PHYS4450 Solid State Physics

SAMPLE QUESTIONS FOR DISCUSSION in Week 11 EXERCISE CLASS (3 April 2013)
You may want to think about them before attending exercise class.

Chapter X discussed energy band theories. SQ20 writes the tight-binding result in terms of a tight-binding Hamiltonian. SQ21 points out that band theory, while with much success in understanding the properties of solids, has its problems. Understanding the problem of band theories is the beginning of many-body physics. SQ22 is related to the density of states in anisotropic bands.

SQ20 **"Tight-Binding Hamiltonian"** (Optional for course contents.) We know that in a 1D simplest tight-binding band that takes into account of the on-site energy ϵ_0 and the nearest neighboring hoping, it has the form of

$$E(k) = \epsilon_0 + 2t\cos(ka)$$

where a is the lattice constant.

Recall that this expression gives the energy eigenvalues. The Schrödinger equation is $\hat{H}\psi = E\psi$. In some books, the authors write the Hamiltonian in terms of the basis set of atomic orbitals centered at different locations R_i. Explicitly, one can use the notation $|i\rangle$ for an atomic orbital centered at the site R_i (or simply i), i.e.,

$$< x|i >= \chi(x - R_i)$$

where $\chi(x - R_i)$ is the wavefunction of the atomic orbital centered at R_i. In this way, the Hamiltonian takes on the form in 1D systems:

$$\hat{H} = \sum_i |i\rangle\epsilon_0\langle i| + \sum_i |i\rangle t\langle i+1|$$

where the second term implied only nearest neighboring hopping is allowed. TA: By forming a Block Sum over the set of atomic orbitals $|i\rangle$, show that the Hamiltonian really gives the band $E(k)$. Note that I have not been very careful about the proper form of the second term. For example, if I want to write it as $\sum_{i,j(n.n.)} |i\rangle t\langle j|$, where the sums are over i and j but they must be nearest neighbors, will it just be the same?

Remark: In general, the tight-binding Hamiltonian can be written in the form

$$\hat{H} = \sum_i |i\rangle\epsilon_i\langle i| + \sum_{i,j} |i\rangle t_{ij}\langle j|$$

where ϵ_i gives the on-site energy (energy of atomic level) of the atom at location $\mathbf{R}_i$ and t_{ij} gives the hopping integral between the atoms at locations $\mathbf{R}_i$ and $\mathbf{R}_j$. This Hamiltonian can now be used to study alloys, e.g., $A_{0.8}B_{0.2}$ so that one can generate a configuration randomly according to the 80% and 20% concentrations and then write down the Hamiltonian accordingly. TA: I have not been careful to include a term of the complex conjugate of the second term. You may check textbooks or literature on the proper way to write it.

SQ21 (**A Problem with Band Theory.**) We have discussed in some length the Energy Band Theory. According to Band Theory (see Chapter XI), a material with partially filled band is a conductor. Think about sodium. The outermost 3s electrons fill (half-fill) partially a band. Indeed, sodium is a metal. However, looking closer, the **same prediction holds** even the sodium atoms are well separated (e.g. separated by 1 m). Would you expect such a system to be a metal? What's wrong? [This leads to the consideration of on-site Coulomb interaction and its energy U. There is then a competition between t (in tight-binding model that characterizes the hopping of electrons) and U, which is the main idea in the Hubbard model (which is the beginning of many-body physics).

SQ22 **Related to Problem 5.3.** It should not be surprising by now to know that in some cases, a band may be anisotropic, i.e., as one goes from $\mathbf{k} = 0$ in different directions in the 1st BZ, the curvature can be different. Here is an example. Consider a two-dimensional anisotropic band of the form

$$\epsilon(\mathbf{k}) = \hbar^2[\frac{k_x^2}{2m_1} + \frac{k_y^2}{2m_2}],$$

where in general $m_1 \neq m_2$. Discuss how can one obtain the density of states $g(\epsilon)$ in this 2D system? When $m_1 = m_2$, what is the result? Does the result reduce to the known result for an isotropic 2D free electron band?