PHY 481/581 - Homework Set 5

Northern Arizona University Due: 11/19/2018

Problem 1. Describe the difference between the free electron and nearly free electron models. Draw the dispersion curves for both models using the extended and reduced zone schemes. What is the origin of the band gap opening at the Brillouin zone boundaries? Be sure to label your drawings clearly.

Problem 2. Consider electrons of mass m moving in a one-dimensional "Dirac comb" potential defined as

$$V(x) = \alpha \sum_{j=1}^{N-1} \delta(x - ja) \tag{1}$$

where α is a "strength parameter" with units of energy, N is the number of lattice points, and a is the spacing between points in the direct lattice.

(a) Show that $\psi(x+a) = e^{ika}\psi(x)$ given that $\psi(x) = e^{ikx}u(x)$, where $u(x) = u(x+a)$ has periodicity matching the lattice.

(b) Show that the solution to the Schrödinger equation is $\psi(x) = A\sin(qx) + B\cos(qx)$, where q is the wavenumber of the electron, for regions with $V(x) = 0$, in particular $0 < x < a$.

(c) Using the continuity of the wave function at $x = 0$, derive

$$B = e^{-ika}\big[A\sin(qa) + B\cos(qa)\big]. \tag{2}$$

(d) Using the discontinuity of the derivative at $x = 0$ given by

$$\left.\frac{d\psi}{dx}\right|_{x=0^+} - \left.\frac{d\psi}{dx}\right|_{x=0^-} = \frac{-2m\alpha}{\hbar^2}\psi(0) \tag{3}$$

derive the following relation:

$$qA - e^{-ika}q\big[A\cos(qa) - B\sin(qa)\big] = \frac{2m\alpha}{\hbar^2}B. \tag{4}$$

(e) Use Eqs. (2) & (4) to derive the relationship for allowed values of q that we discussed in class (see notes from Nov. 09). Draw the resulting curve and indicate the locations of the allowed and disallowed bands. Make sure to mark your axes clearly.