K·p theory for band structure of semiconductor quantum wells

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1 K·p method

The goal of the **k·p** method is solving the Schrödinger equation to find energy and wave function of electron in crystals. The Schrödinger equation describing an electron in crystals reads

$$\left[\frac{p^2}{2m_0} + V_0(\mathbf{r}) + H_{SO}\right]\psi_{m\mathbf{k}}(\mathbf{r}) = E_{m\mathbf{k}}\psi_{m\mathbf{k}}(\mathbf{r}). \tag{1}$$

Here, m_0 is the free-electron mass, $V_0(\mathbf{r})$ is the periodic lattice potential, m denotes the band index, and H_{SO} is the spin-orbit interaction,

$$H_{SO} = \frac{\hbar}{4m_0^2c^2}\boldsymbol{\sigma}\cdot\left(\boldsymbol{\nabla}V_0\times\mathbf{p}\right), \tag{2}$$

where $\boldsymbol{\sigma}$ is the vertor of Pauli matrices. The wave function in the crystal satify the Bloch theorem and is written for the first Brillouin zone as

$$\psi_{m\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{m\mathbf{k}}(\mathbf{r}). \tag{3}$$

Substituting (3) into (1) one obtains the Schrödinger equation for the lattice periodic function $u_{\mathbf{k}}(\mathbf{r})$:

$$\left[\frac{p^2}{2m_0} + V_0(\mathbf{r}) + \frac{\hbar^2k^2}{2m_0} + \frac{\hbar}{m_0}\mathbf{k}\cdot\left(\mathbf{p} + \frac{\hbar}{4m_0c^2}\boldsymbol{\sigma}\times\boldsymbol{\nabla}V_0\right) + \frac{\hbar}{4m_0^2c^2}\boldsymbol{\sigma}\cdot\left(\boldsymbol{\nabla}V_0\times\mathbf{p}\right)\right]u_{m\mathbf{k}}(\mathbf{r}) = E_{m\mathbf{k}}u_{m\mathbf{k}}(\mathbf{r}). \tag{4}$$

We assume that we know the bandenergies and eigenfunctions at a single point k_0 in the Brillouin zone. Since the states for each k are complete, we can expand the Bloch function at an arbitrary k via eigenfunctions at k_0. Typically, the Gamma point $k_0 = 0$, i. e., the center of the Brillouin zone, is chosen as the expansion point. We write

$$u_{m\mathbf{k}}(\mathbf{r}) = \sum_n a^n_{m\mathbf{k}}u_n(\mathbf{r}), \tag{5}$$

where $u_n(\mathbf{r})$ are solutions of the equation

$$\left[\frac{p^2}{2m_0} + V_0(\mathbf{r})\right]u_n(\mathbf{r}) = E^0_n u_n(\mathbf{r}). \tag{6}$$

Substituting (54) into (4), multiplying on the left by u^*_n, and then integrating over unit cell, one obtains an eigen-system problem:

$$\sum_{n'} H_{nn'}(\mathbf{k})\ a^{n'}_{m\mathbf{k}} = E_{m\mathbf{k}}a^n_{m\mathbf{k}}, \tag{7}$$

where

$$
\begin{aligned}
H_{nn'}(\mathbf{k}) &= \left(E_n^0 + \frac{\hbar^2 k^2}{2m_0}\right)\delta_{nn'} + \frac{\hbar}{m_0}\mathbf{k}\cdot\left(\langle u_n|\mathbf{p}|u_{n'}\rangle + \frac{\hbar}{4m_0c^2}\langle u_n|\boldsymbol{\sigma}\times\boldsymbol{\nabla}V_0|u_{n'}\rangle\right) \\
&+ \frac{\hbar}{4m_0^2c^2}\langle u_n|\boldsymbol{\sigma}\cdot(\boldsymbol{\nabla}V_0\times\mathbf{p})\,|u_{n'}\rangle. \qquad (8)
\end{aligned}
$$

Here, the first term in Eq. (8) is diagonal part describing free electron, the second term is off-diagonal part describing the "$k.p$ interaction", and the third term is matrix element of spin-orbit interaction.

2 Extended Kane model

The extended Kane model [1, 2] takes into account fourteen bands including six bonding p-like valence band states, two anti-bonding s-like conduction band states, and six anti-bonding p-like conduction band states. The schematic band structure at Gamma point is showed in Fig. 1. The basis functions are defined as common angular momentum eigenfunctions (atomic orbitals) $|j, j_z\rangle$. In which the quantization axis of angular momentum is the crystallographic direction [001]

$$
\begin{aligned}
u_1 &= \left|\tfrac{3}{2},+\tfrac{3}{2}\right\rangle_{c'} = -\tfrac{1}{\sqrt{2}}\begin{pmatrix}X'+iY'\\0\end{pmatrix} & u_9 &= \left|\tfrac{3}{2},+\tfrac{3}{2}\right\rangle_{v} = -\tfrac{1}{\sqrt{2}}\begin{pmatrix}X+iY\\0\end{pmatrix} \\
u_2 &= \left|\tfrac{3}{2},+\tfrac{1}{2}\right\rangle_{c'} = -\tfrac{1}{\sqrt{6}}\begin{pmatrix}-2Z'\\X'+iY'\end{pmatrix} & u_{10} &= \left|\tfrac{3}{2},+\tfrac{1}{2}\right\rangle_{v} = -\tfrac{1}{\sqrt{6}}\begin{pmatrix}-2Z\\X+iY\end{pmatrix} \\
u_3 &= \left|\tfrac{3}{2},-\tfrac{1}{2}\right\rangle_{c'} = \tfrac{1}{\sqrt{6}}\begin{pmatrix}X'-iY'\\2Z'\end{pmatrix} & u_{11} &= \left|\tfrac{3}{2},-\tfrac{1}{2}\right\rangle_{v} = \tfrac{1}{\sqrt{6}}\begin{pmatrix}X-iY\\2Z\end{pmatrix} \\
u_4 &= \left|\tfrac{3}{2},-\tfrac{3}{2}\right\rangle_{c'} = \tfrac{1}{\sqrt{2}}\begin{pmatrix}0\\X'-iY'\end{pmatrix} & u_{12} &= \left|\tfrac{3}{2},-\tfrac{3}{2}\right\rangle_{v} = \tfrac{1}{\sqrt{2}}\begin{pmatrix}0\\X-iY\end{pmatrix} \\
u_5 &= \left|\tfrac{1}{2},+\tfrac{1}{2}\right\rangle_{c'} = -\tfrac{1}{\sqrt{3}}\begin{pmatrix}Z'\\X'+iY'\end{pmatrix} & u_{13} &= \left|\tfrac{1}{2},+\tfrac{1}{2}\right\rangle_{v} = -\tfrac{1}{\sqrt{3}}\begin{pmatrix}Z\\X+iY\end{pmatrix} \\
u_6 &= \left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle_{c'} = -\tfrac{1}{\sqrt{3}}\begin{pmatrix}X'-iY'\\-Z'\end{pmatrix} & u_{14} &= \left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle_{v} = -\tfrac{1}{\sqrt{3}}\begin{pmatrix}X-iY\\-Z\end{pmatrix} \\
u_7 &= \left|\tfrac{1}{2},+\tfrac{1}{2}\right\rangle_{c} = \begin{pmatrix}S\\0\end{pmatrix} \\
u_8 &= \left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle_{c} = \begin{pmatrix}0\\S\end{pmatrix}
\end{aligned}
$$

One defines the matrix elements of momentum and spin-orbit interaction by parameters as follows [2, 3]:

$$
\begin{aligned}
&\frac{\hbar}{m_0}\langle S|p_x|X\rangle = \frac{\hbar}{m_0}\langle S|p_y|Y\rangle = \frac{\hbar}{m_0}\langle S|p_z|Z\rangle = P, \\
&\frac{\hbar}{m_0}\langle S|p_x|X'\rangle = \frac{\hbar}{m_0}\langle S|p_y|Y'\rangle = \frac{\hbar}{m_0}\langle S|p_z|Z'\rangle = iP', \\
&\frac{\hbar}{m_0}\langle X|p_y|Z'\rangle = \frac{\hbar}{m_0}\langle Y|p_z|X'\rangle = \frac{\hbar}{m_0}\langle Z|p_x|Y'\rangle = Q, \\
&\frac{-3i\hbar}{4m_0^2c^2}\langle X|\,(\boldsymbol{\nabla}V_0\times\mathbf{p})_y\,|Z\rangle = \frac{-3i\hbar}{4m_0^2c^2}\langle Y|\,(\boldsymbol{\nabla}V_0\times\mathbf{p})_z\,|X\rangle = \frac{-3i\hbar}{4m_0^2c^2}\langle Z|\,(\boldsymbol{\nabla}V_0\times\mathbf{p})_x\,|Y\rangle = \Delta, \\
&\frac{-3i\hbar}{4m_0^2c^2}\langle X'|\,(\boldsymbol{\nabla}V_0\times\mathbf{p})_y\,|Z'\rangle = \frac{-3i\hbar}{4m_0^2c^2}\langle Y'|\,(\boldsymbol{\nabla}V_0\times\mathbf{p})_z\,|X'\rangle = \frac{-3i\hbar}{4m_0^2c^2}\langle Z'|\,(\boldsymbol{\nabla}V_0\times\mathbf{p})_x\,|Y'\rangle = \Delta', \\
&\frac{-3i\hbar}{4m_0^2c^2}\langle X|\,(\boldsymbol{\nabla}V_0\times\mathbf{p})_y\,|Z'\rangle = \frac{-3i\hbar}{4m_0^2c^2}\langle Y|\,(\boldsymbol{\nabla}V_0\times\mathbf{p})_z\,|X'\rangle = \frac{-3i\hbar}{4m_0^2c^2}\langle Z|\,(\boldsymbol{\nabla}V_0\times\mathbf{p})_x\,|Y'\rangle = i\bar{\Delta}, \\
&-\frac{1}{2\sqrt{3}}\frac{\hbar^2}{m_0^2c^2}\langle X|\frac{\partial V_0}{\partial y}|Z\rangle = -\frac{1}{2\sqrt{3}}\frac{\hbar^2}{m_0^2c^2}\langle Y|\frac{\partial V_0}{\partial z}|X\rangle = -\frac{1}{2\sqrt{3}}\frac{\hbar^2}{m_0^2c^2}\langle Z|\frac{\partial V_0}{\partial x}|Y\rangle = C_k. \qquad (9)
\end{aligned}
$$

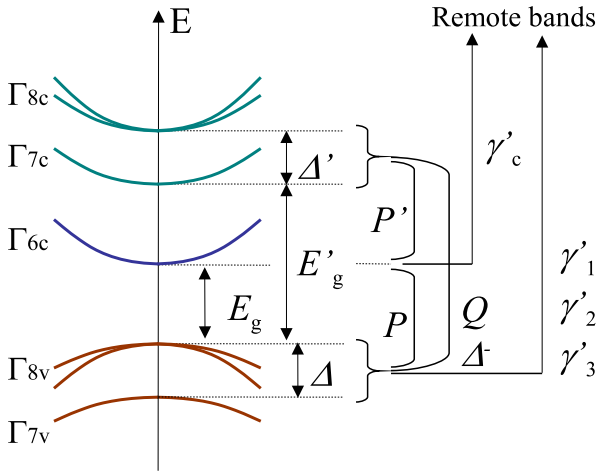

Figure 1: Schematic band structure at Γ point for extended Kane model[2].

