

Physics 140A: Homework Problem Set 7

Assigned 3/8/05. Due 3/15/05.

1. Fermi Surface, and Counting Electrons. 20 points.

(a) Consider electrons in a fcc crystal, assuming the free electron model. Find the electron density for which the spherical Fermi surface lies within the fcc Brillouin zone, but just touches it.

(b) Do the same problem, but for the (simpler) case of a simple square lattice in 2D.

2. Lattice Potential. 20 points.

Consider a 2D square lattice of lattice constant a and take

$$V(r) = -4V_0 \cos\left(\frac{2\pi x}{a}\right) \cos\left(\frac{2\pi y}{a}\right).$$

Find the Fourier transform V_G for all \vec{G} from

$$V_G = \frac{1}{V_{\text{cell}}} \int_{\text{cell}} V(\vec{r}) e^{-i\vec{G}\cdot\vec{r}}.$$

3. Nearly Free Electrons and Band Gaps. 30 points.

(a) Consider exactly the problem done in class, and also in the text in slightly more general form, of $k \approx \pi/a$, and there is a potential Fourier component V_G mixing the two lowest free electron bands with energies $\varepsilon_k, \varepsilon_{k-G}$, where $\varepsilon_k \equiv \hbar^2 k^2 / 2m$. Write the matrix equation (2×2) that must be solved, and solve it, as done in class, showing all work.

(b) Solve also for the wavefunction components $u_O(k), u_G(k)$, again only for $k \approx \pi/a$, the interesting region. It is clearest to expand in Taylor series form around $k = \pi/a$. Explain the dependence of the wavefunction on the quantities that enter; think about (and provide) the various energy scales of relevance.

(c) In a crystal (the 1D model we are using) with lattice constant of 4 \AA , what magnitude of Fourier component is necessary to produce a gap of 1 eV ? Describe explicitly the corresponding potential in the unit cell (real space).