, the unit cubes and the spacing between the n_i are so small that we may consider them to have an essentially continuous distribution. In that case, the number of states up to a given n is just the volume of a sphere of radius n:

$$N(n) = \frac{4}{3}\pi n^3 \tag{3}$$

Since n and E are related, this is equivalent to finding the number of states with energies less than E:

$$N(E) = \frac{4}{3}\pi n^3 = \frac{4\pi}{3} \left(\frac{E}{E_o}\right)^{3/2} = \left(\frac{8ml^2}{h^2}\right)^{3/2} E^{3/2}$$
(4)

If we want to know the number of states with energy less than E+dE, we just make a substitution, and the number of states is

$$N(E + dE) = \left(\frac{8ml^2}{h^2}\right)^{3/2} (E + dE)^{3/2}$$
(5)

If the number of states at an energy E is N(E), then the number of states having energies between E+dE and E is N(E) dE. Recognizing a derivative when we see one,ⁱ

$$N(E) dE = N(E + dE) - N(E) = \left(\frac{8ml^2}{h^2}\right)^{3/2} \left[(E + dE)^{3/2} - E^{3/2} \right] = 2\pi \left(\frac{8ml^2}{h^2}\right)^{3/2} \sqrt{E} dE$$
(6)

We made one mistake so far, however. We know that the n_i can only be positive, but in the analysis above we considered only n^2 . In short, we considered the volume of an entire sphere in n-space, when really we are only allowed to consider the region where all $n_i > 0$. Thus, we over-counted by

ⁱThe form we have is g(x) dx = f(x+dx) - f(x), or g(x) = [f(x+dx) - f(x)]/dx. That is the definition of a derivative, so g(x) = f'(x), or g(x) dx = f'(x) dx.

a factor of 8. Dividing by 8, and noting that each state can actually have both a spin up and spin down electron (an extra factor of 2), we need to divide the above by 4, giving us

$$N(E) dE = \frac{4\pi L^3 (2m)^{3/2}}{h^3} \sqrt{E} dE$$
(7)

3. (a) Obtain an expression for the Fermi energy at T=0 K for an electron gas in a metal in terms of the total number of electrons, the volume, and fundamental constants. (b) At T=0 K, what is the rms speed, in terms of the Fermi energy, of an electron gas in a metal?

Solution: The Fermi energy at T=0 is given by

$$\mathsf{E}_{\mathsf{F}}\big|_{\mathsf{T}=0} = \frac{\hbar^2}{2\mathfrak{m}} \left(\frac{3\pi^2 \mathsf{N}}{\mathsf{V}}\right)^{2/3} \tag{8}$$

where N is the number of electrons in a volume V. A derivation may be found here:

http://en.wikipedia.org/wiki/Fermi_energy

This is the energy of the highest-energy electrons in a metal at T=0. If all this energy is available as kinetic energy,

$$\mathsf{E}_{\mathsf{f}} = \frac{1}{2}\mathfrak{m}\nu^2 \qquad \Longrightarrow \qquad \nu = \sqrt{\frac{2\mathsf{E}_{\mathsf{F}}}{\mathfrak{m}}} \tag{9}$$

4. Show that the average kinetic energy of a conduction electron in a metal at 0 K is $E_{av} = \frac{3}{5}E_F$. Hint: in general, the average kinetic energy is

$$\mathsf{E}_{\mathrm{av}} = \frac{1}{\mathsf{n}_e} \int \mathsf{E} \,\mathsf{N}(\mathsf{E}) \,\mathsf{d}\mathsf{E} \tag{10}$$

where n_e is the density of particles, N(E) dE is the number of electrons per unit volume that have energies in [E, E + dE], and the integral is over all possible values of energy.

Solution: The Fermi energy, the energy of the highest occupied quantum state in a system of fermions at absolute zero temperature, is a function of the number of fermions as found in the last problem. If there are N particles in a volume V, then the highest occupied state has an energy

$$E_{\rm F}({\rm T}=0) = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 {\rm N}}{{\rm V}}\right)^{2/3}$$
(11)

Thus, as more and more particles are added, it takes more and more energy to add the last particle. The total energy of the system, if there are enough particles to consider the distribution of states to be quasi-continuous, is given by

$$\mathsf{E}_{\rm tot} = \int_{0}^{\mathsf{N}} \mathsf{E}_{\mathsf{F}}(\mathsf{N}') \, \mathsf{d}\mathsf{N}' \tag{12}$$

