PHYS4450 Solid State Physics

SAMPLE QUESTIONS FOR DISCUSSION in Week 10 EXERCISE CLASS (27 March 2013)
You may want to think about them before attending exercise class.

Chapter X discussed energy band theories. SQ17 discusses the Kronig-Penney model, which is the simplest example of band formation in QM. SQ18 discusses how to apply the tight-binding method of a solid with more than one atom per unit cell. SQ19 discussed the Fermi surface in a 2D tight-binding band ($2N$ states) with only N electrons (half-filled case).

SQ17 **Kronig-Penney Model.** This are very few "exactly solvable" band structure problems. The Kronig-Penney model is one of them.

In 1930, Kronig and Penney published a paper in Proceedings of the Royal Society (London), A **130**, 499 (1930). They introduced a one-dimensional periodic square wells model to illustrate the formation of bands (ranges of energies in which there are energy eigenvalues). Their model has become standard textbook contents. Their model can be described by a 1D potential energy function with **repeating units** of the following form:

$$\begin{aligned} V(x) &= V_0 \quad -b < x < 0 \\ &= 0 \quad\;\; 0 < x < c \end{aligned}$$

and thus there is a period of $a = b + c$.

TA: Set up the problem in a concisely way. Write down the solutions in the two regions in a unit cell, and then illustrate clearly the steps in which the Bloch's theorem is applied to set up a closed set of equations. Then illustrate that the solutions really give bands and band gaps.

Remarks: There are variations on the Kronig-Penney Model. For example, one can consider a 1D periodic array of δ-functions as a model of solid. This is interesting in that one can do it as in SQ17 or in terms of tight-binding the bound states of each δ-function to form a band. [If you know the quantum mechanics of a single δ-function, then you know there is a bound state.] Kronig also contributed much to the idea of spin (in 1925) and then a casuality relation called the Kramers-Kronig (or KK) relation that relates the real and imaginary parts of response functions (such as the real and imaginary parts of a complex conductivity or a complex dielectric function as you did in Problem Set 4).

SQ18 **Tight-binding Model – 2 atoms per unit cell.** In Ch.X, We introduced the tight-binding method in the simplest possible situation, where there is only one atom per unit cell AND each atom contributes only one atomic orbital. The result is the formation of a single tight-binding band. The method of TBM is, of course, more general than that.

Here, the TA will illustrate how to **generalize TBM** to two atoms per unit cell (but in the simple case of a 1D solid). Consider a 1D solid of lattice constant a of the form ...ABABABABAB..., where A and B refer to two different types of atoms. Let's say they are separated by $a/2$ (this really doesn't matter though). For simplicity, we consider each atom contributes only one atomic orbital to form bands. Thus, an A atom contributes a χ_A atomic state and a B atom contributes a χ_B atomic state. By constructing two Bloch sums, one corresponding to A atoms and another for B atoms, and using the tight-binding model, calculate the band structures that originated from linearly combining the atomic orbitals. TA: More important to illustrate the approach (than the mathematics). You will get at a 2×2 matrix problem for each k-value.

Remarks: Some results are studying conducting polymers for their presentation. The polymer polyacetylene $(C_2H_2)_n$ is an example of the problem (A and B are the same atom but there are alternating single and double bonds).

SQ19 **Fermi surface – 2D tight-binding half-filled band.** This Sample Question serves to explain the figure on class notes page XI-25 for the constant energy contours ("surfaces") of a 2D tight-binding band.

For a 2D solid with a structure of a square lattice of lattice constant a and one atom sitting at the lattice site, the tight-binding model gives a band of the form

$$E(\mathbf{k}) = E(k_x, k_y) = -2t\left(\cos k_x a + \cos k_y a\right) \ .$$

The band can hold a maximum of $2N$ electrons, where N is the number of unit cells in the system.

(a) Determine the Fermi surface for the case of a 1/4-filled band, i.e., there are $N/2$ electrons filling the 2D tight-binding band.

(b) Now there are N electrons (N is the number of unit cells) in the band. This is referred to as the half-filled case (why?). Construct the Fermi surface.

[**Remark:** The half-filled case is believed to be relevant to high T_c superconductors such as YBCO. In YBCO, there are layers of CuO_2 planes. It is believed that these 2D layers are fundamental to the understanding of superconductivity. In the half-filled case, a special feature of the Fermi surface is that pairs of points on opposite sides of the surface are connected by some (and the same) vector in the reciprocal space. This feature is called the "nesting" of Fermi surface. TA: If you know something more about this "nesting" effect, please point it out.]