Physics 155- Winter 2016

Introduction to Condensed Matter Physics

Solution of Test-3: 100 points, Time 1.20 hours 29 February, 2016

1. (a) If the atoms given below are arranged in a hypothetical 1-d lattice, list the ones expected to be metals. ([Ar] stands for Argon)

   (i) Sc: $[Ar]3d^1 4s^2$ (ii) V: $[Ar]3d^3 4s^2$ (iii) Cr: $[Ar]3d^4 4s^2$ (iv) Cu: $[Ar]3d^{10}4s^1$ ......[10]

   Except for Cr all other atoms have an odd number of electrons in the d-s combined levels. Hence they are all metals except Cr, in this 1-d example.

   (b) Consider a 2-d square lattice with 2 electrons per atom. Assuming that the periodic potential is negligible, calculate k_F. How much is the area of the Fermi circle relative to the area of the first Brillouin zone? ......[15]

   Area $A_F = \pi k_F^2$ follows from equation for the number electrons $N_e = 2 \times L^2 \times A_F/(4\pi^2)$, where the factor of 2 is from spin. However we have 2 electrons per atom, and the number of atoms $N_A = L^2/a^2$ for the square lattice. Hence $N_e = 2L^2/a^2$, and so comparing the two equations for N_e we get

   $$A_F = \pi k_f^2 = 4\pi^2/a^2.$$

   This is also the area of the first Brillouin zone where both k_x and k_y range between $-\pi/a$ to π/a.

   (c) Give a brief argument explaining if the system in (b) is a metal or an insulator. ......[5]

   This is a metallic state since the circle cannot be made to coincide with the square :-)

2. Consider a 1-d tight binding model with nearest neighbor hopping t and energy dispersion $\varepsilon_k = -2t\cos(ka)$, where a is the lattice constant.

   (a) Calculate the Fermi energy ε_F and Fermi velocity v_F as a function of the electron density $n = N/L$, where N (or L) is the electron number (or length) of the system. ......[15] *We first calculate $k_F = \pi N/(2L)$, so that $\varepsilon_F = \varepsilon_{k_F} = -2t\cos(\pi Na/2L)$. The Fermi velocity $v_F = \partial\varepsilon_k/(\hbar\partial k)/_{k_F} = 2at/\hbar \sin(\pi Na/2L)$.*

(b) Show that the density of states in this model is given by

$$g(\varepsilon) = \frac{2L}{a\pi} \frac{1}{\sqrt{4t^2 - \varepsilon^2}}. \quad \ldots\ldots [25]$$

As we saw in class, the density of states is expressible from $g(\varepsilon)d\varepsilon = 2 \times L/(2\pi)(dk/d\varepsilon)d\varepsilon$ *so that* $g(\varepsilon)L/\pi = |dk/d\varepsilon|$ *(absolute value since* g *is positive). We thus require an expression for* $dk/d\varepsilon$ *in terms of* ε*. The easiest way to get the required answer is to write the dispersion relation in an inverted form*

$$k = (1/a) \times \arccos\left[\varepsilon_k/(-2t)\right].$$

Using the standard identity $d/dx \arccos x = -1/\sqrt{1-x^2}$*, we obtain the required density of states. Another somewhat longer method is to write* $(dk/d\varepsilon) = 1/(\hbar v_F)$*, and convert the earlier expression for* v_F *to the energy by using* $\sin(x) = \sqrt{1 - \cos^2(x)}$*.*

3. (a) Calculate the bandwidth (i.e. difference between the highest and lowest energies in the band) of the tight binding model in 1-d (from the energy dispersion given) and for the 2-d square lattice. ...... [5]
From the known dispersions the bandwidth W *is given as* $W = 4t$ *in 1-d,* $8t$ *in 2-d for the square lattice.*

(b) Consider the tight binding model on the triangular lattice. Write down the nearest neighbor list. Taking the usual definition, show that the energy dispersion is

$$\varepsilon_k = -2t\cos(k_x a) - 4t\cos(k_x a/2)\cos(\sqrt{3}k_y a/2). \quad \ldots\ldots [15]$$

(c) Show that near the bottom of the band $\vec{k} = \{0, 0\}$, the effective mass is given by

$$m^* = \hbar^2/(3ta^2). \quad \ldots\ldots [10]$$

The 6 nearest neighbors $\vec{\eta}$ *are in units of* a *the lattice constant* $\pm\{1, 0\}$, $\pm\{1/2, \sqrt{3}/2\}$ *and* $\pm\{-1/2, \sqrt{3}/2\}$*. Hence the dispersion is*

$$\varepsilon_k = -2t\{\cos(k_x a) + \cos(k_x a/2 + \sqrt{3}/2k_y a) + \cos(k_x a/2 - \sqrt{3}/2k_y a)\}.$$

Now using the trig identity $Cos(A+B)+Cos(A-B) = 2Cos(A)Cos(B)$*, we get the required answer.*

Near $\vec{k} \sim 0$ *we can Taylor expand* ε_k*. Collecting the various terms we find the isotropic result* $\varepsilon_k = -6t + 3/2a^2k^2 + O(k^4)$*. Ignoring the constant and equating the rest to* $\hbar^2k^2/(2m^*)$ *we get the required result.*