The k p Method

Electronic Properties of Semiconductors

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Chapter 2
One-Band Model

2.1 Overview

Much of the physics of the $k \cdot p$ theory is displayed by considering a single isolated band. Such a band is relevant to the conduction band of many semiconductors and can even be applied to the valence band under certain conditions. We will illustrate using a number of derivations for a bulk crystal.

2.2 $k \cdot p$ Equation

The $k \cdot p$ equation is obtained from the one-electron Schrödinger equation

$$H\psi_{n\mathbf{k}}(\mathbf{r}) = E_n(\mathbf{k})\psi_{n\mathbf{k}}(\mathbf{r}) \,, \tag{2.1}$$

upon representing the Bloch functions in terms of a set of periodic functions:

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \mathrm{e}^{\mathbf{i}\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r}). \tag{2.2}$$

The Bloch and cellular functions satisfy the following set of properties:

$$\langle\psi_{n\mathbf{k}}|\psi_{n'\mathbf{k}'}\rangle \equiv \int \mathrm{d}V\, \psi^*_{n\mathbf{k}}(\mathbf{r})\,\psi_{n'\mathbf{k}'}(\mathbf{r}) = \delta_{nn'}\delta(\mathbf{k}-\mathbf{k}'), \tag{2.3}$$

$$\langle u_{n\mathbf{k}}|u_{n'\mathbf{k}}\rangle \equiv \int \mathrm{d}\Omega\, u^*_{n\mathbf{k}} u_{n'\mathbf{k}} = \delta_{nn'}\frac{\Omega}{(2\pi)^3}, \tag{2.4}$$

where V (Ω) is the crystal (unit-cell) volume.

Let the Hamiltonian only consists of the kinetic-energy operator, a local periodic crystal potential, and the spin-orbit interaction term:

$$H = \frac{p^2}{2m_0} + V(\mathbf{r}) + \frac{\hbar}{4m_0^2c^2}(\boldsymbol{\sigma}\times\nabla V)\cdot\mathbf{p}\,. \tag{2.5}$$

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Here, we only give the formal exact form for a periodic bulk crystal without external perturbations.

In terms of the cellular functions, Schrödinger's equation becomes

$$H(\mathbf{k})\, u_{n\mathbf{k}} = \mathcal{E}_n(\mathbf{k})\, u_{n\mathbf{k}}, \tag{2.6}$$

where

$$H(\mathbf{k}) \equiv H + H_{k\cdot p}, \tag{2.7}$$

$$H_{k\cdot p} = \frac{\hbar}{m_0}\mathbf{k}\cdot\boldsymbol{\pi}, \tag{2.8}$$

$$\boldsymbol{\pi} = \mathbf{p} + \frac{\hbar}{4m_0c^2}(\boldsymbol{\sigma}\times\nabla V), \tag{2.9}$$

$$\mathcal{E}_n(\mathbf{k}) = E_n(\mathbf{k}) - \frac{\hbar^2k^2}{2m_0}. \tag{2.10}$$

Equation (2.6) is the $k\cdot p$ equation. If the states $u_{n\mathbf{k}}$ form a complete set of periodic functions, then a representation of $H(\mathbf{k})$ in this basis is exact; i.e., diagonalization of the infinite matrix

$$\langle u_{n\mathbf{k}}|H(\mathbf{k})|u_{m\mathbf{k}}\rangle$$

leads to the dispersion relation throughout the whole Brillouin zone. Note, in particular, that the off-diagonal terms are only linear in k. However, practical implementations only solve the problem in a finite subspace. This leads to approximate dispersion relations and/or applicability for only a finite range of k values. For GaAs and AlAs, the range of validity is of the order of 10% of the first Brillouin zone [7].

An even more extreme case is to only consider one $u_{n\mathbf{k}}$ function. This is then known as the one-band or effective-mass (the latter terminology will become clear below) model. Such an approximation is good if, indeed, the semiconductor under study has a fairly isolated band—at least, again, for a finite region in k space. This is typically true of the conduction band of most III–V and II–VI semiconductors. In such cases, one also considers a region in k space near the band extremum. This is partly driven by the fact that this is the region most likely populated by charge carriers in thermal equilibrium and also by the fact that linear terms in the energy dispersion vanish, i.e.,

$$\frac{\partial E_n(\mathbf{k}_0)}{\partial k_i} = 0.$$

A detailed discussion of the symmetry constraints on the locations of these extremum points was provided by Bir and Pikus [1]. In the rest of this chapter, we will discuss how to obtain the energy dispersion relation and analyze a few properties of the resulting band.

