

Assignment 3

EE 698N, Advanced Semiconductor Physics

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1 Bandstructure - $\vec{k} \cdot \vec{p}$ Theory

By using the Bloch functions $\psi(\vec{k}, \vec{r}) = e^{i\vec{k} \cdot \vec{r}} u(\vec{k}, \vec{r})$ in the Schrodinger equation $H_0 \psi(\vec{k}, \vec{r}) = E(\vec{k}) \psi(\vec{k}, \vec{r})$, show that one gets the $\vec{k} \cdot \vec{p}$ Hamiltonian

$$\left(H_0 + \underbrace{\frac{\hbar}{m_0} \vec{k} \cdot \vec{p} + \frac{\hbar^2 k^2}{2m_0}}_{\text{perturbation}} \right) u(\vec{k}, \vec{r}) = E(k) u(\vec{k}, \vec{r}) \quad (1)$$

The Hamiltonian operator is the kinetic energy term $H_0 = -\hbar^2 \nabla^2 / 2m_0$, m_0 being the free electron mass, and $\nabla = \partial / \partial r$ is the spatial gradient.

- Verify the conduction and valence band effective masses upon spin-orbit splitting of a typical direct-gap semiconductor covered in class notes.
- For many semiconductors, the approximation involved in k.p theory $E_n(k) \approx E_n(0)$ starts becoming a bad one for even small values of k ; in such cases, the bands cease to be parabolic. Considering a single CB interacting with a single VB, show that by eliminating the momentum matrix element, the conduction bandstructure for small effective masses $m_c^* \ll m_0$ can be rewritten as

$$E_C(k)[E_C(k) + E_G] = \frac{\hbar^2 k^2}{2m_c^*} E_g. \quad (2)$$

Here, E_g is the bandgap. Plot this non-parabolic CB bandstructure for a narrow bandgap semiconductor (InSb, $m_c^* = 0.014m_0$, $E_g = 0.17\text{eV}$) together with the parabolic approximation. This result from $\vec{k} \cdot \vec{p}$ theory is one of the most popular ways of taking non-parabolicity into account.

- Prove the ‘‘Sum Rule’’ for effective masses at the Γ point ($k = 0$). Consider N bands - the sum rule says that if I take the effective mass at the Γ -point of each band m_i^* , and add the terms m_0/m_i^* for each band, the number I get is N -

$$\sum_i \frac{m_0}{m_i^*} = N \quad (3)$$

This implies that if I know effective masses of $N - 1$ bands, I can find that of the one unknown band.

2 Bandstructure - PseudoPotential, LCAO

For this problem, find all relevant parameters from Yu/Cardona’s book, or any other handbooks; if you can’t find the parameters, assume reasonable values.

- a) Modify the Tight-binding Mathematica Program and calculate bandstructure for Germanium. Plot the bandstructure similar to those in Yu/Cardona Fig 2.13.
- b) Modify the Pseudopotential Mathematica Program and calculate bandstructure for InAs, similar to that for GaAs in Yu/Cardona Fig 2.14.

3 Transport of Bloch Electrons

In a fictitious 2-Dimensional crystal, the bandstructure of the lowest band with a square lattice (lattice constant a) is given by

$$E(k_x, k_y) = -E_0 \cdot [\cos k_x a + \cos k_y a] \quad (4)$$

- a) Make a semi-quantitative contour plot of constant energies in the reduced Brillouin Zone, and highlight energies $E = 0, \pm E_0$.
- b) Make a semi-quantitative plot of the effective mass in the (1,0) or x -direction, and the (2,1) direction in the reduced Brillouin Zone.
- c) An electron is initially located at $\mathbf{k} = 0$ in \mathbf{k} -space, and $\mathbf{r} = 0$ in real space. At $t = 0$, a force \mathbf{F} (from an electric field) is turned on which points in an oblique direction, such that $F_x = 2F_y$. Show the trajectory of the electron through the reduced zone in the \mathbf{k} -space, including umklapp processes, for the time interval $0 \leq t \leq 4T$, where

$$T = \frac{\pi \hbar}{a F_x} \quad (5)$$

- d) Calculate and plot the x - and y -components of the velocity and the position of the electron, all functions of time, for $0 \leq t \leq 4T$.
- e) Make a graph of the trajectory of the electron in the x - y plane of real space.
- f) Explain the phenomena in words. What is such motion called?

4 Bloch Oscillations

We saw in class that electrons in typical semiconductors do not exhibit Bloch oscillations since the Brillouin Zone edge is too far in k -space; electrons are scattered before they make it to the BZ edge. However, it is possible to artificially engineer the bandstructure so that this problem can be solved. How can you change the bandstructure to achieve this? Search, and mention one reference paper that (experimentally) uses your approach.