Otherwise, the matrix elements are zeros.

By using definitions (9) the Hamiltonian matrix (8) takes the form [2]

$$H_{14\times14} = \begin{pmatrix} H_{8c8c} & H_{8c7c} & H_{8c6c} & H_{8c8v} & H_{8c7v} \\ H_{7c8c} & H_{7c7c} & H_{7c6c} & H_{7c8v} & H_{7c7v} \\ H_{6c8c} & H_{6c7c} & H_{6c6c} & H_{6c8v} & H_{6c7v} \\ H_{8v8c} & H_{8v7c} & H_{8v6c} & H_{8v8v} & H_{8v7v} \\ H_{7v8c} & H_{7v7c} & H_{7v6c} & H_{7v8v} & H_{7v7v} \end{pmatrix}, \tag{10}$$

where

$$H_{8c8c} = \begin{pmatrix} E'_g+\Delta' & 0 & 0 & 0 \\ 0 & E'_g+\Delta' & 0 & 0 \\ 0 & 0 & E'_g+\Delta' & 0 \\ 0 & 0 & 0 & E'_g+\Delta' \end{pmatrix}, \quad H_{8c7c} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix},$$

$$H_{8c6c} = \begin{pmatrix} \sqrt{\frac{1}{2}}iP'k_- & 0 \\ -\sqrt{\frac{2}{3}}iP'k_z & \sqrt{\frac{1}{6}}iP'k_- \\ -\sqrt{\frac{1}{6}}iP'k_+ & -\sqrt{\frac{2}{3}}iP'k_z \\ 0 & -\sqrt{\frac{1}{2}}iP'k_+ \end{pmatrix}, \quad H_{8c8v} = \begin{pmatrix} \frac{i\bar{\Delta}}{3} & \sqrt{\frac{1}{3}}iQk_+ & \sqrt{\frac{1}{3}}iQk_z & 0 \\ -\sqrt{\frac{1}{3}}iQk_- & \frac{i\bar{\Delta}}{3} & 0 & \sqrt{\frac{1}{3}}iQk_z \\ -\sqrt{\frac{1}{3}}iQk_z & 0 & \frac{i\bar{\Delta}}{3} & -\sqrt{\frac{1}{3}}iQk_+ \\ 0 & -\sqrt{\frac{1}{3}}iQk_z & \sqrt{\frac{1}{3}}iQk_- & \frac{i\bar{\Delta}}{3} \end{pmatrix},$$

$$H_{8c7v} = \begin{pmatrix} -\sqrt{\frac{1}{6}}iQk_+ & -\sqrt{\frac{2}{3}}iQk_z \\ 0 & \sqrt{\frac{1}{2}}iQk_+ \\ -\sqrt{\frac{1}{2}}iQk_- & 0 \\ -\sqrt{\frac{2}{3}}iQk_z & \sqrt{\frac{1}{6}}iQk_- \end{pmatrix}, \quad H_{7c7c} = \begin{pmatrix} E'_g & 0 \\ 0 & E'_g \end{pmatrix}, \quad H_{7c6c} = \begin{pmatrix} \sqrt{\frac{1}{3}}iP'k_z & \sqrt{\frac{1}{3}}iP'k_- \\ \sqrt{\frac{1}{3}}iP'k_+ & -\sqrt{\frac{1}{3}}iP'k_z \end{pmatrix},$$

$$H_{7c8v} = \begin{pmatrix} \sqrt{\frac{1}{6}}iQk_- & 0 & \sqrt{\frac{1}{2}}iQk_+ & \sqrt{\frac{2}{3}}iQk_z \\ \sqrt{\frac{2}{3}}iQk_z & -\sqrt{\frac{1}{2}}iQk_- & 0 & -\sqrt{\frac{1}{6}}iQk_+ \end{pmatrix}, \quad H_{7c7v} = \begin{pmatrix} -\frac{2}{3}i\bar{\Delta} & 0 \\ 0 & -\frac{2}{3}i\bar{\Delta} \end{pmatrix},$$

$$H_{6c6c} = \begin{pmatrix} E_g+\frac{\hbar^2k^2}{2m_0} & 0 \\ 0 & E_g+\frac{\hbar^2k^2}{2m_0} \end{pmatrix}, \quad H_{6c8v} = \begin{pmatrix} -\sqrt{\frac{1}{2}}Pk_+ & \sqrt{\frac{2}{3}}Pk_z & \sqrt{\frac{1}{6}}Pk_- & 0 \\ 0 & -\sqrt{\frac{1}{6}}Pk_+ & \sqrt{\frac{2}{3}}Pk_z & \sqrt{\frac{1}{2}}Pk_- \end{pmatrix},$$

$$H_{6c7v} = \begin{pmatrix} -\sqrt{\frac{1}{3}}Pk_z & -\sqrt{\frac{1}{3}}Pk_- \\ -\sqrt{\frac{1}{3}}Pk_+ & \sqrt{\frac{1}{3}}Pk_z \end{pmatrix}, \quad H_{8v8v} = \begin{pmatrix} \frac{\hbar^2k^2}{2m_0} & -\frac{1}{2}C_kk_+ & C_kk_z & -\frac{\sqrt{3}}{2}C_kk_- \\ -\frac{1}{2}C_kk_- & \frac{\hbar^2k^2}{2m_0} & \frac{\sqrt{3}}{2}C_kk_+ & -C_kk_z \\ C_kk_z & \frac{\sqrt{3}}{2}C_kk_- & \frac{\hbar^2k^2}{2m_0} & -\frac{1}{2}C_kk_+ \\ -\frac{\sqrt{3}}{2}C_kk_+ & -C_kk_z & -\frac{1}{2}C_kk_- & \frac{\hbar^2k^2}{2m_0} \end{pmatrix},$$

$$H_{8v7v} = \begin{pmatrix} \frac{1}{2\sqrt{2}}C_kk_- & \sqrt{\frac{1}{2}}C_kk_z \\ 0 & -\frac{\sqrt{3}}{2\sqrt{2}}C_kk_+ \\ \frac{\sqrt{3}}{2\sqrt{2}}C_kk_- & 0 \\ \sqrt{\frac{1}{2}}C_kk_z & -\frac{1}{2\sqrt{2}}C_kk_- \end{pmatrix}, \quad H_{7v7v} = \begin{pmatrix} \frac{\hbar^2k^2}{2m_0} - \Delta & 0 \\ 0 & \frac{\hbar^2k^2}{2m_0} - \Delta \end{pmatrix},$$

with $k^2 = k_x^2 + k_y^2 + k_z^2$ and $k_\pm = k_x \pm ik_y$. Parameters E_g, E_g', Δ, Δ', $\bar{\Delta}$, P, P', Q, and C_k are elementary parameters of the "bare" fourteen-band model.

The remote-band contributions are included by introducing electron effective masses. To the second order in perturbation theory, the Hamiltonian blocks H_{6c6c}, H_{8v8v}, H_{8v7v}, and H_{7v7v} become

$$H_{6c6c} = \begin{pmatrix} E_g + \frac{\hbar^2k^2}{2m'} & 0 \\ 0 & E_g + \frac{\hbar^2k^2}{2m'} \end{pmatrix},$$

$$H_{8v8v} = \left(\begin{array}{c|c|c|c} -\frac{\hbar^2(\gamma_1'+\gamma_2')(k_x^2+k_y^2)}{2m_0} & \frac{2\sqrt{3}\hbar^2\gamma_3'k_-k_z}{2m_0} & \frac{\sqrt{3}\hbar^2\gamma_2'(k_x^2-k_y^2)}{2m_0} & -\frac{\sqrt{3}}{2}C_kk_- \\ -\frac{\hbar^2(\gamma_1'-2\gamma_2')k_z^2}{2m_0} & -\frac{1}{2}C_kk_+ & -\frac{2\sqrt{3}i\hbar^2\gamma_3'k_xk_y}{2m_0} & \\ & & +C_kk_z & \\ \hline \frac{2\sqrt{3}\hbar^2\gamma_3'k_+k_z}{2m_0} & -\frac{\hbar^2(\gamma_1'-\gamma_2')(k_x^2+k_y^2)}{2m_0} & \frac{\sqrt{3}}{2}C_kk_+ & \frac{\sqrt{3}\hbar^2\gamma_2'(k_x^2-k_y^2)}{2m_0} \\ -\frac{1}{2}C_kk_- & -\frac{\hbar^2(\gamma_1'+2\gamma_2')k_z^2}{2m_0} & & -\frac{2\sqrt{3}i\hbar^2\gamma_3'k_xk_y}{2m_0} \\ & & & -C_kk_z \\ \hline \frac{\sqrt{3}\hbar^2\gamma_2'(k_x^2-k_y^2)}{2m_0} & \frac{\sqrt{3}}{2}C_kk_- & -\frac{\hbar^2(\gamma_1'-\gamma_2')(k_x^2+k_y^2)}{2m_0} & -\frac{2\sqrt{3}\hbar^2\gamma_3'k_-k_z}{2m_0} \\ +\frac{2\sqrt{3}i\hbar^2\gamma_3'k_xk_y}{2m_0} & & -\frac{\hbar^2(\gamma_1'+2\gamma_2')k_z^2}{2m_0} & -\frac{1}{2}C_kk_+ \\ +C_kk_z & & & \\ \hline -\frac{\sqrt{3}}{2}C_kk_+ & \frac{\sqrt{3}\hbar^2\gamma_2'(k_x^2-k_y^2)}{2m_0} & -\frac{2\sqrt{3}\hbar^2\gamma_3'k_+k_z}{2m_0} & -\frac{\hbar^2(\gamma_1'+\gamma_2')(k_x^2+k_y^2)}{2m_0} \\ & +\frac{2\sqrt{3}i\hbar^2\gamma_3'k_xk_y}{2m_0} & -\frac{1}{2}C_kk_- & -\frac{\hbar^2(\gamma_1'-2\gamma_2')k_z^2}{2m_0} \\ & -C_kk_z & & \end{array}\right),$$

$$H_{8v7v} = \begin{pmatrix} -\frac{\sqrt{6}\hbar^2}{2m_0}\gamma_3'k_-k_z + \frac{1}{2\sqrt{2}}C_kk_- & -\frac{\sqrt{6}\hbar^2}{2m_0}\left(\gamma_2'(k_x^2-k_y^2) - 2i\gamma_3'k_xk_y\right) + \sqrt{\frac{1}{2}}C_kk_z \\ -\frac{\sqrt{2}\hbar^2}{2m_0}\gamma_3'(k_x^2+k_y^2-2k_z^2) & \frac{3\sqrt{2}\hbar^2}{2m_0}\gamma_3'k_-k_z - \frac{\sqrt{3}}{2\sqrt{2}}C_kk_+ \\ \frac{3\sqrt{2}\hbar^2}{2m_0}\gamma_3'k_+k_z + \frac{\sqrt{3}}{2\sqrt{2}}C_kk_- & \frac{\sqrt{2}\hbar^2}{2m_0}\gamma_3'(k_x^2+k_y^2-2k_z^2) \\ \frac{\sqrt{6}\hbar^2}{2m_0}\left(\gamma_2'(k_x^2-k_y^2) + 2i\gamma_3'k_xk_y\right) + \sqrt{\frac{1}{2}}C_kk_z & -\frac{\sqrt{6}\hbar^2}{2m_0}\gamma_3'k_+k_z - \frac{1}{2\sqrt{2}}C_kk_- \end{pmatrix},$$

and

$$H_{7v7v} = \begin{pmatrix} -\frac{\hbar^2k^2}{2m_0}\gamma_1' - \Delta & 0 \\ 0 & -\frac{\hbar^2k^2}{2m_0}\gamma_1' - \Delta \end{pmatrix},$$

respectively. Here, m' is electron effective mass and $\gamma_{1,2,3}'$ are modified Luttinger parameters. These parameters account for remote-band effects. Their explicit expressions are given in Section 4. Note that, without remote-band contributions we have $m' = m_0$, $\gamma_1' = -1$, and $\gamma_2' = \gamma_3' = 0$.