2.3 Perturbation Theory

One can apply nondegenerate perturbation theory to the $k \cdot p$ equation, Eq. (2.6), for an isolated band. Given the solutions at $\mathbf{k} = \mathbf{0}$, one can find the solutions for finite k via perturbation theory:

$$E_n(\mathbf{k}) = E_n(\mathbf{0}) + \frac{\hbar^2 k^2}{2m_0} + \frac{\hbar \mathbf{k}}{m_0} \cdot \langle n\mathbf{0}|\boldsymbol{\pi}|n\mathbf{0}\rangle + \frac{\hbar^2}{m_0^2} \sideset{}{'}\sum_l \frac{|\langle n\mathbf{0}|\boldsymbol{\pi}|l\mathbf{0}\rangle \cdot \mathbf{k}|^2}{E_n(\mathbf{0}) - E_l(\mathbf{0})} \tag{2.11}$$

to second order and where

$$\langle n\mathbf{0}|\boldsymbol{\pi}|l\mathbf{0}\rangle = \frac{(2\pi)^3}{\Omega} \int \mathrm{d}\Omega \, u_{n\mathbf{0}}^* \boldsymbol{\pi} u_{l\mathbf{0}}. \tag{2.12}$$

This is the basic effective-mass equation.

2.4 Canonical Transformation

A second technique for deriving the effective-mass equation is by the use of the canonical transformation introduced by Luttinger and Kohn in 1955 [6]. Here, one expands the cellular function in terms of a complete set of periodic functions:

$$u_{n\mathbf{k}}(\mathbf{r}) = \sum_{n'} A_{nn'}(\mathbf{k}) \, u_{n'\mathbf{0}}(\mathbf{r}). \tag{2.13}$$

Then the $k \cdot p$ equation, Eq. (2.6), becomes

$$\begin{aligned}\sum_{n'} A_{nn'}(\mathbf{k}) \left[H + H_{k \cdot p}\right] u_{n'\mathbf{0}}(\mathbf{r}) &= \sum_{n'} A_{nn'}(\mathbf{k}) \left[E_{n'}(\mathbf{0}) + H_{k \cdot p}\right] u_{n'\mathbf{0}}(\mathbf{r}) \\ &= \mathcal{E}_n(\mathbf{k}) \sum_{n'} A_{nn'}(\mathbf{k}) \, u_{n'\mathbf{0}}(\mathbf{r}).\end{aligned} \tag{2.14}$$

Multiplying by $(2\pi)^3/\Omega \int_\Omega \mathrm{d}^3\mathbf{r} \, u_{n\mathbf{0}}^*$ gives

$$E_n(\mathbf{0}) \, A_{nn} + \sum_{n'} \frac{\hbar \mathbf{k}}{m_0} \cdot \mathbf{p}_{nn'} A_{nn'}(\mathbf{k}) = \mathcal{E}_n(\mathbf{k}) \, A_{nn}, \tag{2.15}$$

where

$$\mathbf{p}_{nn'} \equiv \mathbf{p}_{nn'}(\mathbf{0}) = \frac{(2\pi)^3}{\Omega} \int \mathrm{d}\Omega \, u_{n\mathbf{0}}^* \mathbf{p} u_{n'\mathbf{0}}, \tag{2.16}$$

and we have left out the spin-orbit contribution to the momentum operator for simplicity. Now one can write (dropping one band index)

$$H(\mathbf{k})A = \mathcal{E}(\mathbf{k})A, \quad A = \begin{pmatrix} \vdots \\ A_n \\ \vdots \end{pmatrix}. \tag{2.17}$$

