Abstract

This exercise is aimed at refreshing the concepts of band structure from earlier solid state physics courses. There are essentially two different approaches to band structure. One starts by considering electrons as free particles propagating through the background of crystal lattice. The other approach considers electrons to be occupying the atomic orbitals of the individual atoms, and the electrons from outermost shell to hop in between neighbouring sites. We will have a look at both these methods and we also look at how the electron occupancy of the ion relates to the insulating or conducting behaviour of the crystal.

Exercise 1: Nearly free electron model

In this exercise we will start by obtaining the dispersion relation for the nearly free electron model.

a) Consider a 1D periodic lattice with a lattice constant a and with potential energy given by

$$U(x) = \sum_G U_G exp(iGx) \tag{1}$$

Where $G = 2\pi n/a$ is the reciprocal lattice vector. Using the electron wave functions in the Fourier representation

$$\psi(x) = \sum_k C(k) exp(ikx) \tag{2}$$

solve the Schrodinger equation

$$\epsilon\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) \tag{3}$$

and obtain the relation between the coefficients $C(k)$ given by

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

with $\lambda_k = \frac{\hbar^2 k^2}{2m}$

b) Show that each wavefunction (Bloch wave) of the form

$$\psi_k(x) = \sum_k C(k) exp(ikx) \tag{5}$$

indexed by k,where $k \in (-G/2, G/2)$ and the coefficients $C(k)$ satisfy eq(0.4), is a solution to the Schroedinger for the lattice potential given in (0.1).

You should obtain:

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

c) For a very weak potential ($U_G \approx 0$), we can assume that U_G is, in fact, 0. For this case, plot the dispersion relation in the first Brillouin zone.

d) Now the magnitude of the potential is increased, however, it still remains small. The potential modifies the energy spectrum, particularly near the k points where the energies of two states are degenerate (as shown by the crossing of the lines in the dispersion relations for different G values), for example $k = G/2$. Here states with G' = 0 and G' = G have the same energy. Calculate the band gap for the case when all coefficients in Eq (0.1) are the same $U_G = U$.

Exercise 2: Tight-binding model

Consider a 1D periodic lattice with the lattice constant a with one orbital per site. The tight binding Hamiltonian in the nearest neighbour approximation for this lattice is given by:

$$H_{TB} = -\sum_{<ij>} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} \tag{7}$$

taking only a nearest neighbour hopping i.e $t_{ij} = t$ if $i = j \pm 1$ and 0 otherwise.

a) Using the Fourier transform on the fermionic operators, show that the band energy $\epsilon(k)$ is given by:

$$\epsilon_k = -2t\cos(ka) \tag{8}$$

Note: The Fourier transform of the creation and annihilation operators is given by:

$$c_i = \frac{1}{\sqrt{N}} \sum_k c_k e^{ikr_i}, \; c^{\dagger}_i = \frac{1}{\sqrt{N}} \sum_k c^{\dagger}_k e^{-ikr_i} \tag{9}$$

Exercise 3:Insulator vs Conductor

a) How many electrons can be filled per band for a 1D lattice with n sites ?
b) When do we obtain a partially filled band?
c) How does this translate to insulating or conducting behaviour of the lattice ?