3 Euler rotation

In Section 2 we used the coordinate system in which x-, y-, and z-axes are along to crystal directions [100], [010], and [001], respectively. One can change the coordinate system by applying Euler's rotations for the referred frame [4]. Here, we perform rotations around axes z-y-z by angles α-β-γ.

For the wave vector $\mathbf{k}$, the rotation operator is

$$\begin{aligned} R &= R_z(\alpha)R_y(\beta)R_z(\gamma) \\ &= \begin{pmatrix} \cos(\alpha) & -\sin(\alpha) & 0 \\ \sin(\alpha) & \cos(\alpha) & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos(\beta) & 0 & \sin(\beta) \\ 0 & 1 & 0 \\ -\sin(\beta) & 0 & \cos(\beta) \end{pmatrix} \begin{pmatrix} \cos(\gamma) & -\sin(\gamma) & 0 \\ \sin(\gamma) & \cos(\gamma) & 0 \\ 0 & 0 & 1 \end{pmatrix}. \end{aligned} \tag{11}$$

Old and new components of vector $\mathbf{k}$ are related via the transformation

$$\begin{pmatrix} k_x \\ k_y \\ k_z \end{pmatrix} = R \begin{pmatrix} \tilde{k}_x \\ \tilde{k}_y \\ \tilde{k}_z \end{pmatrix}. \tag{12}$$

For angular momentum vectors with $j = 1/2$ and $j = 3/2$, the rotation operators are

$$D_{1/2} = \begin{pmatrix} \exp(-i\frac{\alpha}{2}) & 0 \\ 0 & \exp(i\frac{\alpha}{2}) \end{pmatrix} \begin{pmatrix} \cos(\frac{\beta}{2}) & -\sin(\frac{\beta}{2}) \\ \sin(\frac{\beta}{2}) & \cos(\frac{\beta}{2}) \end{pmatrix} \begin{pmatrix} \exp(-i\frac{\gamma}{2}) & 0 \\ 0 & \exp(i\frac{\gamma}{2}) \end{pmatrix} \tag{13}$$

and

$$\begin{aligned} D_{3/2} &= \begin{pmatrix} \exp(-i\frac{3}{2}\alpha) & 0 & 0 & 0 \\ 0 & \exp(-i\frac{1}{2}\alpha) & 0 & 0 \\ 0 & 0 & \exp(i\frac{1}{2}\alpha) & 0 \\ 0 & 0 & 0 & \exp(i\frac{3}{2}\alpha) \end{pmatrix} \\ &\times \begin{pmatrix} \cos^3(\frac{\beta}{2}) & -\sqrt{3}\cos^2(\frac{\beta}{2})\sin(\frac{\beta}{2}) & \sqrt{3}\cos(\frac{\beta}{2})\sin^2(\frac{\beta}{2}) & -\sin^3(\frac{\beta}{2}) \\ \sqrt{3}\cos^2(\frac{\beta}{2})\sin(\frac{\beta}{2}) & \cos^3(\frac{\beta}{2}) - 2\cos(\frac{\beta}{2})\sin^2(\frac{\beta}{2}) & -2\cos^2(\frac{\beta}{2})\sin(\frac{\beta}{2}) + \sin^3(\frac{\beta}{2}) & \sqrt{3}\cos(\frac{\beta}{2})\sin^2(\frac{\beta}{2}) \\ \sqrt{3}\cos(\frac{\beta}{2})\sin^2(\frac{\beta}{2}) & 2\cos^2(\frac{\beta}{2})\sin(\frac{\beta}{2}) - \sin^3(\frac{\beta}{2}) & \cos^3(\frac{\beta}{2}) - 2\cos(\frac{\beta}{2})\sin^2(\frac{\beta}{2}) & -\sqrt{3}\cos^2(\frac{\beta}{2})\sin(\frac{\beta}{2}) \\ \sin^3(\frac{\beta}{2}) & \sqrt{3}\cos(\frac{\beta}{2})\sin^2(\frac{\beta}{2}) & \sqrt{3}\cos^2(\frac{\beta}{2})\sin(\frac{\beta}{2}) & \cos^3(\frac{\beta}{2}) \end{pmatrix} \\ &\times \begin{pmatrix} \exp(-i\frac{3}{2}\gamma) & 0 & 0 & 0 \\ 0 & \exp(-i\frac{1}{2}\gamma) & 0 & 0 \\ 0 & 0 & \exp(i\frac{1}{2}\gamma) & 0 \\ 0 & 0 & 0 & \exp(i\frac{3}{2}\gamma) \end{pmatrix}, \end{aligned} \tag{14}$$

respectively.

Hamiltonian in the new coordinate system can be obtained by

$$\begin{aligned} \tilde{H}_{14\times14} &= \begin{pmatrix} \tilde{H}_{8c8c} & \tilde{H}_{8c7c} & \tilde{H}_{8c6c} & \tilde{H}_{8c8v} & \tilde{H}_{8c7v} \\ \tilde{H}_{7c8c} & \tilde{H}_{7c7c} & \tilde{H}_{7c6c} & \tilde{H}_{7c8v} & \tilde{H}_{7c7v} \\ \tilde{H}_{6c8c} & \tilde{H}_{6c7c} & \tilde{H}_{6c6c} & \tilde{H}_{6c8v} & \tilde{H}_{6c7v} \\ \tilde{H}_{8v8c} & \tilde{H}_{8v7c} & \tilde{H}_{8v6c} & \tilde{H}_{8v8v} & \tilde{H}_{8v7v} \\ \tilde{H}_{7v8c} & \tilde{H}_{7v7c} & \tilde{H}_{7v6c} & \tilde{H}_{7v8v} & \tilde{H}_{7v7v} \end{pmatrix} \\ &= \begin{pmatrix} D^\dagger_{3/2}H_{8c8c}D_{3/2} & D^\dagger_{3/2}H_{8c7c}D_{1/2} & D^\dagger_{3/2}H_{8c6c}D_{1/2} & D^\dagger_{3/2}H_{8c8v}D_{3/2} & D^\dagger_{3/2}H_{8c7v}D_{1/2} \\ D^\dagger_{1/2}H_{7c8c}D_{3/2} & D^\dagger_{1/2}H_{7c7c}D_{1/2} & D^\dagger_{1/2}H_{7c6c}D_{1/2} & D^\dagger_{1/2}H_{7c8v}D_{3/2} & D^\dagger_{1/2}H_{7c7v}D_{1/2} \\ D^\dagger_{1/2}H_{6c8c}D_{3/2} & D^\dagger_{1/2}H_{6c7c}D_{1/2} & D^\dagger_{1/2}H_{6c6c}D_{1/2} & D^\dagger_{1/2}H_{6c8v}D_{3/2} & D^\dagger_{1/2}H_{6c7v}D_{1/2} \\ D^\dagger_{3/2}H_{8v8c}D_{3/2} & D^\dagger_{3/2}H_{8v7c}D_{1/2} & D^\dagger_{3/2}H_{8v6c}D_{1/2} & D^\dagger_{3/2}H_{8v8v}D_{3/2} & D^\dagger_{3/2}H_{8v7v}D_{1/2} \\ D^\dagger_{1/2}H_{7v8c}D_{3/2} & D^\dagger_{1/2}H_{7v7c}D_{1/2} & D^\dagger_{1/2}H_{7v6c}D_{1/2} & D^\dagger_{1/2}H_{7v8v}D_{3/2} & D^\dagger_{1/2}H_{7v7v}D_{1/2} \end{pmatrix}. \end{aligned} \tag{15}$$

We carry out the rotations with Euler angles $\alpha = \pi/4$, $\beta = \pi/2$, and $\gamma = 0$. The new coordinate system has axes $x \parallel [00\bar{1}]$, $y \parallel [\bar{1}10]$, and $z \parallel [110]$. The Hamiltonian matrices in this case read

$$\tilde{H}_{8c8c} = \begin{pmatrix} E'_g + \Delta' & 0 & 0 & 0 \\ 0 & E'_g + \Delta' & 0 & 0 \\ 0 & 0 & E'_g + \Delta' & 0 \\ 0 & 0 & 0 & E'_g + \Delta' \end{pmatrix}, \quad \tilde{H}_{8c7c} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix},$$

$$\tilde{H}_{8c6c}=\begin{pmatrix}\sqrt{\frac{1}{2}}iP'\tilde{k}_- & 0\\ -\sqrt{\frac{2}{3}}iP'\tilde{k}_z & \sqrt{\frac{1}{6}}iP'\tilde{k}_-\\ -\sqrt{\frac{1}{6}}iP'\tilde{k}_+ & -\sqrt{\frac{2}{3}}iP'\tilde{k}_z\\ 0 & -\sqrt{\frac{1}{2}}iP'\tilde{k}_+\end{pmatrix},\ \tilde{H}_{8c8v}=\begin{pmatrix}\frac{Q\tilde{k}_x}{2}+\frac{i\bar{\Delta}}{3} & \sqrt{\frac{1}{3}}Q\tilde{k}_z & \frac{Q(\tilde{k}_x+2i\tilde{k}_y)}{2\sqrt{3}} & 0\\ \sqrt{\frac{1}{3}}Q\tilde{k}_z & -\frac{Q\tilde{k}_x}{2}+\frac{i\bar{\Delta}}{3} & 0 & \frac{Q(\tilde{k}_x+2i\tilde{k}_y)}{2\sqrt{3}}\\ \frac{Q(\tilde{k}_x-2i\tilde{k}_y)}{2\sqrt{3}} & 0 & -\frac{Q\tilde{k}_x}{2}+\frac{i\bar{\Delta}}{3} & -\sqrt{\frac{1}{3}}Q\tilde{k}_z\\ 0 & \frac{Q(\tilde{k}_x-2i\tilde{k}_y)}{2\sqrt{3}} & -\sqrt{\frac{1}{3}}Q\tilde{k}_z & \frac{Q\tilde{k}_x}{2}+\frac{i\bar{\Delta}}{3}\end{pmatrix},$$

$$\tilde{H}_{8c7v}=\begin{pmatrix}-\sqrt{\frac{1}{6}}Q\tilde{k}_z & -\frac{Q(\tilde{k}_x+2i\tilde{k}_y)}{\sqrt{6}}\\ \sqrt{\frac{1}{2}}Q\tilde{k}_x & \sqrt{\frac{1}{2}}Q\tilde{k}_z\\ \sqrt{\frac{1}{2}}Q\tilde{k}_z & -\sqrt{\frac{1}{2}}Q\tilde{k}_x\\ \frac{Q(\tilde{k}_x-2i\tilde{k}_y)}{\sqrt{6}} & -\sqrt{\frac{1}{6}}Q\tilde{k}_z\end{pmatrix},\quad \tilde{H}_{7c7c}=\begin{pmatrix}E'_g & 0\\ 0 & E'_g\end{pmatrix},\quad \tilde{H}_{7c6c}=\begin{pmatrix}\sqrt{\frac{1}{3}}iP'\tilde{k}_z & \sqrt{\frac{1}{3}}iP'\tilde{k}_-\\ \sqrt{\frac{1}{3}}iP'\tilde{k}_+ & -\sqrt{\frac{1}{3}}iP'\tilde{k}_z\end{pmatrix},$$

