PHY4905 Spring 2013

Homework E

Instructor: Yoonseok Lee

Submit only HW's. EX's are additional problems that I encourage you to work on.

(**a**.**b**) means problem number **b** of chapter **a** in *Introduction to Solid State Physics* (8th ed.) by Kittel.

Use SI unit.

Due February 27

HW 1: Follow the Kronig-Penny model described in Kittel and derive Eq. (21a) and (21b). (10 pt)

HW 2: (7.3) (10 pt)

HW 3: To help you understand the way real band structures are presented we will consider a simple case of two dimensional square lattice with lattice spacing a without periodic potential. So this simple model will give you free electron dispersion in the same way the band structures are plotted. The reciprocal vector is represented by

$$\vec{G} = \frac{2\pi}{a}\left(n_1\hat{x} + n_2\hat{y}\right)$$

where $n_i = 0, \pm 1, \pm 2, ...$

(a) Draw the 1st, 2nd, and 3rd Brillouin zones. (10 pt)

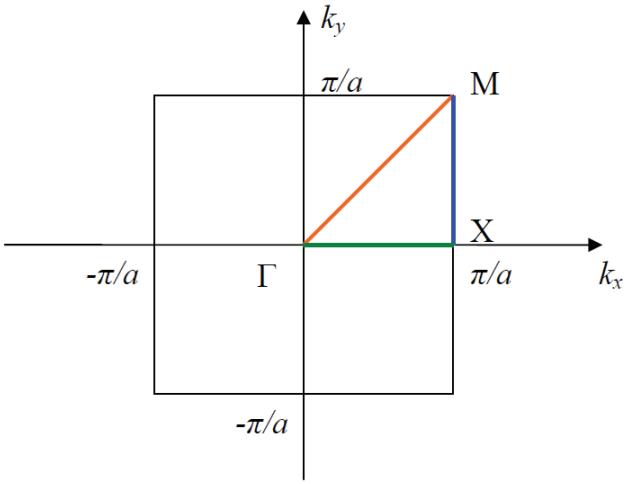
(b) The figure below shows the 1st Brillouin zone of the square lattice with three points Γ, M, and X points, which are conventionally designated high symmetry points. You find that the energy eigenvalues of a free electron in a crystal structure is given by

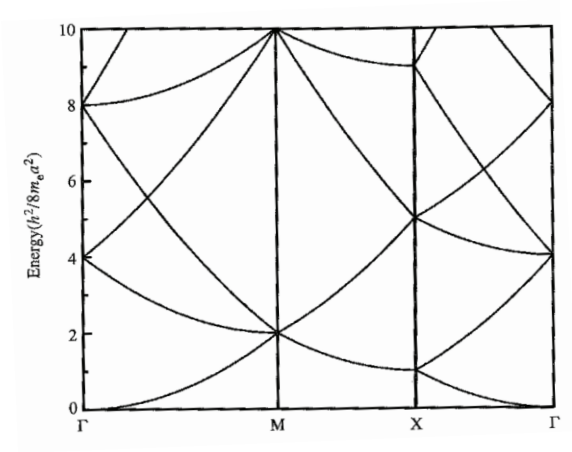
$$E(\vec{k}) = \frac{\hbar^2}{2m}(\vec{k} - \vec{G})^2.$$

Plot the energies of the free electron bands up to $E = \frac{h^2}{ma^2}$ as k traverses the path $\Gamma - M - X - \Gamma$ as shown in the figure below. Indicate each branch with proper reciprocal vector(s). The answer is provided below upto $E = 10\frac{h^2}{8ma^2}$. (10 pt)

Introducing a weak periodic potential will lift degeneracy at the zone boundary and consequently inducing band gaps. That is what you will see in papers or presentations.

HW 4: (7.6)





HW 5: Consider a 1D free electron gas of size L. The single electron energy is simply given by $\epsilon^o = \frac{\hbar^2}{2m}k^2$. Let's introduce a weak periodic potential given by $V(x) = V_o \cos 2k_F x$ where k_F is the Fermi wavenumber. *The wavenumber of the potential being $2k_F$ is the unique point of this problem.*

(a) Find the Fourier component V_G of the potential: $V(x) = \Sigma_G V_G e^{iGx}$. (5 pt)

(b) Provide your qualitative and physical argument based on the ideas developed in electron bands in a crystal on what you expect in the single electron energy $\epsilon(k)$. (5 pt)

(c) Apply the band theory (central equations) to solve for the lowest band dispersion $\epsilon^-(k)$ for $0 \leq k \leq k_F$. Notice that $\epsilon(k) = \epsilon(-k)$. You will get

$$\epsilon^- - \epsilon^o = \frac{1}{2}\left(\frac{\hbar^2}{2m}\right)\left[2k_F\tilde{k} - \sqrt{(2k_F\tilde{k})^2 + \left(\frac{2m}{\hbar^2}\right)^2 V_o^2}\right]$$

where $\tilde{k} = k_F - k$. (10 pt)

(d) Calculate the difference in total energy of the electron system with and without the periodic potential for $V_o << \frac{\hbar^2}{2m}k_F^2$ at $T = 0$. Do you get $\delta E = (2)(2)\frac{L}{2\pi}\int_0^{k_F}(\epsilon^-(k) - \epsilon^o(k))\,dk$ for $-k_F \leq k \leq k_F$ including the spin degeneracy? You will find $\delta E < 0$ for arbitrarily small V_o. (10 pt)

Instability at the Fermi wavenumber: *A 1D free electron system is always unstable against any weak periodic potentials with a $2k_F$ Fourier component. e.g. Peierls instability which drives a 1D metal into an insulator.*
Ans:

$$\delta E = \frac{L}{\pi}\frac{mV_o^2}{\hbar^2(2k_F)^2}\ln\left(\frac{2mV_o}{\hbar^2(2k_F)^2}\right).$$