4012 Condensed Matter Theory: Tutorial 3

1. The group velocity associated with a Bloch's state ψ_k is defined as:

$$v_k = \frac{1}{m}\langle\psi_k|p|\psi_k\rangle \quad \text{with} \quad p = \frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x}\ .$$

Demonstrate that the group velocity can also be written as:

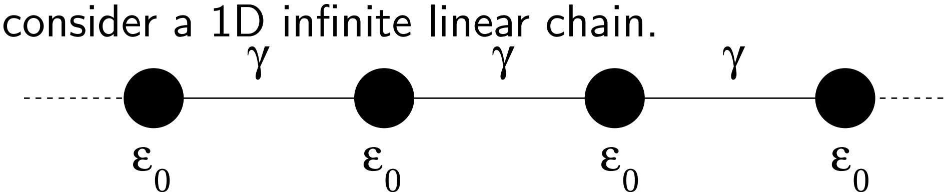
$$v_k = \frac{1}{\hbar}\frac{\mathrm{d}E(k)}{\mathrm{d}k}\ .$$

(*Hint.:* Write the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi_k(x) + V(x)\psi_k = E(k)\psi_k$$

for the Bloch's function $\psi_k(x) = \mathrm{e}^{ikx}u(x)$ and differentiate with respect to k ....)

Then consider a 1D infinite linear chain.



Consider a one orbital, orthogonal, nearest neighbors tight-binding model where the on-site energy is ϵ_0=3 eV, the hopping integral γ=-1 eV and the lattice constant a_0=1Å. In this case calculate the maximum group velocity.

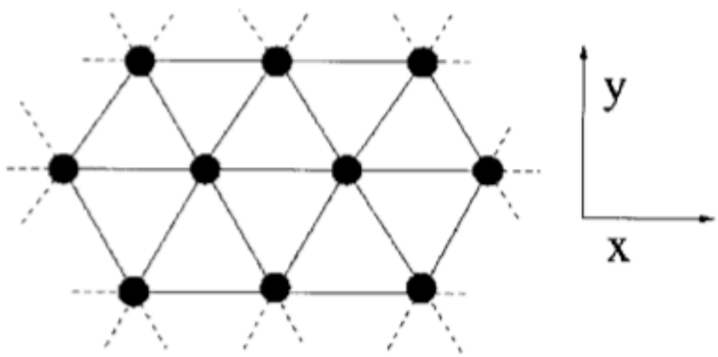
2. Consider a periodic solid and let $|\mathbf{R}\rangle$ denote an atomic orbital placed at the position $\mathbf{R}$. The generic molecular state for the solid is

$$|\psi_k\rangle = \sum_{\mathbf{R}} c_k(\mathbf{R})|\mathbf{R}\rangle$$

where the sun runs over all the atomic sites.

(a) Bloch's Theorem imposes a condition over the coefficients $c_k(\mathbf{R})$. By using such a condition write an expression for the energy associated to the state $|\psi_k\rangle$ (band equation), assuming $\langle\mathbf{R}'|\mathbf{R}\rangle = \delta_{\mathbf{R}'\mathbf{R}}$

(b) Consider now the following triangular lattice of Carbon atoms, where each C atom sits at the corner of an equilateral triangle of side a_0.



Using the Carbon p_z orbital as basis set, calculate the band structure equation for such a lattice, assuming only nearest neighbour interaction (the on-site energy is ϵ and the hopping integral γ).

(c) Consider now $\epsilon = 0$ and $\gamma = 1$, plot the bandstructure along the directions $\Gamma \to A \to B \to C$, where $\Gamma = (0, 0)$, $A = (\pi/a_0, 0)$,

$B = (\pi/a_0, \pi/\sqrt{3}a_0)$ and $C = (0, \pi/\sqrt{3}a_0)$.