

k·p Calculation of Band Structure in Semiconductors

The Physics of Semiconductors, Brennan
Section 8.7

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Substitution of Bloch function into Schrödinger's Equation

In Chapter 7.4 the wave function in a crystal was rewritten as a Bloch function to show the periodicity in the crystal's lattice

$$\Psi^{(r)} = e^{i\vec{k}\cdot\vec{r}} u_{nk}(r) \quad \text{where } k \text{ is defined as the crystalline momentum}$$

If this wave function is substituted into the Schrödinger's Equation then it becomes

$$H\Psi = E\Psi \Rightarrow \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)u_{nk}(r)e^{i\vec{k}\cdot\vec{r}} = Eu_{nk}(r)e^{i\vec{k}\cdot\vec{r}}$$

Taking the Laplacian of the term $e^{i\vec{k}\cdot\vec{r}} u_{nk}(r)$ yields:

$$\nabla^2 \left[e^{i\vec{k}\cdot\vec{r}} u_{nk}(r) \right] = -k^2 e^{i\vec{k}\cdot\vec{r}} u_{nk} + e^{i\vec{k}\cdot\vec{r}} \nabla^2 u_{nk} + 2ie^{i\vec{k}\cdot\vec{r}} \vec{k} \cdot \nabla u_{nk}$$

Substitute this into the previous equation

$$-\frac{\hbar^2}{2m} \left(-k^2 e^{i\vec{k}\cdot\vec{r}} u_{nk} + e^{i\vec{k}\cdot\vec{r}} \nabla^2 u_{nk} + 2ie^{i\vec{k}\cdot\vec{r}} \vec{k} \cdot \nabla u_{nk} \right) + Vu_{nk} e^{i\vec{k}\cdot\vec{r}} = Eu_{nk} e^{i\vec{k}\cdot\vec{r}}$$

$$\left[-\frac{\hbar^2}{2m} \left(-k^2 + \nabla^2 + 2i\vec{k} \cdot \nabla \right) u_{nk} + Vu_{nk} \right] e^{i\vec{k}\cdot\vec{r}} = Eu_{nk} e^{i\vec{k}\cdot\vec{r}}$$

$$-\frac{\hbar^2}{2m} \left(-k^2 + \nabla^2 + 2i\vec{k} \cdot \nabla \right) u_{nk} + Vu_{nk} = Eu_{nk}$$

Substitution of Bloch function into Schrödinger's Equation

(cont'd)

$$-\frac{\hbar^2}{2m} (-k^2 + \nabla^2 + 2i\vec{k} \cdot \nabla) u_{nk} + V u_{nk} = E u_{nk}$$
$$\left(\frac{\hbar^2 k^2}{2m} + \frac{(-i\hbar\nabla)(-i\hbar\nabla)}{2m} + \left(\frac{\hbar\vec{k}}{m} \right) (-i\nabla) + V \right) u_{nk} = E u_{nk}$$

Remember that the linear momentum operator is defined as

$$\vec{p} = -i\hbar\nabla$$

Substitute in p to get

$$\left(\frac{\hbar^2 k^2}{2m} + \frac{p^2}{2m} + \frac{\hbar}{m} \vec{k} \cdot \vec{p} + V \right) u_{nk} = E u_{nk}$$

Now choose a specific point in k-space labeled k_0 .

Since $u_{nk}(r)$ forms a complete set for any given k, then the wave function for any value of k can be written in terms of k_0 as the summation

$$u_{nk}(r) = \sum_{n'} c_{n'} (k - k_0) u_{n'k_0}(r)$$

where n' is a dummy variable

Evaluation around $k = k_0$

Define the Hamiltonian operator at the point $k = k_0$ to be

$$H_{k_0} = \frac{p^2}{2m} + \frac{\hbar}{2m} \bar{k}_0 \cdot \bar{p} + \frac{\hbar^2 k_0^2}{2m} + V$$

Then $\frac{p^2}{2m}$ equals

$$\frac{p^2}{2m} = H_{k_0} - \frac{\hbar}{2m} \bar{k}_0 \cdot \bar{p} - \frac{\hbar^2 k_0^2}{2m} - V(r)$$

Substituting the new value of $\frac{p^2}{2m}$ into the expanded Schrödinger's Equation yields

$$\left[H_{k_0} - \frac{\hbar}{2m} \bar{k}_0 \cdot \bar{p} - \frac{\hbar^2 k_0^2}{2m} - V(r) + \frac{\hbar^2 k^2}{2m} + \frac{\hbar}{2m} \bar{k} \cdot \bar{p} + V(r) \right] u_{nk} = E u_{nk}$$

$$\left[H_{k_0} + \frac{\hbar}{m} (\bar{k} - \bar{k}_0) \cdot \bar{p} + \frac{\hbar^2}{2m} (\bar{k}^2 - \bar{k}_0^2) \right] u_{nk} = E u_{nk}$$

