

Physics 155- Winter 2016

Introduction to Condensed Matter Physics

Test-4: 100 points, Time 1.20 hours 11 March, 2016

Your Name (Capitals)

***** Notes on reversed page *****

1. A free electron like metal in a simple cubic system with lattice constant a , has r electrons per atom.

(i) Find the ratio of the volume of the Fermi surface to the volume of the first Brillouin zone. [10]

First note that $V_{BZ} = 8\pi^3/a^3$. The FS volume is $4\pi k_F^3/3$, where k_F is determined from the number of electrons N_{el} through $N_{el} = (V/8\pi^3) \times 2 \times 4\pi k_F^3/3$, so that $V_{FS} = 4\pi^3 N_{el}/V$. Now $N_{el} = rN$, where N is the number of cells. Using the property of the simple cubic lattice $V = a^3 N$ we get $V_{FS} = r \times 4\pi^3/a^3$. Thus the answer is

$$V_{FS}/V_{BZ} = r/2.$$

(ii) Calculate the area of the Fermi surface. [10]

The above calculation also gives us $k_F = (3\pi^2 r)^{1/3}/a$, and the area of the FS = $4\pi(3\pi^2 r)^{2/3}/a^2$.

(iii) At $r = 1, 2$ is this system a metal or insulator? [5]

A metal in both cases. For $r=2$ we have a sphere which cannot fit into a cube and hence the FS is not fully gapped.

2. The thermal average of the magnetic moment of a collection of N non interacting atoms with angular momentum J is given by $M = N\mu_B g_J J B_J(x)$, where $x = g_J \mu_B \beta H$, and the Brillouin function is given by:

$$B_J(x) = \frac{J + 1/2}{J} \coth x(J + 1/2) - \frac{1}{2J} \coth x/2.$$

At high temperatures we can expand using $\coth(a) = 1/a + a/3 + O(a^3)$. Carry out this expansion to lowest relevant order and show that the susceptibility χ equals

$$\chi = N p_{eff}^2 / (3k_B T),$$

with $p_{eff} = g_J \mu_B \sqrt{J(J+1)}$ [10]

This is straightforward algebra.

Specializing to the case of $J = 1/2$, and using the standard properties of the coth function, show that the thermal average of the magnetic moment is given by

$$M = N \mu_B \tanh \mu_B \beta H. \quad \dots\dots [10]$$

This is also straightforward algebra where we additionally use the doubling formulas $\sinh(2x) = 2\sinh(x)\cosh(x)$ and $\cosh(2x) = 2\cosh^2(x) - 1$.

3. For each of the following cases find the total L, S and J and the magnetic moment at $T = 0$ in units of the Bohr magneton.

(i) A Cobalt compound in the Co^{3+} state, using the electronic configuration $Co = [Ar]3d^7 4s^2$ [15]

Here we have $3d^6$ configuration. By Hund's rule $L=2, S=2$ and $J=4$. The Lande g factor is $3/2$ using the given formula. Hence the magnetic moment at $T=0$ is $M/N = g_J \mu_B J = 6\mu_B$.

(ii) A Niobium compound in the Nb^{2+} state, using the electronic configuration $Nb = [Kr]4d^4 5s^1$ [15]

Here we get a $4d^3$ configuration with $L=3, S=3/2$ and $J=3/2$. Hence $g = 2/5$ using the given formula. Hence the magnetic moment is $M/N = 3/5\mu_B$

4. The bound state of a donor atom in a semiconductor is found to have a radius $a_B \sim 900$ Angstroms. Given that the principal quantum number $n = 3$, and the conduction band mass $m_c = m_e/10$.

For solving both these problems, we express the energy and Bohr radius in terms of the principal quantum number n , mass ratio m_c/m_e and dielectric constant ϵ as

$$E_B = E_{Hydrogen} \times (m_c/m_e)/(n^2\epsilon^2), \dots (a)$$

and

$$a_B = a_B^0 \times n^2 \times \epsilon \times m_e/m_c, \dots (b)$$

where $a_B^0 = 0.52$ Angstrom.

(i) Find the dielectric constant of the semiconductor. [15]

Using (b) and the given data, we get $\epsilon = 19.2$.

(ii) Find the binding energy relative to the bottom of the conduction band in eV. [10]

Using (a) and the given data plus the computed ϵ we get $E_B = -13.6/(90 \times 19.2^2) = -.00041$ eV.

Notes

- The Landè factor is given by:

$$g_J = 3/2 - (L(L + 1) - S(S + 1))/(2J(J + 1)).$$

- The ground state energy of Hydrogen atom is -13.6 eV, and the corresponding Bohr radius is ~ 0.52 Angstrom.
- m_e is the electron mass in vacuum. Its numerical value is not needed in the above problems.