Physics 481: Condensed Matter Physics - Homework 10

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due date: April 15, 2011

Problem 1: Fermi surfaces in two dimensions (10 points)

Consider a two-dimensional system of nearly free electrons (weak periodic potential) with a square unit cell (lattice constant a). Determine the Fermi surfaces for the cases of 1, 2, 3, and 5 electrons per unit cell. To this end, first project the free electron Fermi surface into the 1st Brillouin zone and then think about at what points gaps open.

Plot the Fermi surfaces in the Brillouin zone. It might be useful to make separate plots for the different bands. (Note: Semi-quantitative plots are OK, i.e., you need to get the topology right, the exact positions are not so important.)

Problem 2: Kronig-Penney model (Marder, problem 7.5, 15 points + 10 BONUS points)

Consider an electron in 1D in the presence of the periodic potential (Kronig-Penney model)

$$U(x) = \sum_{m=-\infty}^{\infty} U_0\, \Theta(x - ma)\, \Theta(ma + b - x) \ .$$

a) Restrict your attention to a single unit cell, and write down the boundary conditions for the wave function as required by Bloch's theorem.

b) Solve the Schrödinger equation by constructing $\psi(x)$ from plane waves and imposing suitable boundary conditions at $x = 0, b, a$. The results is a relation between the Bloch index k and the energy.

c) Take the limit $b \to 0$, $U_0 \to \infty$ with $U_0 b \to W_0 a \frac{\hbar^2 a^{-2}}{m}$. Show that the condition for the Bloch index simplifies to

$$\cos(ka) = \frac{W_0}{qa}\sin(qa) + \cos(qa)$$

where q is related to the eigenenergy ϵ via $q = (2m\epsilon/\hbar^2)^{1/2}$.

d) Produce plots of the lowest two energy bands $\epsilon_{n\mathbf{k}}$ ($n = 0, 1$) in the limit of part c) with $a = 1$, $m = 1$, $\hbar = 1$, and $W_0 = 0.5$.

Problem 3: 2D tight-binding model (15 points)

Consider electrons in a two-dimensional square lattice (lattice constant a) in tight-binding approximation. The dispersion relation is $\epsilon = -2t\cos(k_x a) - 2t\cos(k_y a)$ with $t > 0$.

a) Sketch $\epsilon(\mathbf{k})$ along the lines $\Gamma - X$, $X - W$, and $W - \Gamma$.

b) Plot a few constant energy lines on the k_x, k_y plane.

c) With one electron per site in this crystal, draw the Fermi surface. Is this a metal or an insulator?

d) With two electrons per site, draw the Fermi surface. Is this a metal or an insulator?