QUANTUM MECHANICS II

PHYS 517

Problem Set # 5

Distributed: May 6, 2015

Due: May 15, 2015

Energy Band Theory of Lattices

1. Fourier Coefficients: In Problem #2 you will need the Fourier coefficients of the periodic function $f(\theta) = \frac{1}{3+2\cos\theta}$. Evaluate the first five Fourier coefficients.

2. Energy Bands for One Dimensional Lattice: Schrödinger's equation for a periodic one-dimensional lattice with unit cell size a is

$$\frac{\hbar^2}{2m}(k+G)^2 u_G(k) + \sum_{G'} V_{G-G'} u_{G'}(k) = E u_G(k) \tag{1}$$

Set $\hbar = 1, m = 1, a = 1, V(\theta) = \frac{2.5}{3+2\cos\theta}$, set up this matrix eigenvalue equation for each value of k in the range $0 \leq k \leq \pi/a$ and compute the lowest four bands in this solid.

3. Two Dimensional Solid: Schrödinger's equation in reciprocal space for a periodic two-dimensional square lattice with edgelength a is

$$\frac{\hbar^2}{2m}(\mathbf{k}+\mathbf{G})\cdot(\mathbf{k}+\mathbf{G}) u_{\mathbf{G}}(\mathbf{k}) + \sum_{\mathbf{G}'} V_{\mathbf{G}-\mathbf{G}'} u_{\mathbf{G}'}(\mathbf{k}) = E u_{\mathbf{G}}(\mathbf{k}) \tag{2}$$

The notation is an obvious extension of the notation in Problem #2. Use $V(x,y) = -3+2(\cos(2\pi x/a)+\cos(2\pi y/a))+\cos(2\pi x/a)\cos(2\pi y/a)$ and plot the lowest four bands along these lines in reciprocal space

a. $(0,0) \rightarrow (0,\pi/a)$

b. $(0,\pi/a) \rightarrow (\pi/a,\pi/a)$

c. $(\pi/a,\pi/a) \rightarrow (0,0)$