MATERIALS PHYSICS II FALL 2006 HOMEWORK PROBLEMS 3

Return to Michael by Wednesday 4.10.2006 at noon

1. Derive the dispersion relation $\epsilon(\mathbf{k})$ for fcc and bcc lattices in the tight-binding approximation, assuming one s-electron per lattice site and only the nearest-neighbour interactions. Evaluate the bandwidth in each case and relate it to the coordination number. (**3 points**)

2. *Peierls distortion in an infinite chain (ring).* Consider an infinite ring of atoms with the atomic spacing of a. Let the on-site energy be zero and the hopping integral β. The dispersion relation is then $\epsilon(k) = -2\beta cos(ka)$. Suppose that every second atom is slightly displaced, and this leads to two hopping integrals, β_1 and β_2 in the unit cell.
(a) What are now the max. and min. values of k in the 1st Brillouin zone (BZ)?
(b) Show the eigenstates of the chain,

$$\Psi_k = \sum_{m=-\infty}^{\infty} e^{ik2ma}(c_1(k)|m,1> + c_2(k)|m,2>)$$

obey the Bloch theorem. ($|m,1>$ denotes the eigenstate of atom 1 in unit cell m).
(c) Insert the eigenstates into the Schrodinger equation and obtain two secular equations, tying the coefficients $c_1(k)$ and $c_2(k)$ together.
(d) Find the (two) solutions to the energy band $E(k)$.
(e) Sketch the energy bands in the 1st BZ. What happens at the zone boundary? If each atom has one electron, what can you say about the metal vs. insulator character of this chain? (**4 points**)

3. Read Chapter 5.7 in Elliott. Write a short (2 pages) essay on experimental probes of electronic structure. (**3 points**)