The average energy is simply the total energy divided by the number of particles:

$$\mathsf{E}_{\rm avg} = \frac{1}{\mathsf{N}} \int_{0}^{\mathsf{N}} \mathsf{E}_{\mathsf{F}}(\mathsf{N}') \, \mathsf{d}\mathsf{N}' = \frac{1}{\mathsf{N}} \int_{0}^{\mathsf{N}} \frac{\hbar^2}{2\mathfrak{m}} \left(\frac{3\pi^2 \mathsf{N}'}{\mathsf{V}}\right)^{2/3} \, \mathsf{d}\mathsf{N}' = \frac{1}{\mathsf{N}} \frac{\hbar^2}{2\mathfrak{m}} \left(\frac{3\pi^2}{\mathsf{V}}\right)^{2/3} \left(\frac{3}{5}\mathsf{N}^{5/3}\right) = \frac{3}{5} \mathsf{E}_{\mathsf{F}}$$
(13)

5. Explain the basic operation of a field-effect transistor (FET). How does a field effect transistor uses a small gate voltage to produce large modulations in source to drain current?

Solution: We did this a couple of times in lecture. There is a quick overview here:

http://faculty.mint.ua.edu/~pleclair/PH253/Notes/info_storage.pdf

6. Explain, appealing to band theory, why conductors tend to be opaque and insulators transparent.

Solution: Insulators have a gap of forbidden energies between the highest filled states and lowest occupied states, so photons of energy less than this gap cannot be absorbed (since that would involve promoting an electron to a forbidden state). Thus, insulators are transparent for photon energies less than their energy gap. Metals have no such gap, and can essentially absorb photons of any energy. Also covered in lecture.

7. *Pauli exclusion.* What are the energies of the photons that would be emitted when the fourelectron system in the figure below returns to its ground state? See also: Pfeffer & Nir 3.4.5

Solution: The ground state must consist of a spin up and spin down electron in each of the two lowest energy levels. The possible transitions returning the system to the ground state are shown above. Transitions A and D have the same energy difference, and thus give rise to the same energy photon, and thus only three different photons should be observed:

$$E_{A} = E_{D} = E_{3} - E_{2} = 9.36 \,\text{eV} - 4.16 \,\text{eV} = 5.20 \,\text{eV}$$
(14)

$$\mathsf{E}_{\mathsf{B}} = \mathsf{E}_2 - \mathsf{E}_1 = 4.16 \,\mathrm{eV} - 1.04 \,\mathrm{eV} = 3.12 \,\mathrm{eV} \tag{15}$$

$$E_{C} = E_{3} - E_{1} = 9.36 \,\text{eV} - 1.04 \,\text{eV} = 8.32 \,\text{eV}$$
⁽¹⁶⁾



A system of four electrons with three energy levels, their ground state, and the possible transitions to the ground state.

8. Three non-interacting particles are in their ground state in an infinite square well;ⁱⁱ see the figure above. What happens when a magnetic field is turned on which interacts with the spins of the particles? Draw the new levels and particles (with spin).



A system of three electrons in an infinite square well, and the shift of the energy levels when a magnetic field is applied.

Solution: After the external magnetic field is applied, the new value of each particle's energy level E_i equals the original level E_n plus the interaction (Zeeman) energy:

$$\mathsf{E}_{\mathsf{i}} = \mathsf{E}_{\mathsf{n}} - \vec{\mu}_{\mathsf{s}} \cdot \vec{\mathsf{B}} = \mathsf{E}_{\mathsf{n}} - \mu_{\mathsf{s}z}\mathsf{B} = \mathsf{E}_{\mathsf{n}} + 2\mathsf{m}_{\mathsf{s}}\mu_{\mathsf{B}}\mathsf{B} \tag{17}$$

Since $m_s = \pm \frac{1}{2}$, the new levels will be displaced from the old by an amount $\Delta E = \pm \mu_B B$, with a spin $-\frac{1}{2}$ ("down") particle occupying the lower sublevel and a spin $+\frac{1}{2}$ ("up") particle occupying the upper sublevel. In contrast to the situation without a magnetic field present, the particle in the n=2 level will have its spin $-\frac{1}{2}$ if the system is in the ground state.

 $^{^{\}rm ii}{\rm Recall}$ the energies in an infinite square well are $E\!=\!n^2h^2/8ma^2$