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Structure and Properties of Functional Materials

Exercise Set 7

Friday, 8 March, 2013

1. Recall that in class, when solving the Schrödinger equation in a weak periodic potential, we decided that the solutions would have the form

$$\psi_k(x) = \sum_G c_{k-G} \exp\left(i(k-G)x\right)$$

where G is a reciprocal lattice vector. We also decided that, to a good approximation, one c would be much larger than all the rest – so that the solution just looks like a plane wave for a free electron – except for values of k on a Brillouin zone boundary, $k = \frac{1}{2}G$, in which both c_k and c_{k-G} could be large.

(a) When solving the latter case, we jumped from the simultaneous equations

$$\left(E - \frac{\hbar^2 k^2}{2m}\right) c_k - V_G c_{k-G} = 0$$

$$\left(E - \frac{\hbar^2 (k-G)^2}{2m}\right) c_{k-G} - V_{-G} c_k = 0$$

to the solution, for nonzero c_k and c_{k-G},

$$E = \tfrac{1}{2}(E_0^k + E_0^{k-G}) \pm \sqrt{\tfrac{1}{4}(E_0^{k-G} - E_0^k)^2 + |V_G|^2}$$

where we define

$$E_0^k = \frac{\hbar^2 k^2}{2m} \qquad E_0^{k-G} = \frac{\hbar^2 (k-G)^2}{2m}.$$

Fill in the missing mathematical gaps, and hence prove that the band gap is $2|V_G|$.

Consider a square (2D) lattice with, as usual, real lattice parameter a and reciprocal lattice parameter a^*, in a weak periodic potential given by $V(x,y) = V_0\left(\cos(xa^*) + \cos(ya^*)\right)$.

(b) Express this potential as a Fourier series of the form

$$V = \sum_{\mathbf{G}} V_{\mathbf{G}} \exp(i\mathbf{G}\cdot\mathbf{r}).$$

(Hint: it is probably easier to do this by inspection, using the formula $\exp(ix) + \exp(-ix) = 2\cos(x)$, than to use the general method involving integration for constructing Fourier series.)

(c) Hence calculate the band gap at $\mathbf{k} = \mathrm{X} = (\frac{1}{2}, 0)a^*$ in terms of V_0.

(d) In this approximation, what will the band gap at $\mathbf{k} = \mathrm{M} = (\frac{1}{2}, \frac{1}{2})a^*$ be? Can you explain why?

(e) At what value of V_0 does this system change from being a metal to being an insulator? Sketch the Fermi surface just below and just above this transition.