Problem set 2 *due at 05/04/2020*

Total points = 760 pts

1. Kronig-Penny model (360%)

Assume free electron ($m^* = m_0 = 9.11 \times 10^{-31}$ kg), please plot two figures in slide #113 in lecture note for the following cases:

(a) (60%) a = 10 nm, b = 1 nm, and V_0 = 1 eV
(b) (60%) a = 1 nm, b = 10 nm, and V_0 = 1 eV
(c) (60%) a = 10 nm, b = 1 nm, and V_0 = 0.5 eV
(d) (60%) a = 10 nm, b = 1 nm, and V_0 = 0.1 eV
(e) (120%) please pick random numbers of a, b, and V_0 to make your plots of band structures with clear bands and band gaps.

2. [Nearly Free Electron Approximation] (160%)

Consider a one-dimensional solid whose "empty lattice" E (n, k) is shown in Fig. 1. We are interested in the evolution of the electronic states in this solid as a weak periodic potential is introduced. Use appropriate perturbation theory (1st and 2nd order) to answer the following questions. Let $\psi(n,k)$, $E(n,k)$, and $v(n,k)$ represent the wavefunction, energy, and group velocity of electrons occupying a state (n, k), where n is index and k is wave vector in 1st B.Z. Consider 6 specific k-values as indicated in Fig. 1, where $k_1 = 0$ $k_2 = \frac{\pi}{10a}$, $k_3 = \frac{\pi}{3a}$, $k_4 = \frac{\pi}{2a}$, $k_5 = \frac{9\pi}{10a}$, and $k_6 = \frac{\pi}{a}$

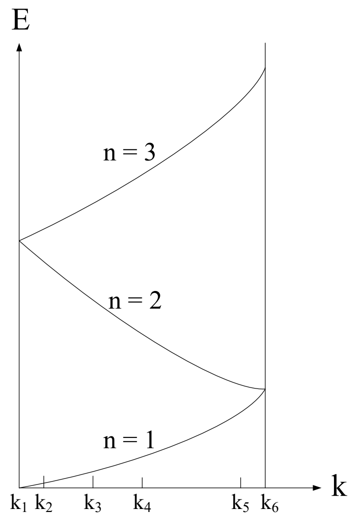

Fig. 1 E-k relation

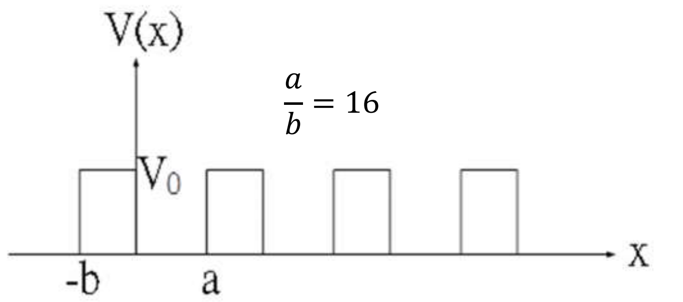

Fig. 2 Kronig-Penney model

(a) (40%) Write down expression for $\psi(n,k)$, $E(n,k)$, and $v(n,k)$ for the states (n = 1, k_5), (n = 2, k_6), (n = 3, k_6), assuming no periodic potential is present (empty lattice or free electron)

(b) (40%) Assuming a periodic potential of the form $U(x) = V_0 \cos\left(\frac{2\pi}{a}x\right)$, where $V_0 = \frac{\hbar^2}{2m}\frac{1}{10}\left(\frac{\pi}{a}\right)^2$ is now introduced. How much does this potential change E (n = 1, k_5), E (n = 1, k_6), E (n = 3, k_6), v (n = 1, k_6), v (n = 2, k_5)? (Give the percentage change)

(c) (40%) For the potential of part (b), write the approximate expressions for $\psi(n = 1, k_5)$ and $\psi(n = 2, k_5)$.

(d) (40%) Suppose that the periodic potential is that of the Kronig-Penney model as shown in Fig. 2. What are the percentage change in E (n = 1, k_6), E (n = 2, k_1), E (n = 3, k_4), E (n = 3, k_6) with respect to the empty lattice energies. Assume $V_0 = \frac{\hbar^2}{2m}\frac{1}{10}\left(\frac{\pi}{a}\right)^2$.

3. Low-dimensional density of states (120%)

(a) (40%) Assume in two-dimension crystal of square of length L and under the periodic boundary condition, at T = 0, the Fermi wave vector is k_F, please find

(i) (10%) electron density

(ii) (10%) energy density

(iii) (10%) average energy

(iv) (10%) density of state

(b) (40%) repeat (a) for 1D crystal (200%)

(c) (40%) Now T > 0, please compare E_F (T > 0) and E_F (T = 0) for 2D and 1D crystal (100%)

4. Carrier density (120%)

(a) (40%) If n-type doping level is 10^{15} cm^{-3}, please draw electron density vs. temperature (50 K to 300 K).

(b) (80%) Replot the following two figures.