MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Physics Department

8.231, Physics of Solids I

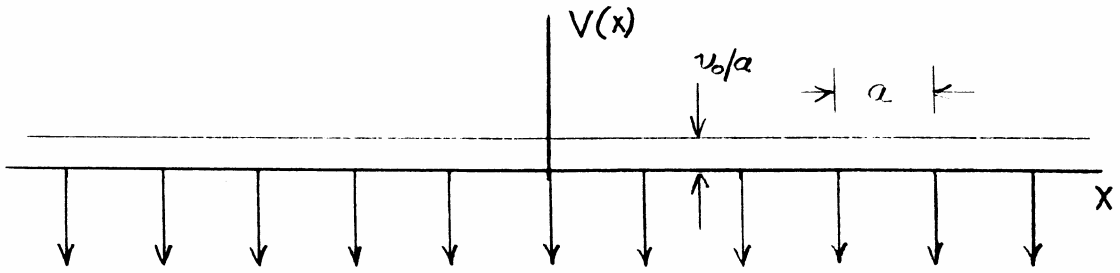
Due in Ses #32
by 2:00 PM

Problem Set #7

Problem 1: Perturbation in One Dimension

A free, non-interacting electron gas in one dimension is perturbed by a zero-mean potential of the form

$$V(x) = \frac{v_o}{a} - \sum_n v_o \, \delta(x - na).$$



a) Indicate on a carefully labeled sketch how the free electron dispersion curve will be modified by this weak interaction.

b) Find an expression for the energy ε_n about which the n^{th} gap occurs. Write down an approximation to the wavefunction at the gap, using two unperturbed wavefunctions as a basis. Just give the *general* form.

c) Using the two-component wavefunction from b), derive an expression for the magnitude, Δ_n, of the n^{th} gap.

d) Find the specific forms of the wavefunctions at the gap and indicate which has the higher energy. Explain physically why the energy of one is higher than that of the other.

e) Calculate the density of states as a function of energy, $D(\varepsilon)$, in the absence of the perturbation. Sketch how $D(\varepsilon)$ will be modified by the interaction.

Problem 2: Higher Brillouin Zones

a) Construct the first 5 Brillouin zones for a two dimensional square lattice. Show in separate figures how zones 2 through 5 would look when mapped into the first zone.

b) Indicate the location of the Fermi surface for free electrons in the reduced zone scheme when there are two and then three electrons per atom.

Problem 3: Lattice with a Basis

Consider the potential energy for a lattice with a basis, where the basis vectors are denoted by $\vec{b}_i$. To a good approximation the total potential energy can be written as a sum of contributions from each individual atom:

$$V(\vec{r}) = \sum_{\vec{R}_j} \sum_{\vec{b}_i} U_i(\vec{r}-\vec{R}_j-\vec{b}_i).$$

Recall that the Fourier component of the lattice potential at the reciprocal lattice vector $\vec{G}$ is given by

$$V_{\vec{G}} = \frac{1}{V}\int V(\vec{r})\, e^{-i\vec{G}\cdot\vec{r}}\, dr^3.$$

a) Show that $V_{\vec{G}} = \frac{N}{V} \sum_{\vec{b}_i} e^{-i\vec{G}\cdot\vec{b}_i} U_{i,\vec{G}}$ where $U_{i,\vec{G}}$ is the Fourier component of the potential due to the i^{th} atom in the basis. Notice the similarity to the structure factor that enters the calculation of intensities in diffraction experiments.

b) If all the atoms in the basis are identical, the $U_{i,\vec{G}}$ will be almost identical. What could prevent them from being exactly identical? If they were identical, some of the bands on some portions of Brillouin zone edge would not be split (no gap opens up) by the usual approximations involving two degenerate states.

c) Consider the case of diamond. Assume that each of the two carbon atoms in the basis do contribute identical $U_{i,\vec{G}}$. Show that $V_{\vec{G}}$ vanishes for $\vec{G} = \frac{4\pi}{a}(\hat{x}+\hat{y}+\hat{z})$. For what other symmetrically equivalent $\vec{G}$s will the Fourier component vanish? We have considered so far the coupling of two degenerate states on opposite sides of the Brillouin zone with wavevectors differing by some $\vec{G}$. In this this case, show on a sketch of the Brillouin zone boundary for diamond the surfaces on which the splitting will not occur because these particular Fourier components of the potential vanish.

Problem 4: Hexagonal Close-Packed Structure

Consider the first Brillouin zone of a crystal with a simple hexagonal lattice in three dimensions with lattice constants a and c. Let $\vec{G}_c$ denote the shortest reciprocal lattice vector parallel to the c axis of the crystal lattice.

a) Show that for a hexagonal close-packed crystal structure the Fourier component $V_{\vec{G}_c}$ of the crystal potential $V(\vec{r})$ is zero.

b) Is $V_{2\vec{G}_c}$ also zero?

c) Why is it possible in principle to obtain an insulator made up of divalent atoms at the lattice points of a simple hexagonal lattice?

d) Why is it not possible to obtain an insulator made up of monovalent atoms in a hexagonal close-packed structure?

Problem 5: Lifting a Degeneracy in a Two-Dimensional Band

Consider the free electron bands associated with a two-dimensional square lattice with lattice spacing a. In the reduced zone scheme, the second energy level occurring at $\vec{k} = 0$ is four fold degenerate with an energy $\lambda \equiv \frac{\hbar^2}{2m}(\frac{2\pi}{a})^2$.

a) On a sketch of the reciprocal lattice, locate the four locations corresponding to these degenerate states before they were translated back into the first Brillouin zone. Indicate the 8 reciprocal lattice vectors $\vec{G}$ that could be used to connect one of the four states with another.

b) Assume that there are Fourier components of the lattice potential corresponding to each of the 8 reciprocal lattice vectors found in a). Find the 4×4 matrix equation from degenerate perturbation theory that would have to be solved to find the new states and their energies.

c) Assume that the potential energy has four fold rotational symmetry about any lattice site. Find the new energies when the Fourier components associated with the $\vec{G}$s with the larger magnitude are zero. Repeat for the case when it is the Fourier components for the $\vec{G}$s with the smaller magnitude which are zero.