Set the potential voltages to be equal so they cancel each other out

Integration over all space

Substitute in the expanded form of $u_{nk}(r)$ to get

$$\left[H_{k_0} + \frac{\hbar}{m} (\bar{k} - \bar{k}_0) \cdot \bar{p} + \frac{\hbar^2}{2m} (\bar{k}^2 - \bar{k}_0^2) \right] \sum_{n'} c_{n'} u_{n'} k_0 = \sum_{n'} c_{n'} E_{n'} u_{n'} k_0$$

Now multiply all terms by $u_{nk_0}^*$ and integrate over all space

$$\int u_{nk_0}^* \left[H_{k_0} + \frac{\hbar}{m} (\bar{k} - \bar{k}_0) \cdot \bar{p} + \frac{\hbar^2}{2m} (\bar{k}^2 - \bar{k}_0^2) \right] \sum_{n'} c_{n'} u_{n'} k_0 = \int u_{nk_0}^* \sum_{n'} c_{n'} E_{n'} u_{n'} k_0$$

Break the integration into four separate terms

A. $\sum_{n'} \int u_{nk_0}^* H_{k_0} c_{n'} u_{n'} k_0$

B. $\sum_{n'} \frac{\hbar}{m} \int u_{nk_0}^* (\bar{k} - \bar{k}_0) \cdot \bar{p} c_{n'} u_{n'} k_0$

C. $\sum_{n'} \frac{\hbar^2}{2m} \int u_{nk_0}^* (\bar{k}^2 - \bar{k}_0^2) c_{n'} u_{n'} k_0$

D. $\sum_{n'} \int u_{nk_0}^* c_{n'} E_{n'} u_{n'} k_0$

Integration of separated terms

For term A:

$$\sum_{n'} \int u_{nk_0}^* H_{k_0} c_n u_n k_0$$

Since H_{k_0} is the Hamiltonian for $k = k_0$ then from the reduced Schrödinger's equation it is possible to derive

$$H_{k_0} u_{nk_0} = E_n(k_0) u_{nk_0}$$

Where $E_n(k_0)$ is defined as the energy for k set to k_0

The equation then becomes

$$\sum_{n'} \int u_{nk_0}^* E_{n'}(k_0) c_n u_n k_0$$

Which integrates to

$$\sum_{n'} E_{n'}(k_0) c_n \delta_{nn'}$$

The Kronecker delta is zero for all terms except when n' is equal to n .

Therefore term A reduces to

$$E_n(k_0) c_n$$

Integration of separated terms

For term B:

$$\sum_{n'} \frac{\hbar}{m} \int u_{nk_0}^* (\bar{k} - \bar{k}_0) \cdot \bar{p} c_{n'} u_{n'} k_0$$

Define $\bar{p}_{nn'}$ so that

$$\bar{p}_{nn'} = \int u_{nk_0}^* \bar{p} u_{n'} k_0$$

then term B reduces to

$$\sum_{n'} \frac{\hbar}{m} (\bar{k} - \bar{k}_0) \cdot \bar{p}_{nn'} c_{n'}$$

Term C:

$$\sum_{n'} \frac{\hbar^2}{2m} \int u_{nk_0}^* (\bar{k}^2 - \bar{k}_0^2) c_{n'} u_{n'} k_0 = \sum_{n'} \frac{\hbar^2}{2m} (\bar{k}^2 - \bar{k}_0^2) c_{n'} \delta_{nn'} = \frac{\hbar^2}{2m} (\bar{k}^2 - \bar{k}_0^2) c_n$$

Term D:

$$\sum_{n'} \int u_{nk_0}^* c_{n'} E_{n'} u_{n'} k_0 = \sum_{n'} c_{n'} E_{n'} u_{n'} k_0 \delta_{nn'} = c_n E_n(k)$$

Putting all the terms together you get

$$E_n(k) c_n + \sum_{n'} \frac{\hbar}{m} (\bar{k} - \bar{k}_0) \cdot \bar{p}_{nn'} c_{n'} + \frac{\hbar^2}{2m} (\bar{k}^2 - \bar{k}_0^2) c_n = c_n E_n(k)$$

Integration of separated terms

(cont'd)

$$E_n(k_0)c_n + \sum_{n'} \frac{\hbar}{m} (\bar{k} - \bar{k}_0) \cdot \bar{p}_{nn'} c_{n'} + \frac{\hbar^2}{2m} (\bar{k}^2 - \bar{k}_0^2) c_n = c_n E_n(k)$$

This leads to a matrix that is of the form:

$$\left[\begin{array}{cccc} E_1(k_0) + \frac{\hbar}{m} (\bar{k} - \bar{k}_0) \cdot \bar{p}_{1,1} + \frac{\hbar^2}{2m} (\bar{k}^2 - \bar{k}_0^2) & \frac{\hbar}{m} (\bar{k} - \bar{k}_0) \cdot \bar{p}_{1,2} & \dots & \frac{\hbar}{m} (\bar{k} - \bar{k}_0) \cdot \bar{p}_{1,n} \\ \frac{\hbar}{m} (\bar{k} - \bar{k}_0) \cdot \bar{p}_{2,1} & E_2(k_0) + \frac{\hbar}{m} (\bar{k} - \bar{k}_0) \cdot \bar{p}_{2,2} + \frac{\hbar^2}{2m} (\bar{k}^2 - \bar{k}_0^2) & & \vdots \\ \vdots & & \ddots & \vdots \\ \frac{\hbar}{m} (\bar{k} - \bar{k}_0) \cdot \bar{p}_{n,1} & \dots & & E_n(k_0) + \frac{\hbar}{m} (\bar{k} - \bar{k}_0) \cdot \bar{p}_{n,n'} + \frac{\hbar^2}{2m} (\bar{k}^2 - \bar{k}_0^2) \end{array} \right]$$

