Exercise 1:

a) Substituting $U(x)$ and $\psi(x)$ in schodinger equation we obtain,

$$\sum_k \frac{\hbar^2 k^2}{2m} C(k) e^{ikx} + \sum_k \sum_G U_G C(k) e^{iGx} e^{ikx} = \epsilon \sum_k C(k) e^{ikx} \tag{1}$$

$$\sum_k C(k) \left(\frac{\hbar^2 k^2}{2m} - \epsilon \right) e^{ikx} + \sum_k \sum_G U_G C(k) e^{i(G+k)x} = 0 \tag{2}$$

defining $\lambda_k = \frac{\hbar^2 k^2}{2m}$, and $k \to k - G$ in second term

$$\sum_k \left[(\lambda_k - \epsilon) C(k) + \sum_G U_G C(k - G) \right] e^{ikx} = 0 \tag{3}$$

since each e^{ikx} are independent vectors, the terms in square brackets must be zero,

$$(\lambda_k - \epsilon) C(k) + \sum_G U_G C(k - G) = 0 \tag{4}$$

b) Substituting the bloch wave $\psi_k(x)$ in schodingers equation:

$$\sum_k \frac{\hbar^2 k^2}{2m} C(k) e^{ikx} + \sum_{k'} \sum_G U_G e^{i(k'+G)x} C(k') = \epsilon \sum_k C(k) e^{ikx} \tag{5}$$

Rename indices with the following equation in the second term: $k' + G = k$ and obtain

$$\sum_k \left[C(k) \left(\frac{\hbar^2 k^2}{2m} - \epsilon \right) + \sum_G U_G C(k - G) \right] e^{ikx} = 0 \tag{6}$$

Since terms like e^{ikx} are independent vectors we expect the coefficients of $e^{i(k-G)x}$ in above equation to be zero, which gives us the same relation as (1). Hence, we observe that each bloch wave $\psi_k(x)$ indexed by 'k' individually satisfies (4)

c) Using the assumption given in the exercise, (6) becomes,

$$C(k - G) \left(\frac{\hbar^2}{2m} (k - G)^2 - \epsilon \right) = 0 \tag{7}$$

The equation has two solutions for every reciprocal lattice vector G: $C(k - G) = 0$ or $\epsilon = \frac{\hbar^2}{2m}(k - G)^2$. Therefore, the electron dispersion consists of a set of parabolas shifted by G (Fig. (1)).

d) Using coefficients $C(G/2)$ and $C(-G/2)$ in the Schroedinger equation in the momentum representation, for $U_G = U$ we get,

$$\begin{cases} (\lambda - \epsilon) C(\frac{G}{2}) + U C(-\frac{G}{2}) = 0 \\ (\lambda - \epsilon) C(\frac{-G}{2}) + U C(\frac{G}{2}) = 0 \end{cases} \tag{8}$$

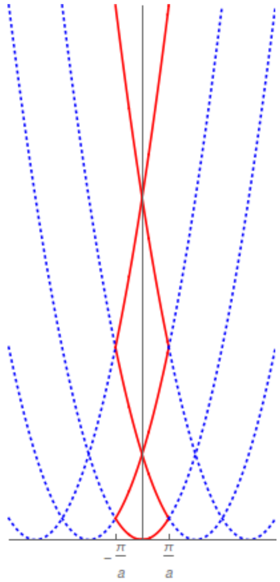

Figure 1: Energy spectrum of free electron bloch bands

$$\begin{vmatrix} \lambda - \epsilon & U \\ U & \lambda - \epsilon \end{vmatrix} = 0 \tag{9}$$

$$\lambda = \epsilon \pm U \tag{10}$$

Therefore a gap of width $\sim 2U$ opens up.

Exercise-2:
Defining the Fourier tranform of creation and annihilation operators as:

$$c_i = \frac{1}{\sqrt{N}} \sum_k c_k e^{ikr_i}, \qquad c_i^\dagger = \frac{1}{\sqrt{N}} \sum_k c_k^\dagger e^{-ikr_i}$$

The Hamiltonian becomes

$$\mathcal{H}_{TB} = -\frac{t}{N} \sum_{r_i} \sum_k \sum_{k'} c_k^\dagger e^{-ikr} c_{k'} e^{ik'(r_i+a)} + c_k^\dagger e^{-ikr} c_{k'} e^{ik'(r_i-a)} \tag{11}$$

Since for each r_i only $r_j = r_i \pm a$ give non-zero terms.

$$\begin{aligned} \mathcal{H}_{TB} &= -\frac{t}{N} \sum_k \sum_{k'} c_k^\dagger c_{k'} \left(e^{ik'a} + e^{-ik'a} \right) \underbrace{\sum_r e^{i(k'-k)r}}_{N\delta_{kk'}} \\ &= \sum_k (-2t\cos(ka)) c_k^\dagger c_k \end{aligned} \tag{12}$$

Hence $\epsilon_k = -2t\cos(ka)$

Exercise 3:
a) For a crystal with N sites the one band can be filled with 2N electrons. One can use particle in a box problems to see why this happens. The energy levels of particle in a box correspond to momenta $k_n = \frac{n\pi}{L}$. Hence the energy difference between subsequent levels

is $\frac{\pi}{L}$. If 1-D crystal has N atoms then $L = Na$ which implies that length of each energy "bin" in a momentum space is π/Na. The length of first brillouin zone(with positive k) is π/a. Hence, the zone can be divided into N bins. Taking two electrons per energy level/bin(spin up and spin down) we have 2N electrons that can be filled in a band.

Note: We take only positive k because $\sin(kx)$ function (wave function for particle in a box) can be expressed as $((e^{ikx} - e^{-ikx})/2)$. The boundary condition of particle in a box enforces the particle to occupy the $+k$ and $-k$ levels simultaneously. One can alternately take a periodic boundary condition and arrive at the same result where length of each bin in $2\pi/Na$ which leads to N bins in the first brillouin zone.

b) We obtain a partially filled band when there are odd number of electrons per site.

c) Since only partially filled bands are conducting we observe that a) compounds with even number of electrons per site are insulators and b) the ones with odd number of electrons per site are conductors.