The linear equations are coupled. The solution involves uncoupling them. This can be achieved by a canonical transformation:

$$A = TB, \tag{2.18}$$

where T is unitary (in order to preserve normalization). Then

$$\overline{H}(\mathbf{k})B = \mathcal{E}(\mathbf{k})B, \tag{2.19}$$

where

$$\overline{H}(\mathbf{k}) = T^{-1}HT. \tag{2.20}$$

Writing $T = \mathrm{e}^{S}, \quad T^{-1} = \mathrm{e}^{-S} = T^{\dagger}$,

$$\begin{aligned} \overline{H} &= \left(1 - S + \frac{1}{2!}S^2 - \cdots\right) H(\mathbf{k}) \left(1 + S + \frac{1}{2!}S^2 + \cdots\right) \\ &= H(\mathbf{k}) + [H(\mathbf{k}), S] + \frac{1}{2!}\,[[H(\mathbf{k}), S], S] + \cdots \\ &= H + H_{k\cdot p} + [H, S] + [H_{k\cdot p}, S] \\ &\quad + \frac{1}{2!}\,[[H, S], S] + \frac{1}{2!}\left[[H_{k\cdot p}, S], S\right] + \cdots \end{aligned} \tag{2.21}$$

Since $H_{k\cdot p}$ induces the coupling, one would like to remove it to order S by

$$H_{k\cdot p} + [H, S] = 0, \tag{2.22}$$

or, with $|n\rangle \equiv |u_{n\mathbf{0}}\rangle$,

$$\begin{aligned} \langle n|H_{k\cdot p}|n'\rangle + \sum_{n''}\Big[\langle n|H|n''\rangle\langle n''|S|n'\rangle - \langle n|S|n''\rangle\langle n''|H|n'\rangle\Big] &= 0, \\ \frac{\hbar}{m_0}\mathbf{k}\cdot\mathbf{p}_{nn'} + E_n(\mathbf{0})\langle n|S|n'\rangle - \langle n|S|n'\rangle E_{n'}(\mathbf{0}) &= 0, \end{aligned}$$

giving, for $n \neq n'$,

$$\langle n|S|n'\rangle = -\frac{\hbar}{m_0}\frac{\mathbf{k}\cdot\mathbf{p}_{nn'}}{[E_n(\mathbf{0}) - E_{n'}(\mathbf{0})]}. \tag{2.23}$$

Now, Eq. (2.21) becomes

$$\overline{H}(\mathbf{k}) = H + \frac{1}{2}[H_{k\cdot p}, S] + \frac{1}{2}[[H_{k\cdot p}, S], S] + \cdots$$

and, to second order,

$$\begin{aligned}\langle n|\,\overline{H}\,(\mathbf{k})|n'\rangle &\approx \langle n|H|n'\rangle + \frac{1}{2}\sum_{n''}\Big[\langle n|H_{k\cdot p}|n''\rangle\langle n''|S|n'\rangle - \langle n|S|n''\rangle\langle n''|H_{k\cdot p}|n'\rangle\Big]\\ &= E_n(\mathbf{0})\delta_{nn'} + \frac{\hbar^2}{2m_0^2}\sum_{n''}\left[\frac{\mathbf{k}\cdot\mathbf{p}_{nn''}\,\mathbf{k}\cdot\mathbf{p}_{n''n'}}{[E_{n'}(\mathbf{0}) - E_{n''}(\mathbf{0})]} + \frac{\mathbf{k}\cdot\mathbf{p}_{nn''}\,\mathbf{k}\cdot\mathbf{p}_{n''n'}}{[E_n(\mathbf{0}) - E_{n''}(\mathbf{0})]}\right]\\ &= \left[E_n(\mathbf{0}) + \frac{\hbar^2}{2}\sum_{\alpha\beta}k_\alpha\left(\frac{1}{m_n}\right)_{\alpha\beta}k_\beta\right]\delta_{nn'} + \text{interband terms of order } k^2,\end{aligned}$$

which is, of course, the same as Eq. (2.11).

