6.730 PHYSICS FOR SOLID STATE APPLICATIONS

Department of Electrical Engineering and Computer Science
Massachusetts Institute of Technology

PROBLEM SET 8

Issued: 4-10-96 Due: 4-17-96, at the beginning of class.

Readings:
3D Band Structure: Chapters 9—11 in Ashcroft and Mermin.
Effective Mass Theorem: Chapter 9.2 in 6.730 notes.
Hydrogenic Impurity States: Chapter 9.3 in 6.730 notes.
Semiclassical Equations of Motion: Chapter 9.4 in 6.730 notes and Chapter 12 in Ashcroft and Mermin.

Problem 8.1 This problem uses the program (`eb2d2.m`) which will be sent to you for calculating the energy bands for a two dimensional solid with lattice spacing of 5 Å. Answer the following by submitting graphs using this program.

Do the following potentials have energy gaps between the first and second bands?

$$V = .2\,\mathrm{eV}\cos(\frac{2\pi x}{a}) \tag{1}$$

$$V = 0.5\,\mathrm{eV}\cos(\frac{2\pi x}{a}) + 5\,\mathrm{eV}\cos(\frac{2\pi y}{a}) \tag{2}$$

$$V = 0.7\,\mathrm{eV}\cos(\frac{2\pi x}{a}) + 0.7\,\mathrm{eV}\cos(\frac{2\pi y}{a}) \tag{3}$$

$$V = 0.7\,\mathrm{eV}\cos(\frac{2\pi x}{a}) + 0.7\,\mathrm{eV}\cos(\frac{2\pi y}{a}) + 0.7\,\mathrm{eV}\left[\cos(\frac{2\pi}{a}(x+y)) + \cos(\frac{2\pi}{a}(x-y))\right] \tag{4}$$

$$V = 0.7\,\mathrm{eV}\cos(\frac{2\pi x}{a}) + 0.7\,\mathrm{eV}\cos(\frac{2\pi y}{a}) - 0.7\,\mathrm{eV}\left[\cos(\frac{2\pi}{a}(x+y)) + \cos(\frac{2\pi}{a}(x-y))\right] \tag{5}$$

Note that the coefficients in front of the three terms correspond to the program variable $V[10]$, $V[01]$ *and* $V[11]$.

Problem 8.2 Assume the potentials in Problem 8.1 are weak. Solve for the eigen values and eigen vectors at the corner point of the First Brillouin Zone, that is at $(k_x, k_y) = (\pi/a, \pi/a)$. You will need to construct the appropriate 4×4 matrix for the 4 degenerate free-particle (plane-wave) states.

For each of the potentials in Problem 8.1, plot in real space for a square of two lattice spacings centered at the origin.

- The potential.
- Each of the probability densities for the four eigen states.

Problem 8.3 A two-dimensional metal in the form of a square lattice has two conduction electrons per atom. In the almost free electron approximation, sketch carefully the fermi surfaces in each Brillouin zone. **Do this problem both from the graphical construction, and by using the computer program.**

Quiz 2 is Friday, April 19, 1996.