

## Phys 155, Winter 2007, Homework 4, due 5pm, Feb 21 for 1,2 and Feb 24 for 3

### 1. *Two free electron states interacting at zone boundary*

In this problem, we will consider an arbitrary dimension for space. Consider a crystal momentum value  $\mathbf{k}$  which is very close to, or on, a plane that is a perpendicular bisector of the line from the origin to a reciprocal lattice vector  $\mathbf{G}$ . Assume that no other perpendicular bisectors corresponding to other reciprocal lattice vectors are close to  $\mathbf{k}$ . Let's also assume that the crystal potential is very weak. These assumptions make it possible to reduce the problem to a 2x2 matrix problem involving two free electron states with wave numbers  $\mathbf{k}$  and  $\mathbf{k}-\mathbf{G}$ .

- (a) Set up the 2x2 problem and solve it. Slide 13 of Lecture 6 may be helpful. Or you can simply work from the Hamiltonian, focusing on the two states with  $\mathbf{k}$  and  $\mathbf{k}-\mathbf{G}$ . Express eigenvalues  $\varepsilon_1(\mathbf{k})$  and  $\varepsilon_2(\mathbf{k})$  in terms of unperturbed eigenvalues (i.e. free electron energies) and relevant Fourier components of the crystal potential.
- (b) For each eigenvalue, show that the group velocity (i.e.  $\frac{\partial \varepsilon(\mathbf{k})}{\partial \mathbf{k}}$ ) is parallel to the bisector plane (namely a zone boundary) if  $\mathbf{k}$  lies on the bisector plane i.e. if  $|\mathbf{k}| = |\mathbf{k}-\mathbf{G}|$ . (Math caution) Obtain the group velocity and set  $|\mathbf{k}| = |\mathbf{k}-\mathbf{G}|$ , not the other way around.
- (c) For  $|\mathbf{k}| = |\mathbf{k}-\mathbf{G}|$ , obtain the eigenfunction corresponding to the each eigenvalue, and show that it is always a standing wave (due to Bragg diffraction).

### 2. *Photoelectric effect requires crystal momentum*

In photoelectric effect, an electron absorbs a photon and becomes more energetic. The photon energy is on the order of a few eV to a few tens of eV, and so is the electron energy, so you won't need to consider relativistic mechanics of the electron.

- (a) Show that if the electron was initially in free space, then this process cannot occur for any finite photon energy values, except for one energy value which is way outside the energy range stated above (and becomes a non-solution when the more correct relativistic equation is considered). (Hint) Consider moving frame and the momentum and energy conservation rules to satisfy.
- (b) If the crystal potential is taken into account, then the photoelectric effect is indeed possible. Let's assume that the crystal potential is very weak so that the effect on the electron dispersion is very small, but is enough to cause zone-folding as in slides 11-12 of Lecture 6. For definiteness, consider a one dimensional crystal with a lattice constant  $3.14 \text{ \AA}$ , and consider a 10 eV photon initially propagating along the crystal. Draw a zone-folded dispersion relation like in the left-most plot of slide 11 of Lecture 6 up to about 15 eV. Assume that states up to about 4 eV are occupied by electrons. Indicate from which occupied state to which unoccupied state an electron can make a transition as the result of absorbing the photon.

### 3. *Formulation of your presentation*

By email, send a paragraph describing what you like to do for the presentation at the end of the course.

1. Summarize roughly what you like to talk about.
2. Make a connection to what we covered (or will cover) in class.
3. It would be ideal if there is a reference or two that you already know you will talk about.
4. Come and talk to me if you need help formulating your subject.

Examples of a format of your paragraph:

I like to present on recent concepts developed in the field of quasi-crystals. Quasi-crystals are materials which do not have repeating unit cells, as conventionally defined, e.g. as in our class. Nevertheless, they display sharp Bragg diffraction lines in X-ray diffraction experiments, baffling scientists and raising fundamental questions to our common assumptions about solids. Therefore, some people suggest that a new definition of crystal is called for and propose that a crystal be defined as "a material that shows a sharp Bragg diffraction line." I will summarize the idea behind this proposal, and will also present about two different kinds of quasi-crystals, namely a conventional crystal whose structure is incommensurately modulated to have no periodicity and a material whose structure can be thought of as a projection of a periodic structure in a higher dimension. The two papers that I will discuss heavily in this presentation are xxx by yyy and zzz by ttt.

My presentation will be on solar cells, which are thought to be an important component for future renewable energy source being sought after. Currently, the push to improve the solar cell technology is being made in two directions, one in improving the quantum efficiency of solar cells and the second in improving the flux of the sun light by better focusing. Of these two the first one is more germane to condensed matter physics, and thus I will present an overview of the efforts being made in the first direction. First, I will summarize the principle of solar cells. Then, I will discuss why the quantum efficiency of single semi-conductor material is limited (to ~ 30 %), and discuss several methods that researchers use to improve the efficiency, e.g. using impurity bands, porous or amorphous materials, superlattices, quantum dots, and multi-junction multi-band-gap materials. I will then summarize the physics issues related to one of these methods - namely using xxx, which I think is the most promising. In this presentation, I will heavily use the concept of semiconductor physics (energy bands, energy gaps and impurity states) that we covered (or will cover) in class, and my main reference will be xxx by yyy.