We now restrict ourselves to zincblende and diamond crystals for which $n = s = \Gamma_1$ (see Appendix B for the symmetry properties), $p_{nn} = 0$, and

$$E(\mathbf{k}) = E_{\Gamma_1} + \frac{\hbar^2 k^2}{2m_0} + \frac{\hbar^2}{m_0^2}\sum_l{}' \frac{|\mathbf{p}_{\Gamma_1 l}\cdot\mathbf{k}|^2}{E_{\Gamma_1} - E_l}. \tag{2.24}$$

Note that, for conciseness, we are also only using the group notation for the electron states in a zincblende crystal. The standard state ordering for zincblende and diamond is given in Fig. 2.1. There are exceptions to these such as the inverted band structure of HgTe [9] and the inverted conduction band of Si. Thus, the interaction of the Γ_1 state with other states via $p_{\Gamma_1 l}$ changes the dispersion relation from that of a free-electron one. The new inverse effective-mass tensor is

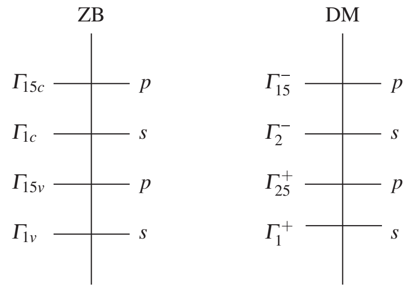

Fig. 2.1 Zone-center states for typical zincblende (ZB) and diamond (DM) crystals

$$\left(\frac{1}{m^*}\right)_{ij} = \frac{1}{m_0}\delta_{ij} + \frac{2}{m_0^2}\sum_l{}' \frac{p^i_{\Gamma_1 l} p^j_{l\Gamma_1}}{E_{\Gamma_1} - E_l}. \tag{2.25}$$

Equation (2.11) or Eqs. (2.24) and (2.25) define the one-band, effective-mass model. The band dispersion can be calculated given the momentum matrix elements and band gaps. Note that Eq. (2.24) is only approximate, giving the parabolic approximation. Constraints on the effective mass can now be written from Eq. (2.25).

2.5 Effective Masses

One can write down simple expressions for the effective masses of nondegenerate bands.

2.5.1 Electron

Because of the energy denominator, distant bands are expected to be less important. The two closest bands to the Γ_{1c} state for cubic semiconductors are the Γ_{15} states $\sim X, Y, Z$. Since $\Gamma_{1c} \sim S$, and

$$\langle S|p_x|X\rangle = \langle S|p_y|Y\rangle = \langle S|p_z|Z\rangle,$$

the conduction mass m_e is isotropic:

$$\begin{aligned}\frac{1}{m_e} &= \frac{1}{m_0} + \frac{2}{m_0^2}\frac{|\langle S|p_x|X_v\rangle|^2}{E_{\Gamma_{1c}} - E_{\Gamma_{15v}}} + \frac{2}{m_0^2}\frac{|\langle S|p_x|X_c\rangle|^2}{E_{\Gamma_{1c}} - E_{\Gamma_{15c}}}\\ &\equiv \frac{1}{m_0} + \frac{2P^2}{\hbar^2 E_0} - \frac{2P'^2}{\hbar^2 E_0'},\end{aligned} \tag{2.26}$$

where

$$P^2 = \frac{\hbar^2}{m_0^2}|\langle S|p_x|X_v\rangle|^2, \tag{2.27}$$

$$P'^2 = \frac{\hbar^2}{m_0^2}|\langle S|p_x|X_c\rangle|^2. \tag{2.28}$$

For diamond,

$$P' = 0 \quad \Longrightarrow \quad 0 < m_e < m_0.$$

For zincblende, typically

$$\frac{P'^2}{E'_0} < \frac{P^2}{E_0} \quad \Longrightarrow \quad 0 < m_e < m_0.$$

Hence, the electron effective mass is usually smaller than the free-electron mass.

2.5.2 Light Hole

Of the three-fold degenerate Γ_{15v} states, only one couples with Γ_{1c} along a given Δ direction, giving rise to the light-hole (lh) mass. Consider $\mathbf{k} = (k_x, 0, 0)$. Then, since the lh state can now be assumed nondegenerate, again m_{lh} is isotropic (though a more accurate model will reveal them to be anisotropic):

$$\frac{1}{m_{lh}} = \frac{1}{m_0} + \frac{2}{m_0^2} \frac{|\langle S|p_x|X_v\rangle|^2}{E_{\Gamma_{15v}} - E_{\Gamma_{1c}}} = \frac{1}{m_0} - \frac{2P^2}{\hbar^2 E_0} \equiv \frac{1}{m_0}\left(1 - \frac{E_P}{E_0}\right), \tag{2.29}$$

with

$$E_P \equiv \frac{2m_0 P^2}{\hbar^2} \tag{2.30}$$

known as the Kane parameter. Typically, $E_p \sim 20\,\text{eV}$, $E_0 \sim 0$–$5\,\text{eV}$. Hence, $-m_0 < m_{lh} < 0$. Note that, contrary to the electron case, the lh mass does not contain the P' term.