A solution to the matrix can be found by implementing perturbation theory

Solution through perturbation theory

A zero order approximation for the energy for each state is given by disregarding the values that are not on the diagonal of the matrix. Therefore the energy for each state is:

$$E_n(k) = E_n(k_0) + \frac{\hbar^2}{2m}(k^2 - k_0^2)$$

The first order approximation term is obtained by setting the perturbation Hamiltonian to

$$H_p = \frac{\hbar}{m}(\bar{k} - \bar{k}_0) \cdot \bar{p}$$

The energy level for the first term then becomes

$$E_n^{(1)} = \langle \Psi_n^{(0)} | H_p | \Psi_n^{(0)} \rangle \text{ where } \Psi_n^{(0)} = e^{i\bar{k} \cdot \bar{r}} u_{nk}(r)$$

$$E_n^{(1)} = \int e^{-i\bar{k} \cdot \bar{r}} u_{nk}(r) \frac{\hbar}{m} (\bar{k} - \bar{k}_0) \cdot \bar{p} e^{i\bar{k} \cdot \bar{r}} u_{nk}(r)$$

Then define \bar{p}_{nn} to be

$$\bar{p}_{nn} = \int u_{nk}(r) \bar{p} u_{nk}(r)$$

The first order energy is then

$$E_n^{(1)} = \frac{\hbar}{m} (\bar{k} - \bar{k}_0) \cdot \bar{p}_{nn}$$

Second order approximation

The second order approximation term is obtained by

$$E_n^{(2)} = \sum_{n'} \left(\frac{\langle \Psi_n^{(0)} | H_p | \Psi_{n'}^{(0)} \rangle}{(E_{n'k_0} - E_{nk_0})} \right) \left(\langle \Psi_n^{(0)} | H_p | \Psi_{n'}^{(0)} \rangle \right)$$
$$E_n^{(2)} = \sum_{n'} \left(\frac{\left(\frac{\hbar}{m} (\bar{k} - k_0) \cdot \bar{p}_{nn'} \right) \left(\frac{\hbar}{m} (\bar{k} - k_0) \cdot \bar{p}_{nn'} \right)}{(E_{n'k_0} - E_{nk_0})} \right) = \sum_{n'} \frac{\hbar^2}{m^2} \frac{|(\bar{k} - \bar{k}_0) \cdot \bar{p}_{nn}|^2}{E_{n'k_0} - E_{nk_0}}$$

The total energy eigenvalue is arrived at by combining the zero, first, and second order approximations

$$E_n(k) = E_n(k_0) + \frac{\hbar^2}{2m} (k^2 - k_0^2) + \frac{\hbar}{m} (\bar{k} - \bar{k}_0) \cdot \bar{p}_{nn} + \sum_{n'} \frac{\hbar^2}{m^2} \frac{|(\bar{k} - \bar{k}_0) \cdot \bar{p}|^2}{E_{n'k_0} - E_{nk_0}}$$

Special cases for k·p

Now consider the case where the crystal is symmetric in every direction from point k_0 . If this were to occur then the first order correction term would go to zero.

If k_0 were set to zero and was also at a center of the symmetry for the crystal then the energy eigenvalue would be reduced to

$$E_n(k) = E_{n0} + \frac{\hbar^2 k^2}{2m} + \sum_{n'} \frac{\hbar^2}{m^2} \frac{|\vec{k} \cdot \langle u_{0n'} | \vec{p} | u_{0n} \rangle|^2}{E_{n'0} - E_{n0}}$$

An equation for the effective mass in the crystal can be obtained by rewriting the energy equation as

$$E_n(k) = E_{n0} + \frac{\hbar^2}{2m} \vec{k} \cdot \frac{\bar{m}}{m^*} \cdot \vec{k}$$

Where $\frac{\bar{m}}{m^*}$ is defined as an effective mass tensor that represents the curvature of the E-k diagram versus the direction in k-space. The effective mass will be different depending on the direction in k-space.

$$\left. \frac{\bar{m}}{m^*} \right|_{ij} = \delta_{ij} + \frac{2}{m} \sum_{n'} \frac{\langle u_{0n'} | \vec{p}_i | u_{0n} \rangle \langle u_{0n'} | \vec{p}_j | u_{0n} \rangle}{E_{n'0} - E_{n0}}$$

Uses for the k·p approximation

The k·p approximation is useful for approximating the band gap energy for materials that have low band gaps, such as InN. This is because as the difference in energy between states becomes larger, then the factor $E_{n'0} - E_{n0}$ causes the second order correction term becomes smaller and smaller.