Due Apr. 21, Thursday.

NOTICE

Two problems at end are removed now, relative to the print-out version that was distributed in class. **Do the following 4 problems**, instead of 6 problems. The now-removed problems will be included in the next homework, and so if you worked on them already, you work won't be lost. For problem 4, please read, at the minimum 2.2.3 and 2.3.4 of the book. Some of these topics were already covered in the HW 1. A more in-depth discussion related to problem 4, will occur in the next lecture.

Problem 1 (20 points) Consider a 1D crystal with lattice constant a. Show that

$$\varepsilon(k) = -2t\cos(ka) - 2t_2\cos(2ka)$$

is a valid band dispersion but

$$\varepsilon(k) = -2t\cos(ka) - 2t_2\cos(ka/2)$$

is not. Make sketches in the k-ε plane, for both functions. In your sketches, carefully mark the special k points, $k = n\pi/a$ with $n = 0, \pm 1, \pm 2, \ldots$, and the overall period of $\varepsilon(k)$. Assume that $t > 0$ and $t_2 > 0$.

Problem 2 (20 points) Consider the following simple dispersion for a 1D crystal with lattice constant $a = 3$ Å.

$$\varepsilon(k) = -2t\cos(ka)$$

We take $t = 2$ eV. In a real band structure t can range from several tenths of eV to several eV's.

(a) Find the group velocity $v = \partial\omega/\partial k$, where ω is defined by $\varepsilon(k) = \hbar\omega$.

(b) Make a sketch of the group velocity as a function of k.

(c) Find the maximum group velocity as a fraction of the speed of light. This would be the so-called **"Fermi velocity"** if this band were exactly half-filled. Note that $\hbar c = 1973$ eV Å. The Fermi velocity is the typical velocity of an electron in a metal (even at $T = 0$!).

Problem 3 (20 points) Consider a cube with a side length 2, and the origin at the center. Namely, the eight vertices of the cube are given by $(\pm 1, \pm 1, \pm 1)$.

(a) Choose four vertices of the cube so that any pair of vertices are diagonally connected to each other on a *face* of the cube. Explain briefly why these four vertices form a tetrahedron. Include a diagram of the cube and the tetrahedron.

(b) Put a Si atom at the origin of the cube. Also, put a Si atom at each vertex that you found in the previous part. This is the tetrahedron motif of a Si crystal, up to a scale. Consider the atomic $3s$ and $3p$ wave functions for the Si atom at the origin: $\psi_s, \psi_x, \psi_y, \psi_z$, corresponding to orbitals commonly referred to as s, p_x, p_y, p_z orbitals, respectively. For this problem, the following information regarding these orbitals would be sufficient: (1) Each of them is normalized. (2) They are orthogonal to each other. That is, they are "ortho-normal:"

$$\int d^3\vec{r}\; \psi_\alpha^* \psi_\beta = \delta_{\alpha,\beta}$$

where α or β can be one of s, x, y, z, and $\delta_{\alpha,\beta} = 1$ if $\alpha = \beta$ and 0 if $\alpha \neq \beta$ ("Kronecker delta symbol"). (Note that all wave functions are real: $\psi_\alpha^* = \psi_\alpha$.)
Consider these four new orbitals:

$$\psi_i = \frac{1}{2}\psi_s + \frac{1}{2}(x_i\psi_x + y_i\psi_y + z_i\psi_z)$$

where x_i, y_i, z_i are the coordinates of each vertex that you found in the previous part, and the vertex index $i = 1, 2, 3,$ or 4. Show that these new orbitals are also "ortho-normal":

$$\int d^3\vec{r}\; \psi_i^* \psi_j = \delta_{i,j}$$

where $\delta_{i,j} = 1$ if $i = j$ and 0 if $i \neq j$. **These four orbitals ψ_i are the sp^3 orbitals of Si**.

(c) (10 points, extra credit) Make rough sketches ("signed lobes") of these orbitals, by first noting that the second part of the wave function ($\propto (x_i\psi_x + y_i\psi_y + z_i\psi_z)$) is a p wave function pointing along the direction of each vertex. That is, the second part has exactly the same shape as the ψ_x orbital but points along the i-th vertex vector. In your sketches, mark clearly the position of the origin relative to the position where the wave function ψ_i is zero.

Problem 4 (10 points for (a,b) and 10 extra credit points for (c,d,e)) Pierret 2.4.