$$\tilde{H}_{7c8v}=\begin{pmatrix}-\sqrt{\frac{1}{6}}Q\tilde{k}_z & \sqrt{\frac{1}{2}}Q\tilde{k}_x & \sqrt{\frac{1}{2}}Q\tilde{k}_z & \sqrt{\frac{1}{6}}Q(\tilde{k}_x+2i\tilde{k}_y)\\ -\sqrt{\frac{1}{6}}Q(\tilde{k}_x-2i\tilde{k}_y) & \sqrt{\frac{1}{2}}Q\tilde{k}_z & -\sqrt{\frac{1}{2}}Q\tilde{k}_x & -\sqrt{\frac{1}{6}}Q\tilde{k}_z\end{pmatrix},\ \tilde{H}_{7c7v}=\begin{pmatrix}-\frac{2}{3}i\bar{\Delta} & 0\\ 0 & -\frac{2}{3}i\bar{\Delta}\end{pmatrix},$$

$$\tilde{H}_{6c6c}=\begin{pmatrix}E_g+\frac{\hbar^2\tilde{k}^2}{2m'} & 0\\ 0 & E_g+\frac{\hbar^2\tilde{k}^2}{2m'}\end{pmatrix},\ \tilde{H}_{6c8v}=\begin{pmatrix}-\sqrt{\frac{1}{2}}P\tilde{k}_+ & -\sqrt{\frac{2}{3}}P\tilde{k}_z & \sqrt{\frac{1}{6}}P\tilde{k}_- & 0\\ 0 & -\sqrt{\frac{1}{6}}P\tilde{k}_+ & \sqrt{\frac{2}{3}}P\tilde{k}_z & \sqrt{\frac{1}{2}}P\tilde{k}_-\end{pmatrix},$$

$$\tilde{H}_{6c7v}=\begin{pmatrix}-\sqrt{\frac{1}{3}}P\tilde{k}_z & -\sqrt{\frac{1}{3}}P\tilde{k}_-\\ -\sqrt{\frac{1}{3}}P\tilde{k}_+ & \sqrt{\frac{1}{3}}P\tilde{k}_z\end{pmatrix},$$

$$\tilde{H}_{8v8v}=\left(\begin{array}{c|c|c|c}
\begin{array}{c}-\frac{\hbar^2(\gamma'_1+\gamma'_2)\tilde{k}_x^2}{2m_0}\\ -\frac{\hbar^2(2\gamma'_1-\gamma'_2+3\gamma'_3)\tilde{k}_y^2}{4m_0}\\ -\frac{\hbar^2(2\gamma'_1-\gamma'_2-3\gamma'_3)\tilde{k}_z^2}{4m_0}\\ -\frac{\sqrt{3}}{4}C_k\tilde{k}_y\end{array} & \begin{array}{c}\frac{2\sqrt{3}\hbar^2(\gamma'_3\tilde{k}_x-i\gamma'_2\tilde{k}_y)\tilde{k}_z}{2m_0}\\ -\frac{i}{4}C_k\tilde{k}_z\end{array} & \begin{array}{c}\frac{\sqrt{3}\hbar^2\gamma'_2\tilde{k}_x^2}{2m_0}\\ -\frac{\sqrt{3}\hbar^2(\gamma'_2+\gamma'_3)\tilde{k}_y^2}{4m_0}\\ -\frac{\sqrt{3}\hbar^2(\gamma'_2-\gamma'_3)\tilde{k}_z^2}{4m_0}\\ -\frac{2\sqrt{3}i\hbar^2\gamma'_3\tilde{k}_x\tilde{k}_y}{2m_0}\\ +\frac{1}{4}C_k(\tilde{k}_y+4i\tilde{k}_x)\end{array} & -\frac{3\sqrt{3}}{4}iC_k\tilde{k}_z\\ \hline
\begin{array}{c}\frac{2\sqrt{3}\hbar^2(\gamma'_3\tilde{k}_x+i\gamma'_2\tilde{k}_y)\tilde{k}_z}{2m_0}\\ +\frac{i}{4}C_k\tilde{k}_z\end{array} & \begin{array}{c}-\frac{\hbar^2(\gamma'_1-\gamma'_2)\tilde{k}_x^2}{2m_0}\\ -\frac{\hbar^2(2\gamma'_1+\gamma'_2-3\gamma'_3)\tilde{k}_y^2}{4m_0}\\ -\frac{\hbar^2(2\gamma'_1+\gamma'_2+3\gamma'_3)\tilde{k}_z^2}{4m_0}\\ +\frac{3\sqrt{3}}{4}C_k\tilde{k}_y\end{array} & \frac{\sqrt{3}}{4}iC_k\tilde{k}_z & \begin{array}{c}\frac{\sqrt{3}\hbar^2\gamma'_2\tilde{k}_x^2}{2m_0}\\ -\frac{\sqrt{3}\hbar^2(\gamma'_2+\gamma'_3)\tilde{k}_y^2}{4m_0}\\ -\frac{\sqrt{3}\hbar^2(\gamma'_2-\gamma'_3)\tilde{k}_z^2}{4m_0}\\ -\frac{2\sqrt{3}i\hbar^2\gamma'_3\tilde{k}_x\tilde{k}_y}{2m_0}\\ -\frac{1}{4}C_k(\tilde{k}_y+4i\tilde{k}_x)\end{array}\\ \hline
\begin{array}{c}\frac{\sqrt{3}\hbar^2\gamma'_2\tilde{k}_x^2}{2m_0}\\ -\frac{\sqrt{3}\hbar^2(\gamma'_2+\gamma'_3)\tilde{k}_y^2}{4m_0}\\ -\frac{\sqrt{3}\hbar^2(\gamma'_2-\gamma'_3)\tilde{k}_z^2}{4m_0}\\ +\frac{2\sqrt{3}i\hbar^2\gamma'_3\tilde{k}_x\tilde{k}_y}{2m_0}\\ +\frac{1}{4}C_k(\tilde{k}_y-4i\tilde{k}_x)\end{array} & -\frac{\sqrt{3}}{4}iC_k\tilde{k}_z & \begin{array}{c}-\frac{\hbar^2(\gamma'_1-\gamma'_2)\tilde{k}_x^2}{2m_0}\\ -\frac{\hbar^2(2\gamma'_1+\gamma'_2-3\gamma'_3)\tilde{k}_y^2}{4m_0}\\ -\frac{\hbar^2(2\gamma'_1+\gamma'_2+3\gamma'_3)\tilde{k}_z^2}{4m_0}\\ -\frac{3\sqrt{3}}{4}C_k\tilde{k}_y\end{array} & \begin{array}{c}-\frac{2\sqrt{3}\hbar^2(\gamma'_3\tilde{k}_x-i\gamma'_2\tilde{k}_y)\tilde{k}_z}{2m_0}\\ -\frac{i}{4}C_k\tilde{k}_z\end{array}\\ \hline
\frac{3\sqrt{3}}{4}iC_k\tilde{k}_z & \begin{array}{c}\frac{\sqrt{3}\hbar^2\gamma'_2\tilde{k}_x^2}{2m_0}\\ -\frac{\sqrt{3}\hbar^2(\gamma'_2+\gamma'_3)\tilde{k}_y^2}{4m_0}\\ -\frac{\sqrt{3}\hbar^2(\gamma'_2-\gamma'_3)\tilde{k}_z^2}{4m_0}\\ +\frac{2\sqrt{3}i\hbar^2\gamma'_3\tilde{k}_x\tilde{k}_y}{2m_0}\\ -\frac{1}{4}C_k(\tilde{k}_y-4i\tilde{k}_x)\end{array} & \begin{array}{c}-\frac{2\sqrt{3}\hbar^2(\gamma'_3\tilde{k}_x+i\gamma'_2\tilde{k}_y)\tilde{k}_z}{2m_0}\\ +\frac{i}{4}C_k\tilde{k}_z\end{array} & \begin{array}{c}-\frac{\hbar^2(\gamma'_1+\gamma'_2)\tilde{k}_x^2}{2m_0}\\ -\frac{\hbar^2(2\gamma'_1-\gamma'_2+3\gamma'_3)\tilde{k}_y^2}{4m_0}\\ -\frac{\hbar^2(2\gamma'_1-\gamma'_2-3\gamma'_3)\tilde{k}_z^2}{4m_0}\\ +\frac{\sqrt{3}}{4}C_k\tilde{k}_y\end{array}
\end{array}\right),$$

$$\tilde{H}_{8v7v} = \left(\begin{array}{c|c} -\frac{\sqrt{6}\hbar^2(\gamma_3'\tilde{k}_x - i\gamma' - 2\tilde{k}_y)\tilde{k}_z}{2m_0} - \frac{iC_k\tilde{k}_z}{2\sqrt{2}} & -\frac{\sqrt{6}\hbar^2\left(2\gamma_2'\tilde{k}_x^2 - (\gamma_2'+\gamma_3')\tilde{k}_y^2 - (\gamma_2'-\gamma_3')\tilde{k}_z^2 - 4i\gamma_3'\tilde{k}_x\tilde{k}_y\right)}{4m_0} + \frac{C_k(2\tilde{k}_y - i\tilde{k}_x)}{2\sqrt{2}} \\ \hline -\frac{\hbar^2\left(2\gamma_2'\tilde{k}_x^2 - (\gamma_2'-3\gamma_3')\tilde{k}_y^2 - (\gamma_2'+3\gamma_3')\tilde{k}_z^2\right)}{2\sqrt{2}m_0} + \frac{\sqrt{3}iC_k\tilde{k}_x}{2\sqrt{2}} & \frac{3\sqrt{2}\hbar^2(\gamma_3'\tilde{k}_x - i\gamma_2'\tilde{k}_y)\tilde{k}_z}{2m_0} + \frac{\sqrt{3}iC_k\tilde{k}_z}{2\sqrt{2}} \\ \hline \frac{3\sqrt{2}\hbar^2(\gamma_3'\tilde{k}_x + i\gamma_2'\tilde{k}_y)\tilde{k}_z}{2m_0} + \frac{\sqrt{3}iC_k\tilde{k}_z}{2\sqrt{2}} & \frac{\hbar^2\left(2\gamma_2'\tilde{k}_x^2 - (\gamma_2'-3\gamma_3')\tilde{k}_y^2 - (\gamma_2'+3\gamma_3')\tilde{k}_z^2\right)}{2\sqrt{2}m_0} - \frac{\sqrt{3}iC_k\tilde{k}_x}{2\sqrt{2}} \\ \hline \frac{\sqrt{6}\hbar^2\left(2\gamma_2'\tilde{k}_x^2 - (\gamma_2'+\gamma_3')\tilde{k}_y^2 - (\gamma_2'-\gamma_3')\tilde{k}_z^2 + 4i\gamma_3'\tilde{k}_x\tilde{k}_y\right)}{4m_0} + \frac{C_k(2\tilde{k}_y + i\tilde{k}_x)}{2\sqrt{2}} & -\frac{\sqrt{6}\hbar^2(\gamma_3'\tilde{k}_x + i\gamma' - 2\tilde{k}_y)\tilde{k}_z}{2m_0} - \frac{iC_k\tilde{k}_z}{2\sqrt{2}} \end{array}\right),$$

$$\tilde{H}_{7v7v} = \begin{pmatrix} -\frac{\hbar^2\tilde{k}^2}{2m_0}\gamma_1' - \Delta & 0 \\ 0 & -\frac{\hbar^2\tilde{k}^2}{2m_0}\gamma_1' - \Delta \end{pmatrix}.$$