To compare the lh and e masses,

$$\frac{1}{m_e} + \frac{1}{m_{lh}} = \frac{2}{m_0} - \frac{2P'^2}{\hbar^2 E'_0} = \frac{1}{m_0}\left(2 - \frac{E'_P}{E'_0}\right).$$

For diamond, $E'_P = 0$, giving

$$\frac{1}{m_e} + \frac{1}{m_{lh}} > 0 \quad \text{(always)}, \tag{2.31}$$

and

$$|m_{lh}| > m_e. \tag{2.32}$$

For zincblende, $E'_P \sim 1$–$10\,\text{eV}$, $E'_0 \sim 3$–$5\,\text{eV}$, and the masses are closer in magnitude. The qualitative effect of the e–lh interaction on the effective masses is sketched in Fig. 2.2. This is also known as a two-band model.

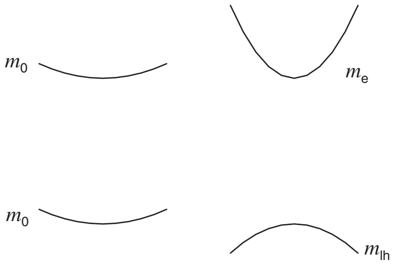

Fig. 2.2 Two-band model. The $k \cdot p$ interaction changes the curvatures

2.5.3 Heavy Hole

One may define the heavy-hole (hh) states as the partners in the Γ_{15v} representation which do not couple to the conduction s electron. In so far as the Γ_{15c} states are not considered, the hh state has the free-electron mass. Including the Γ_{15c} state and again assuming that the Γ_{15v} states are nondegenerate, the isotropic mass is

$$\frac{1}{m_{hh}} = \frac{1}{m_0} - \frac{2}{m_0^2} \frac{|\langle Y_v | p_x | Z_c \rangle|^2}{E_0 + E_0'} = \frac{1}{m_0} \left(1 - \frac{E_Q}{E_0 + E_0'} \right). \tag{2.33}$$

Typically, $E_Q \sim$20–25 eV, $E_0 + E_0' \sim 10\,\text{eV}$, and $0 > m_{hh} > -m_0$.

We have seen how the simple one-band model can provide a semi-quantitative description of various bands for zincblende and diamond semiconductors, particularly the sign and relative magnitudes of the associated effective masses. The necessity of describing the band structure quantitatively and more accurately (such as nonparabolicity and anisotropy) leads to the consideration of multiband models.

2.6 Nonparabolicity

So far, we have presented the simplest one-band model in order to illustrate the theory; it does allow for anisotropy via an anisotropic effective mass. Still, a one-band model can be made to reproduce more detailed features of a real band including nonparabolicity, anisotropy and spin splitting. An example of such a model is the k^4 dispersion relation given by Rössler [23]:

$$\begin{aligned} E(\mathbf{k}) = \tfrac{\hbar^2 k^2}{2m^*} &+ \alpha k^4 + \beta \left(k_y^2 k_z^2 + k_z^2 k_x^2 + k_x^2 k_y^2 \right) \\ &\pm \gamma \left\{ k^2 \left(k_y^2 k_z^2 + k_z^2 k_x^2 + k_x^2 k_y^2 \right) - 9 k_x^2 k_y^2 k_z^2 \right\}^{1/2}. \end{aligned} \tag{2.34}$$

The first term on the right-hand side is the familiar isotropic and parabolic effective-mass term. The remaining terms give nonparabolicity, warping and spin splitting, respectively. We will derive them later in the book.

2.7 Summary

We have set up the fundamental $k \cdot p$ equation and shown, using a variety of techniques, how a one-band model (the so-called effective-mass model) can be obtained from it. This model was then used to derive a semi-quantitative understanding of the magnitude of the effective masses of band-edge states for cubic semiconductors. In particular, it was shown that the simplest effective-mass model for electrons and light holes gives isotropic masses.