
Assignment 1

EE 80724, Wide Bandgap Device Physics, Fall 2009

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1 Bloch Equation

The Hamiltonian operator for electrons in a 1D crystal is periodic: $H(x + na) = H(x)$, where a is a lattice constant and n is an integer. If the length of the 1D crystal is $L = Ma$, then we impose periodic boundary conditions on the wavefunction, requiring it to follow $\psi(x + L) = \psi(x)$. If T is an operator that translates the wavefunction from $x \rightarrow x + a$, then $T\psi(x) = \psi(x + a)$. Periodic boundary conditions then require that $T^M = 1$. Therefore, there are M distinct values of T , each being a ' M^{th} ' root of unity: $T_n = e^{i\frac{2\pi}{M}n}$ where $n = 0, 1, \dots, M - 1$.

- In class, we saw that if we rewrite this relation as $T_n = e^{ik_n a}$, then $k_n = \frac{2\pi}{a} \frac{n}{M}$. Show then that the wavefunction has to satisfy $\psi(k, x + ma) = e^{ikma}\psi(k, x)$. This is of course trivial.
- Now show that if $\psi(k, x + ma) = e^{ikma}\psi(k, x)$, it is *equivalent* to saying (one implies the other) that the wavefunction can be written as $\psi(k, x) = e^{ikx}u(k, x)$, where $u(k, x + ma) = u(k, x)$. This is Bloch's theorem. The function u has the same periodicity of the lattice, and the 'envelope' function is the phase factor e^{ikx} which has the periodicity of the entire crystal.

2 Empty Lattice Bandstructure: 1D

Argue why in an ideal 1D crystal, energy degeneracies (or band crossings) can *only* occur at $k = 0$ or at the Brillouin Zone edges, but never at any other k points. Since degeneracy points lead to bandgaps, what does this say about ideal 1D semiconductors: will they be direct or indirect bandgap? What about 2D and 3D crystals?

3 Empty Lattice Bandstructure: 2D

Consider the ideal 2D crystal of graphene. Identify the primitive real-space lattice vectors ($\mathbf{a}_1, \mathbf{a}_2$). Find the primitive reciprocal lattice vectors ($\mathbf{b}_1, \mathbf{b}_2$). The general reciprocal lattice vector may be written as $\mathbf{G} = n\mathbf{b}_1 + m\mathbf{b}_2$, written more compactly as (n, m) .

- Starting from the expression for the energy bandstructure of the empty lattice model $\mathcal{E}(\mathbf{k}) = \frac{\hbar^2(\mathbf{k} + \mathbf{G})^2}{2m_0}$, draw up a table with expressions of energy bands along the k_x and k_y directions. Associate each band with the respective (n, m) reciprocal lattice vector.
- Plot the bandstructure along $(k_x, 0)$ for (n, m) : $(0, 0)$ through $(2, 2)$ with all possible (\pm) combinations. Also make a 2D plot of the energy bandstructure. Superimpose and compare with the known bandstructure of graphene and comment.

4 Empty Lattice Bandstructure: 3D - Wurtzite GaN

Do the same as in the previous problem, but for 3D GaN. Use the wurtzite crystal structure (you have 3 reciprocal lattice vectors). Plot the energy bands along the typical high-symmetry directions in the k -space. Superimpose and compare with the known bandstructure.