4 Löwdin perturbation approach

The Hamiltonian matrix H can be expressed as a sum of two parts: the diagonal part H^0 and the off-diagonal H'

$$H = H^0 + H', \tag{16}$$

in which H' is regarded as a perturbation. Since the ordinary perturbation theory does not work properly for degenerate systems one needs some further treatments. One assumes that the basis set can be divided into weakly interacting subsets A and B in which one is interested only in the subset A. The interactions between A and B are treated by perturbation theory. To avoid singularities due to the degenerate of states that may appear in perturbation calculations, the subsets A and B always be chosen such that they are separated in energy. The resulting Hamiltonian for subset A in the perturbation approximation is given by [2]

$$\breve{H}_A = H^{(0)} + H^{(1)} + H^{(2)} + H^{(3)} + H^{(4)} + \dots\,, \tag{17}$$

where

$$\begin{aligned}
H^{(0)}_{ii'} &= H^0_{ii'}\,,\\
H^{(1)}_{ii'} &= H'_{ii'}\,,\\
H^{(2)}_{ii'} &= \frac{1}{2}\sum_n H'_{in}H'_{ni'}\left[\frac{1}{E_i^0 - E_n^0} + \frac{1}{E_{i'}^0 - E_n^0}\right]\,,\\
H^{(3)}_{ii'} &= -\frac{1}{2}\sum_{i'',n}\left[\frac{H'_{in}H'_{ni''}H'_{i''i'}}{(E_{i'}^0 - E_n^0)(E_{i''}^0 - E_n^0)} + \frac{H'_{ii''}H'_{i''n}H'_{ni'}}{(E_i^0 - E_n^0)(E_{i''}^0 - E_n^0)}\right]\,,\\
&\quad + \frac{1}{2}\sum_{n,n'} H'_{in}H'_{nn'}H'_{n'i'}\left[\frac{1}{(E_i^0 - E_n^0)(E_i^0 - E_{n'}^0)} + \frac{1}{(E_{i'}^0 - E_n^0)(E_{i'}^0 - E_{n'}^0)}\right],\\
H^{(4)}_{ii'} &= \frac{1}{2}\sum_{i'',i''',n}\frac{1}{(E_{i''}^0 - E_n^0)(E_{i'''}^0 - E_n^0)}\left[\frac{H'_{ii''}H'_{i''i'''}H'_{i'''n}H'_{ni'}}{E_i^0 - E_n^0} + \frac{H'_{in}H'_{ni''}H'_{i''i'''}H'_{i'''i'}}{E_{i'}^0 - E_n^0}\right]\\
&\quad - \frac{1}{2}\sum_{i'',n,n'}\left[\frac{H'_{in}H'_{nn'}H'_{n'i''}H'_{i''i'}}{(E_{i''}^0 - E_n^0)(E_{i'}^0 - E_{n'}^0)}\left(\frac{1}{E_{i''}^0 - E_n^0} + \frac{1}{E_{i'}^0 - E_{n'}^0}\right) + \frac{H'_{ii''}H'_{i''n}H'_{nn'}H'_{n'i'}}{(E_i^0 - E_{n'}^0)(E_{i''}^0 - E_n^0)}\left(\frac{1}{E_{i''}^0 - E_{n'}^0} + \frac{1}{E_i^0 - E_n^0}\right)\right]\\
&\quad - \frac{1}{24}\sum_{i'',n,n'} H'_{in}H'_{ni''}H'_{i''n'}H'_{n'i'}\left[\frac{8}{(E_i^0 - E_n^0)(E_i^0 - E_{n'}^0)(E_{i''}^0 - E_{n'}^0)} + \frac{8}{(E_{i'}^0 - E_n^0)(E_{i'}^0 - E_{n'}^0)(E_{i''}^0 - E_n^0)}\right.\\
&\qquad + \frac{4}{(E_i^0 - E_{n'}^0)(E_{i''}^0 - E_n^0)}\left(\frac{1}{E_i^0 - E_n^0} + \frac{1}{E_{i''}^0 - E_{n'}^0}\right) + \frac{4}{(E_{i'}^0 - E_n^0)(E_{i''}^0 - E_{n'}^0)}\left(\frac{1}{E_{i'}^0 - E_{n'}^0} + \frac{1}{E_{i''}^0 - E_n^0}\right)\\
&\qquad \left. - \frac{1}{(E_{i''}^0 - E_n^0)(E_{i''}^0 - E_{n'}^0)}\left(\frac{1}{E_i^0 - E_n^0} + \frac{1}{E_{i'}^0 - E_{n'}^0}\right) - \frac{3}{(E_i^0 - E_n^0)(E_{i'}^0 - E_{n'}^0)}\left(\frac{1}{E_{i''}^0 - E_n^0} + \frac{1}{E_{i''}^0 - E_{n'}^0}\right)\right]\\
&\quad + \frac{1}{2}\sum_{n,n',n''} H'_{in}H'_{nn'}H'_{n'n''}H'_{n''i'}\left[\frac{1}{(E_i^0 - E_n^0)(E_i^0 - E_{n'}^0)(E_i^0 - E_{n''}^0)} + \frac{1}{(E_{i'}^0 - E_n^0)(E_{i'}^0 - E_{n'}^0)(E_{i'}^0 - E_{n''}^0)}\right],
\end{aligned} \tag{18}$$

with $i, i', i'', i''' \in A$ and $n, n', n'' \in B$.

By choosing the subset A consisting of two anti-bonding s-like conduction band states and applying the perturbation expansion up to third order, one obtains the reduced Hamiltonian for the conduction band

$$\breve{H}_{2\times 2} = H^{m^*}_{2\times 2} + H^{D}_{2\times 2}, \tag{19}$$

where $H^{m^*}_{2\times 2}$ contains k^2 terms and $H^{D}_{2\times 2}$ contains k^3 terms which describes the Dresselhaus spin-splitting in bulk inversion asymmetric materials.

For both coordinate systems with $z \parallel [001]$ and $z \parallel [001]$, $H^{m^*}_{2\times 2}$ has the form

$$H^{m^*}_{2\times 2} = \begin{pmatrix} E_g + \frac{\hbar^2 k^2}{2m^*} & 0 \\ 0 & E_g + \frac{\hbar^2 k^2}{2m^*} \end{pmatrix}, \tag{20}$$

where

$$\frac{m_0}{m^*} = \frac{m_0}{m'} + \frac{2m_0}{3\hbar^2}\left[P^2\left(\frac{2}{E_g} + \frac{1}{E_g+\Delta}\right) + P'^2\left(\frac{1}{E_g - E'_g} + \frac{2}{E_g - E'_g - \Delta'}\right) + \frac{4}{3}PP'\bar{\Delta}\left(\frac{1}{(E_g+\Delta)(E_g - E'_g)} - \frac{1}{E_g(E_g - E'_g - \Delta')}\right)\right]. \tag{21}$$

We identify m^* with electron effective mass measured by experiments (given in Table 1). Eq. (21) allows us to evaluate the value of m' from m^* and elementary parameters of the "bare" fourteen-band model.

The Dresselhaus term $H^{D}_{2\times 2}$ reads for the coordinate system with $z \parallel [001]$:

$$H^{D}_{2\times 2} = D^c \begin{pmatrix} (k_x^2 - k_y^2)k_z & -k_+ k_z^2 + ik_- k_x k_y \\ -k_- k_z^2 - ik_+ k_x k_y & -(k_x^2 - k_y^2)k_z \end{pmatrix} \tag{22}$$

and for the coordinate system with $z \parallel [110]$:

$$H^{D}_{2\times 2} = D^c \begin{pmatrix} \frac{1}{2}(2k_x^2 - k_y^2 + k_z^2)k_y & -\frac{i}{2}(2k_x^2 + k_y^2 - 4ik_x k_y - k_z^2)k_z \\ \frac{i}{2}(2k_x^2 + k_y^2 + 4ik_x k_y - k_z^2)k_z & -\frac{1}{2}(2k_x^2 - k_y^2 + k_z^2)k_y \end{pmatrix}, \tag{23}$$

where

$$D^c = \frac{4}{3}PP'Q\left(\frac{1}{(E_g+\Delta)(E_g - E'_g - \Delta')} - \frac{1}{E_g(E_g - E'_g)}\right). \tag{24}$$

Similarly, by choosing the subset A consisting of heavy and light hole states, the simplified Hamiltonian for the valence band in the third order of perturbation theory reads

$$\breve{H}_{4\times 4} = H^{L}_{4\times 4} + H^{D}_{4\times 4}. \tag{25}$$

The term $H^{L}_{4\times 4}$ is given for the coordinate system with $z \parallel [001]$ by:

$$H^{L}_{4\times 4} = \left(\begin{array}{c|c|c|c} -\frac{\hbar^2(\gamma_1+\gamma_2)(k_x^2+k_y^2)}{2m_0} & \frac{2\sqrt{3}\gamma_3 k_- k_z}{2m_0} & \frac{\sqrt{3}\hbar^2\gamma_2(k_x^2-k_y^2)}{2m_0} & -\frac{\sqrt{3}}{2}C_k k_- \\ -\frac{\hbar^2(\gamma_1-2\gamma_2)k_z^2}{2m_0} & -\frac{1}{2}C_k k_+ & -\frac{2\sqrt{2}i\hbar^2\gamma_3 k_x k_y}{2m_0} & \\ & & +C_k k_z & \\ \hline c.c. & -\frac{\hbar^2(\gamma_1-\gamma_2)(k_x^2+k_y^2)}{2m_0} & \frac{\sqrt{3}}{2}C_k k_+ & \frac{\sqrt{3}\hbar^2\gamma_2(k_x^2-k_y^2)}{2m_0} \\ & -\frac{\hbar^2(\gamma_1+2\gamma_2)k_z^2}{2m_0} & & -\frac{2\sqrt{2}i\hbar^2\gamma_3 k_x k_y}{2m_0} \\ & & & -C_k k_z \\ \hline c.c. & c.c. & -\frac{\hbar^2(\gamma_1-\gamma_2)(k_x^2+k_y^2)}{2m_0} & -\frac{2\sqrt{3}\gamma_3 k_- k_z}{2m_0} \\ & & -\frac{\hbar^2(\gamma_1+2\gamma_2)k_z^2}{2m_0} & -\frac{1}{2}C_k k_+ \\ \hline c.c. & c.c. & c.c. & -\frac{\hbar^2(\gamma_1+\gamma_2)(k_x^2+k_y^2)}{2m_0} \\ & & & -\frac{\hbar^2(\gamma_1-2\gamma_2)k_z^2}{2m_0} \end{array}\right), \tag{26}$$

and for the coordinate system with $z \parallel [110]$ by:

$$H^L_{4\times4} = \left(\begin{array}{c|c|c|c} \begin{array}{c} -\frac{\hbar^2(\gamma_1+\gamma_2)k_x^2}{2m_0} \\ -\frac{\hbar^2(2\gamma_1-\gamma_2+3\gamma_3)k_y^2}{4m_0} \\ -\frac{\hbar^2(2\gamma_1-\gamma_2-3\gamma_3)k_z^2}{4m_0} \\ -\frac{\sqrt{3}}{4}C_k k_y \end{array} & \begin{array}{c} \frac{2\sqrt{3}\hbar^2(\gamma_3 k_x - i\gamma_2 k_y)k_z}{2m_0} \\ -\frac{i}{4}C_k k_z \end{array} & \begin{array}{c} \frac{\sqrt{3}\hbar^2\gamma_2 k_x^2}{2m_0} \\ -\frac{\sqrt{3}\hbar^2(\gamma_2+\gamma_3)k_y^2}{4m_0} \\ -\frac{\sqrt{3}\hbar^2(\gamma_2-\gamma_3)k_z^2}{4m_0} \\ +\frac{C_k(k_y+4ik_x)}{4} \end{array} & -\frac{3\sqrt{3}}{4}iC_k k_z \\ \hline c.c. & \begin{array}{c} -\frac{\hbar^2(\gamma_1-\gamma_2)k_x^2}{2m_0} \\ -\frac{\hbar^2(2\gamma_1+\gamma_2-3\gamma_3)k_y^2}{4m_0} \\ -\frac{\hbar^2(2\gamma_1+\gamma_2+3\gamma_3)k_z^2}{4m_0} \\ +\frac{3\sqrt{3}}{4}C_k k_y \end{array} & -\frac{\sqrt{3}}{4}iC_k k_z & \begin{array}{c} \frac{\sqrt{3}\hbar^2\gamma_2 k_x^2}{2m_0} \\ -\frac{\sqrt{3}\hbar^2(\gamma_2+\gamma_3)k_y^2}{4m_0} \\ -\frac{\sqrt{3}\hbar^2(\gamma_2-\gamma_3)k_z^2}{4m_0} \\ -\frac{C_k(k_y+4ik_x)}{4} \end{array} \\ \hline c.c. & c.c. & \begin{array}{c} -\frac{\hbar^2(\gamma_1-\gamma_2)k_x^2}{2m_0} \\ -\frac{\hbar^2(2\gamma_1+\gamma_2-3\gamma_3)k_y^2}{4m_0} \\ -\frac{\hbar^2(2\gamma_1+\gamma_2+3\gamma_3)k_z^2}{4m_0} \\ -\frac{3\sqrt{3}}{4}C_k k_y \end{array} & -\frac{2\sqrt{3}\hbar^2(\gamma_3 k_x - i\gamma_2 k_y)k_z}{2m_0} \\ & & & -\frac{i}{4}C_k k_z \\ \hline c.c. & c.c. & c.c. & \begin{array}{c} -\frac{\hbar^2(\gamma_1+\gamma_2)k_x^2}{2m_0} \\ -\frac{\hbar^2(2\gamma_1-\gamma_2+3\gamma_3)k_y^2}{4m_0} \\ -\frac{\hbar^2(2\gamma_1-\gamma_2-3\gamma_3)k_z^2}{4m_0} \\ +\frac{\sqrt{3}}{4}C_k k_y \end{array} \end{array}\right), \quad (27)$$

where

$$\begin{aligned} \gamma_1 &= \gamma_1' + \frac{2m_0}{3\hbar^2}\left(\frac{P^2}{E_g} + \frac{Q^2}{E_g'} + \frac{Q^2}{E_g'+\Delta'} + \frac{2}{3}\frac{PP'\bar{\Delta}}{E_g(E_g'+\Delta')}\right), \\ \gamma_2 &= \gamma_2' + \frac{2m_0}{3\hbar^2}\left(\frac{1}{2}\frac{P^2}{E_g} - \frac{1}{2}\frac{Q^2}{E_g'} + \frac{1}{3}\frac{PP'\bar{\Delta}}{E_g(E_g'+\Delta')}\right), \\ \gamma_3 &= \gamma_3' + \frac{2m_0}{3\hbar^2}\left(\frac{1}{2}\frac{P^2}{E_g} + \frac{1}{2}\frac{Q^2}{E_g'} + \frac{1}{3}\frac{PP'\bar{\Delta}}{E_g(E_g'+\Delta')}\right). \end{aligned} \quad (28)$$

We indentify $\gamma_{1,2,3}$ with original Luttinger parameters (given in Table 1). From Eq. (28) we can evaluate $\gamma'_{1,2,3}$ via $\gamma_{1,2,3}$ and elementary parameters of "pure" fourteen-band model.

The Dresselhaus term $H^D_{4\times4}$ reads for the coordinate system with $z \parallel [001]$:

$$H^D_{4\times4} = \left(\begin{array}{c|c|c|c} \begin{array}{c} -3(D_1^v + D_2^v) \\ \times(k_x^2 - k_y^2)k_z \end{array} & \begin{array}{c} \frac{D_1^v - D_2^v}{\sqrt{3}}(k_x^3 + ik_y^3) \\ -\frac{5D_1^v + D_2^v}{\sqrt{3}}ik_x k_y k_- \\ +\frac{2(2D_1^v + D_2^v)}{\sqrt{3}}k_+ k_z^2 \end{array} & \begin{array}{c} \frac{1}{\sqrt{3}}(D_1^v - D_2^v) \\ \times(k_x^2 + k_y^2 - 2k_z^2)k_z \end{array} & \begin{array}{c} (D_1^v - D_2^v)\left(k_x^3 - ik_y^3\right. \\ \left. -ik_x k_y k_+ - 2k_- k_z^2\right) \end{array} \\ \hline c.c. & \begin{array}{c} -(3D_1^v - D_2^v) \\ \times(k_x^2 - k_y^2)k_z \end{array} & \begin{array}{c} (D_2^v - D_1^v)(k_x^3 + ik_y^3) \\ -(D_1^v + 3D_2^v)ik_x k_y k_- \\ +\frac{2(D_1^v + D_2^v)}{3}k_+ k_z^2 \end{array} & \begin{array}{c} -\frac{1}{\sqrt{3}}(D_1^v - D_2^v) \\ \times(k_x^2 + k_y^2 - 2k_z^2)k_z \end{array} \\ \hline c.c. & c.c. & \begin{array}{c} (3D_1^v - D_2^v) \\ \times(k_x^2 - k_y^2)k_z \end{array} & \begin{array}{c} \frac{D_1^v - D_2^v}{\sqrt{3}}(k_x^3 + ik_y^3) \\ -\frac{5D_1^v + D_2^v}{\sqrt{3}}ik_x k_y k_- \\ +\frac{2(2D_1^v + D_2^v)}{\sqrt{3}}k_+ k_z^2 \end{array} \\ \hline c.c. & c.c. & c.c. & \begin{array}{c} 3(D_1^v + D_2^v) \\ \times(k_x^2 - k_y^2)k_z \end{array} \end{array}\right), \quad (29)$$

and for the coordinate system with $z \parallel [110]$:

$$H^D_{4\times4} = \left(\begin{array}{c|c|c|c} -2(2D_1^v+D_2^v)k_x^2k_y & \frac{2D_1^v+D_2^v}{\sqrt{3}}ik_y^2k_z & -\frac{D_1^v-D_2^v}{\sqrt{3}}\left(2ik_x^3-k_y^3\right. & -3(D_1^v-D_2^v)k_-k_yk_z \\ +(2D_1^v+D_2^v)k_y^3 & +\frac{D_1^v+2D_2^v}{\sqrt{3}}2ik_x^2 & -ik_xk_y^2+2k_x^2k_y & \\ -(D_1^v+2D_2^v)k_yk_z^2 & -\frac{D_1^v+2D_2^v}{\sqrt{3}}ik_z^3 & \left.+2k_yk_z^2-ik_xk_z^2\right) & \\ & +\sqrt{3}(3D_1^v+D_2^v) & & \\ & \times k_xk_yk_z & & \\ \hline c.c. & -D_2^v(2k_x^2-k_y^2)k_y & 2D_1^vi(2k_x^2-k_z^2)k_z & \frac{D_1^v-D_2^v}{\sqrt{3}}\left(2ik_x^3-k_y^3\right. \\ & -(3D_2^v-2D_2^v)k_yk_z^2 & +(D_1^v+D_2^v)ik_y^2k_z & -ik_xk_y^2+2k_x^2k_y \\ & & +(3D_1^v+5D_2^v)k_xk_yk_z & \left.+2k_yk_z^2-ik_xk_z^2\right) \\ \hline c.c. & c.c. & -D_2^v(2k_x^2-k_y^2)k_y & \frac{2D_1^v+D_2^v}{\sqrt{3}}ik_y^2k_z \\ & & -(3D_2^v-2D_2^v)k_yk_z^2 & +\frac{D_1^v+2D_2^v}{\sqrt{3}}2ik_x^2 \\ & & & -\frac{D_1^v+2D_2^v}{\sqrt{3}}ik_z^3 \\ & & & +\sqrt{3}(3D_1^v+D_2^v) \\ & & & \times k_xk_yk_z \\ \hline c.c. & c.c. & c.c. & -2(2D_1^v+D_2^v)k_x^2k_y \\ & & & +(2D_1^v+D_2^v)k_y^3 \\ & & & -(D_1^v+2D_2^v)k_yk_z^2 \end{array}\right), \quad (30)$$

where

$$D_1^v = \frac{1}{3}\frac{PP'Q}{E_gE_g'}, \quad D_2^v = \frac{1}{3}\frac{PP'Q}{E_g(E_g'+\Delta')}. \quad (31)$$

Table 1: Band parameters for GaAs and $Al_xGa_{1-x}As$ bulk, taken from [2, 5, 6].

	GaAs	$Al_{0.35}Ga_{0.65}As$
E_g (eV)	1.519	1.972
E_g' (eV)	4.488	4.527
Δ (eV)	0.341	0.317
Δ' (eV)	0.171	0.171
$\bar{\Delta}$ (eV)	-0.05	-0.085
P (eV.nm)	1.0493	0.944
P' (eV.nm)	0.478	0.117
Q (eV.nm)	0.8165	0.626
C_k (eV.nm)	-0.00034	-0.00017
γ_1	6.85	5.59
γ_2	2.1	1.59
γ_3	2.9	2.31
m^*/m_0	0.067	0.095
g^*	-0.44	0.61
κ	1.20	0.54
q	0.01	0.01

Valence band offset is $0.35\Delta E_g$.

To compute band structure for semiconductor bulk we can diagonalize either the full 14×14 Hamiltonian (10) or the simplified Hamiltonians (19) and (25). Band energy for GaAs bulk using parameters in Table 1 is showed in Fig. 2. We notice that due to the inversion asymmetry of zinc-blende crystal structure, there is a spin splitting in the dispersion for $k \parallel [110]$. The parameters that are responsible for spin splitting are P', $\bar{\Delta}$, and C_k. In crystals having inversion symmetry, e.g. Si, Ge, $P' = \bar{\Delta} = C_k = 0$ [2].

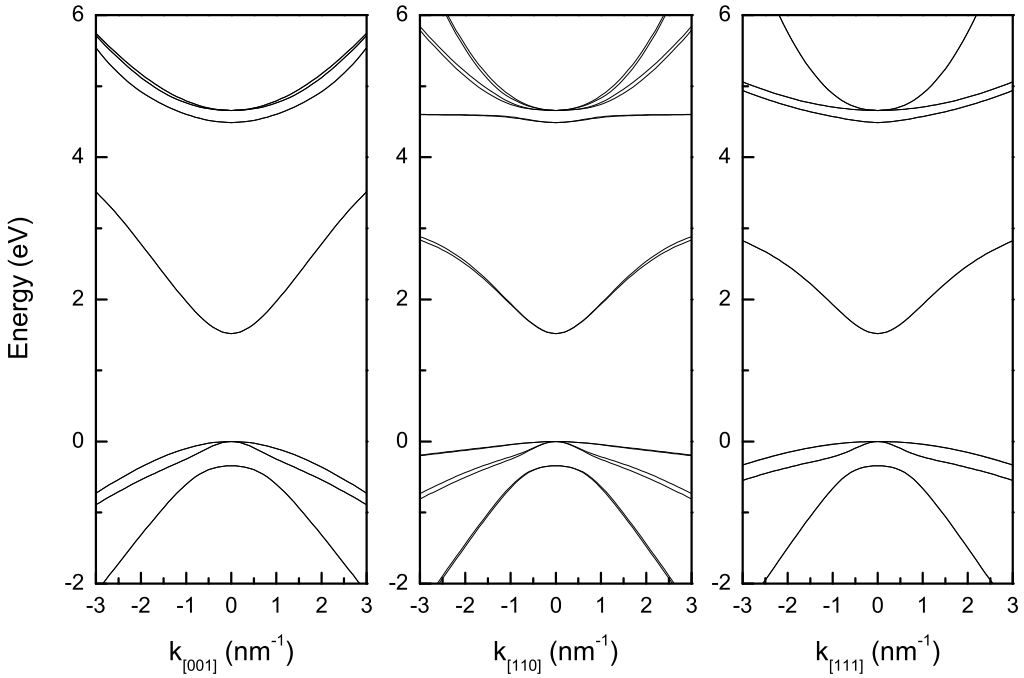

Figure 2: Band structure of GaAs bulk for various **k** directions.

The comparison between exact and perturbation solutions is given in Fig. 3. The exact solution is showed by blue lines and third-order perturbation solution is showed by red lines. As we can see, the perturbation result works well for small k but deviates from the exact one for large k.

5 External electric and magnetic field

5.1 Electric field $\mathbf{E} = (0, 0, E_z)$

In the presence of an external electric field **E** the Hamiltonian reads

$$\hat{H}_{14\times14} = H_{14\times14}(\mathbf{k}) + e\mathbf{E}\cdot\mathbf{r}\ I_{14\times14}, \tag{32}$$

where **r** is the position operator and $I_{14\times14}$ is the identity matrix.

We consider an electric field along to z-axis ($\mathbf{E} = (0, 0, E_z)$) and apply the perturbation approach to block-diagonalize the Hamiltonian $\hat{H}$. Note that the commutation relation $[z, k_z] = i$ holds in the calculation. Third-order Löwdin perturbation theory gives us simplified Hamiltonians

$$\breve{H}_{2\times2} = H^{m^*}_{2\times2} + H^{D}_{2\times2} + H^{R}_{2\times2} + eE_z z\ I_{2\times2} \tag{33}$$

for the conduction band and

$$\breve{H}_{4\times4} = H^{L}_{4\times4} + H^{D}_{4\times4} + H^{R}_{4\times4} + eE_z z\ I_{4\times4} \tag{34}$$

for the valence band. Here, $H^{m^*}_{2\times2}$, $H^{D}_{2\times2}$, $H^{L}_{4\times4}$, and $H^{D}_{4\times4}$ are given in Section 4, $H^{R}_{2\times2}$ and $H^{R}_{4\times4}$ Rashba terms. In both coordinate systems with $z \parallel [001]$ and $z \parallel [110]$, $H^{R}_{2\times2}$ has the form

$$H^{R}_{2\times2} = R^c \begin{pmatrix} 0 & ik_- \\ ik_+ & 0 \end{pmatrix}, \tag{35}$$

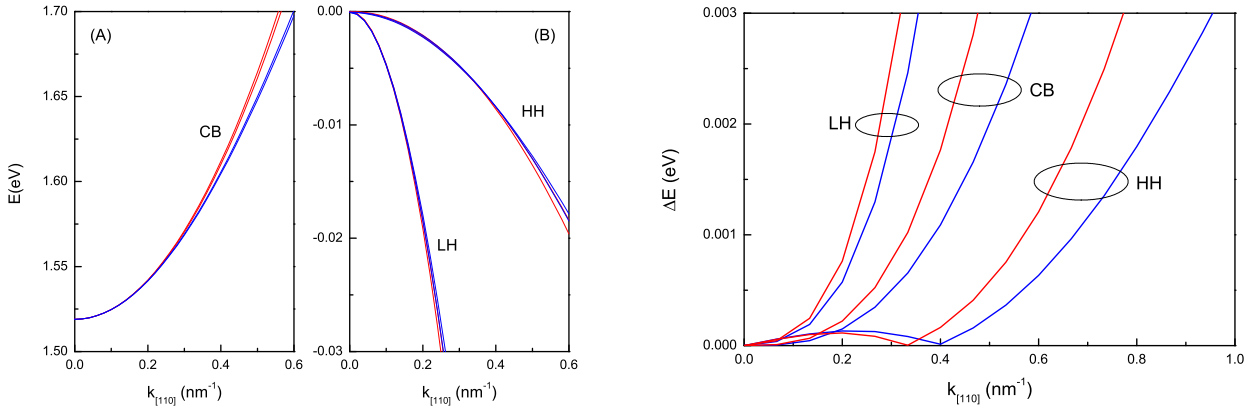

Figure 3: Band structure of GaAs bulk calculated in two approaches: by solving full 14×14 Hamiltonian (blue lines) and by using perturbation theory (red lines). (A) Conduction band dispersion, (B) Valence band dispersion, and (C) Spin splitting $\Delta E(k_{[110]}) = |E(k_{[110]}, \uparrow) - E(k_{[110]}, \downarrow)|$.

where

$$R^c = \frac{eE_z}{3}\left[P^2\left(\frac{1}{E_g^2} - \frac{1}{(E_g+\Delta)^2}\right) + P'^2\left(\frac{1}{(E_g - E_g' - \Delta')^2} - \frac{1}{(E_g - E_g')^2}\right)\right]. \tag{36}$$

The term $H^R_{4\times4}$ has ther form in the coordinate system with $z \parallel [001]$:

$$H^R_{4\times4} = \begin{pmatrix} 0 & (R_2^v - R_1^v)ik_- & 0 & \frac{2(R_2^v - R_3^v)}{\sqrt{3}}ik_+ \\ c.c. & 0 & \frac{2(R_3^v - R_1^v)}{\sqrt{3}}ik_- & 0 \\ 0 & c.c. & 0 & (R_2^v - R_1^v)ik_- \\ c.c. & 0 & c.c. & 0 \end{pmatrix} \tag{37}$$

and in the coordinate system with $z \parallel [110]$:

$$H^R_{4\times4} = \begin{pmatrix} 0 & \begin{matrix}(R_3^v - R_1^v)ik_x \\ +(R_2^v - E_1^v)k_y\end{matrix} & 0 & \frac{R_2^v - R_3^v}{\sqrt{3}}(ik_x - 2k_y) \\ c.c. & 0 & \begin{matrix}\frac{3R_2^v - 2R_1^v - R_3^v}{\sqrt{3}}ik_x \\ +\frac{2(R_3^v - R_1^v)}{\sqrt{3}}k_y\end{matrix} & 0 \\ 0 & c.c. & 0 & \begin{matrix}(R_3^v - R_1^v)ik_x \\ +(R_2^v - E_1^v)k_y\end{matrix} \\ c.c. & 0 & c.c. & 0 \end{pmatrix} \tag{38}$$

where

$$R_1^v = \frac{eE_z}{2\sqrt{3}}\frac{P^2}{E_g^2}, \quad R_2^v = \frac{eE_z}{2\sqrt{3}}\frac{Q^2}{E_g'^2}, \quad R_3^v = \frac{eE_z}{2\sqrt{3}}\frac{Q^2}{(E_g' + \Delta')^2}. \tag{39}$$

5.2 Magnetic field $\mathbf{B} = (B_x, B_y, 0)$

To describe the presence of magnetic field we replace wave vector $\mathbf{k}$ by canonical wave vector $\hat{\mathbf{k}} = \mathbf{k} + \frac{e}{\hbar}\mathbf{A}$, where $\mathbf{A}$ is vector potential and $\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}$. The Hamiltonian reads

$$\hat{H}_{14\times14} = H_{14\times14}(\hat{\mathbf{k}}) + H^Z_{14\times14}, \tag{40}$$

where $H^Z_{14\times14}$ is the effective Zeeman Hamiltonian:

$$H^Z_{14\times14} = \mu_B \mathbf{B}\cdot \begin{pmatrix} 0_{4\times4} & 0 & 0 & 0 & 0 \\ 0 & 0_{2\times2} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2}g'\boldsymbol{\sigma} & 0 & 0 \\ 0 & 0 & 0 & -2\left(\kappa'\mathbf{J}+q'\mathbf{J}^3\right) & -3\kappa'\mathbf{U} \\ 0 & 0 & 0 & -3\kappa'\mathbf{U}^\dagger & -2\kappa'\boldsymbol{\sigma} \end{pmatrix}, \tag{41}$$

where $\mu_B = e\hbar/(2m_0)$, $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector of Pauli matrices, $\mathbf{J} = (J_x, J_y, J_z)$ is the vector of angular momentum matrices for $j = 3/2$, $\mathbf{J}^3 = \left(J_x^3, J_y^3, J_z^3\right)$, and $\mathbf{U}$ is the vector of off-diagonal 4×2 matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$J_x = \begin{pmatrix} 0 & \frac{\sqrt{3}}{2} & 0 & 0 \\ \frac{\sqrt{3}}{2} & 0 & 1 & 0 \\ 0 & 1 & 0 & \frac{\sqrt{3}}{2} \\ 0 & 0 & \frac{\sqrt{3}}{2} & 0 \end{pmatrix}, \; J_y = i\begin{pmatrix} 0 & -\frac{\sqrt{3}}{2} & 0 & 0 \\ \frac{\sqrt{3}}{2} & 0 & -1 & 0 \\ 0 & 1 & 0 & -\frac{\sqrt{3}}{2} \\ 0 & 0 & \frac{\sqrt{3}}{2} & 0 \end{pmatrix}, \; J_z = \begin{pmatrix} \frac{3}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{3}{2} \end{pmatrix},$$

$$U_x = \frac{1}{3\sqrt{2}}\begin{pmatrix} -\sqrt{3} & 0 \\ 0 & -1 \\ 1 & 0 \\ 0 & \sqrt{3} \end{pmatrix}, \; U_y = \frac{i}{3\sqrt{2}}\begin{pmatrix} \sqrt{3} & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & \sqrt{3} \end{pmatrix}, \; U_z = \frac{\sqrt{2}}{3}\begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix}. \tag{42}$$

g' is effective electron g-factor, κ' and q' describe effective hole g-factor which accounting for remote-band contributions. Without remote bands one has $g' = 2$, $\kappa' = \frac{1}{3}$, and $q' = 0$.

For an in-plane magnetic field $\mathbf{B} = (B_x, B_y, 0)$ we choose the gauge $\mathbf{A} = (zB_y, -zB_x, 0)$. By applying the perturbation theory up to third order we obtain a simplified Hamiltonian for the conduction band:

$$\breve{H}_{2\times2} = H^{m^*}_{2\times2}(\hat{\mathbf{k}}) + H^D_{2\times2}(\mathbf{k}) + H^Z_{2\times2}, \tag{43}$$

where $H^{m^*}_{2\times2}$ and $H^D_{2\times2}$ are given in Section 4, $H^Z_{2\times2}$ is the effective Zeeman Hamiltnian for conduction band:

$$H^Z_{2\times2} = \frac{g^*}{2}\mu_B(\sigma_x B_x + \sigma_y B_y), \tag{44}$$

where

$$\frac{g^*}{2} = \frac{g'}{2} + \frac{2m_0}{3\hbar^2}\left[P^2\left(\frac{1}{E_g+\Delta} - \frac{1}{E_g}\right) + P'^2\left(\frac{1}{E_g - E'_g} - \frac{1}{E_g - E'_g - \Delta'}\right) + \frac{2PP'\bar{\Delta}}{3}\left(\frac{2}{(E_g+\Delta)(E_g-E'_g)} + \frac{1}{E_g(E_g-E'_g-\Delta')}\right)\right]. \tag{45}$$

We identify g^* with the electron g-factor parameter in Table 1 and derive g' from Eq. (45).

For the heavy and light hole band, third-order Löwdin perturbation theory gives

$$\breve{H}_{4\times4} = H^L_{4\times4}(\hat{\mathbf{k}}) + H^D_{4\times4}(\mathbf{k}) + H^Z_{4\times4}, \tag{46}$$

where $H^L_{4\times4}$ and $H^D_{4\times4}$ are given in Section 4, $H^Z_{4\times4}$ is the effective Zeeman Hamiltonian for valence band which reads for the coordinate system with $z \parallel [001]$ [2]:

$$H^Z_{4\times4} = -2\kappa\mu_B\begin{pmatrix} 0 & \frac{\sqrt{3}}{2}B_- & 0 & 0 \\ \frac{\sqrt{3}}{2}B_+ & 0 & B_- & 0 \\ 0 & B_+ & 0 & \frac{\sqrt{3}}{2}B_- \\ 0 & 0 & \frac{\sqrt{3}}{2}B_+ & 0 \end{pmatrix} - 2q\mu_B\begin{pmatrix} 0 & \frac{7\sqrt{3}}{8}B_- & 0 & \frac{3}{4}B_+ \\ \frac{7\sqrt{3}}{8}B_+ & 0 & \frac{5}{2}B_- & 0 \\ 0 & \frac{5}{2}B_+ & 0 & \frac{7\sqrt{3}}{8}B_- \\ \frac{3}{4}B_- & 0 & \frac{7\sqrt{3}}{8}B_+ & 0 \end{pmatrix} \tag{47}$$

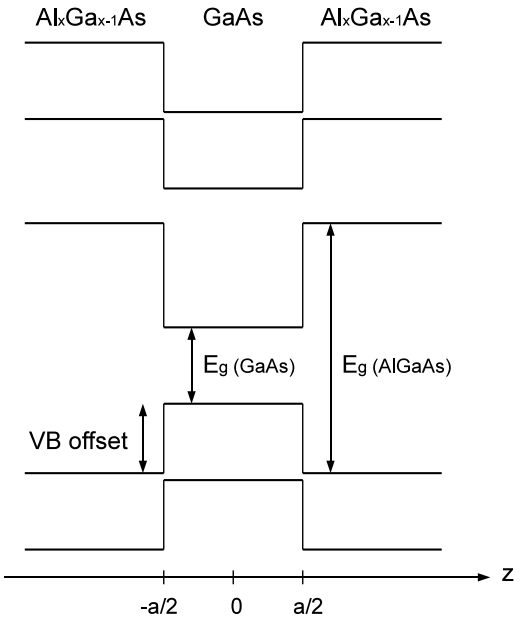

Figure 4: Band offsets at the Gamma point.

and for the coordinate system with $z \parallel [110]$:

$$H^Z_{4\times4} = -2\kappa\mu_B \begin{pmatrix} 0 & \frac{\sqrt{3}}{2}B_- & 0 & 0 \\ \frac{\sqrt{3}}{2}B_+ & 0 & B_- & 0 \\ 0 & B_+ & 0 & \frac{\sqrt{3}}{2}B_- \\ 0 & 0 & \frac{\sqrt{3}}{2}B_+ & 0 \end{pmatrix}$$
$$-2q\mu_B \begin{pmatrix} 0 & \frac{7\sqrt{3}}{8}\left(B_x - \frac{10}{7}iB_y\right) & 0 & \frac{3}{4}\left(B_x + \frac{1}{2}iB_y\right) \\ \frac{7\sqrt{3}}{8}\left(B_x + \frac{10}{7}iB_y\right) & 0 & \frac{5}{2}\left(B_x - \frac{11}{20}iB_y\right) & 0 \\ 0 & \frac{5}{2}\left(B_x + \frac{11}{20}iB_y\right) & 0 & \frac{7\sqrt{3}}{8}\left(B_x - \frac{10}{7}iB_y\right) \\ \frac{3}{4}\left(B_x - \frac{1}{2}iB_y\right) & 0 & \frac{7\sqrt{3}}{8}\left(B_x + \frac{10}{7}iB_y\right) & 0 \end{pmatrix} \quad (48)$$

with $B_\pm = B_x \pm iB_y$ and

$$\kappa = \kappa' + \frac{2m_0}{\hbar^2}\left(\frac{7}{18}\frac{Q^2}{E'_g + \Delta'} - \frac{5}{9}\frac{Q^2}{E'_g} + \frac{1}{6}\frac{P^2}{E_g}\right), \quad (49)$$

$$q = q' + \frac{2m_0}{\hbar^2}\left(\frac{2}{9}\frac{Q^2}{E'_g} - \frac{2}{9}\frac{Q^2}{E'_g + \Delta'}\right). \quad (50)$$

Note that, to obtain Eqs. (47)-(50), in the perturbation calculation we use relations $[z, k_z] = i$, $k_z z = \frac{1}{2}(zk_z + k_z z) - \frac{i}{2}$, and $zk_z = \frac{1}{2}(zk_z + k_z z) + \frac{i}{2}$.

6 Quantum well systems

We use the envelope function approximation to find band energy and wave function of electron in semiconductor quantum wells. By choosing z-axis as the growth direction of the quantum well, the electron wave function has the form

$$\psi_{m\mathbf{k}_\parallel}(\mathbf{r}) = e^{i\mathbf{k}_\parallel\cdot\mathbf{r}_\parallel}\sum_n f^n_{m\mathbf{k}_\parallel}(z)u_n(\mathbf{r}), \quad (51)$$

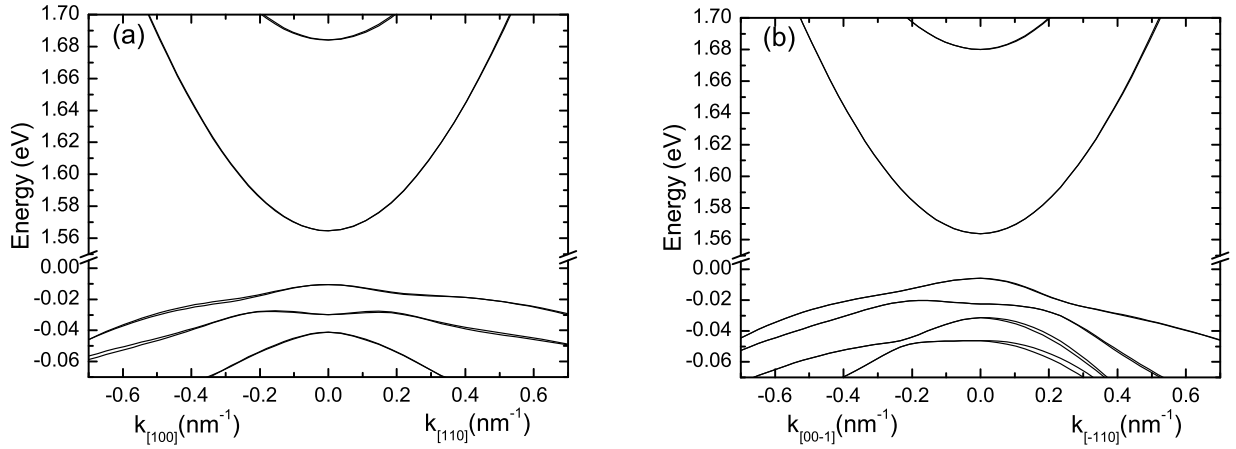

Figure 5: Band structure of 8 nm-wide GaAs/$Al_{0.35}Ga_{0.65}As$ quantum wells grown in the directions (a) [001] and (b) [110]. Band-gap energy for these two quantum wells are 1.575 eV and 1.570 eV, respectively.

where $\mathbf{k}_\parallel$ is the in-plane wave vector and $f^n_{m\mathbf{k}_\parallel}(z)$ is a slowly varying envelope function which satises the effective-mass equation

$$\sum_{n'=1}^{14}\left[H_{nn'}(\mathbf{k}_\parallel,\hat{k}_z)+V_n(z)\delta_{nn'}\right]f^{n'}_{m\mathbf{k}_\parallel}(z)=E_{m\mathbf{k}_\parallel}f^n_{m\mathbf{k}_\parallel}(z). \tag{52}$$

Here, H is the bulk Hamiltonian in which $\hat{k}_z$ is replaced by $-i\partial/\partial z$ and $V(z)$ is the well potential. Square potential wells defined from band offsets at Gamma point are shown in Fig. 4. To account for the spatial dependence of the band parameters we use the Hermitian forms for operator terms $h(z)\hat{k}_z$ and $h(z)\hat{k}_z^2$, where $h(z)$ is an arbitrary function,

$$h(z)\hat{k}_z\rightarrow-\frac{i}{2}\left(\frac{\partial}{\partial z}h(z)+h(z)\frac{\partial}{\partial z}\right),\quad h(z)\hat{k}_z^2\rightarrow-\frac{\partial}{\partial z}h(z)\frac{\partial}{\partial z}. \tag{53}$$

To solve Eq. (52) we expand the envelope function via plane waves [6, 7, 8]

$$f^n_{m\mathbf{k}_\parallel}=\sum_{l=1}^{N}a^{n,l}_{m\mathbf{k}_\parallel}\varphi_l(z) \tag{54}$$

with

$$\varphi_l(z)=\begin{cases}\sqrt{\frac{2}{L_z}}\sin\left[\frac{l\pi}{L_z}\left(z+\frac{L_z}{2}\right)\right] & \text{if } -\frac{L_z}{2}\le z\le\frac{L_z}{2},\\ 0 & \text{otherwise.}\end{cases} \tag{55}$$

Here, L_z is a constant and is chosen to be several times larger than the quantum well thickness a. This basis functions are suitable for describing a quantum well centered at $z=0$.

Substitute the expansion (54) into (52), left multiply by φ^*, and take integral over z we obtain a $14N\times14N$ matrix eigensystem problem:

$$\sum_{n'=1}^{14}\sum_{l'=1}^{N}\langle\varphi_l|H_{nn'}+V_n\delta_{nn'}|\varphi_{l'}\rangle a^{n',l'}_{\mu\mathbf{k}_\parallel}=E_{\mu\mathbf{k}_\parallel}a^{n,l}_{\mu\mathbf{k}_\parallel}. \tag{56}$$

Numerical diagonalizing the $14N \times 14N$ matrix provides us the band energy and expansion coefficients for envelope functions.

Bandstructure of 8-nm-wide GaAs/$Al_{0.35}Ga_{0.65}As$ quantum wells with parameters in Table 1 is shows in Fig. 5. Due to the inversion asymmetry of GaAs lattice structure a small spin splitting of energy bands is obtained.

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