# 半导体能带结构理论

# Theory of Band Structures in Semiconductors

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2007-4-22

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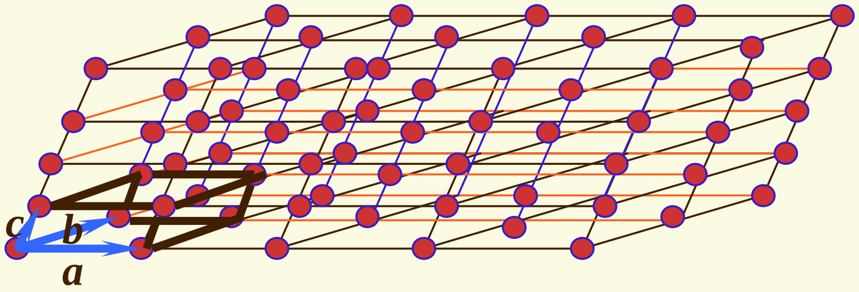
# Bloch定理

- 晶体内的周期势

$$V(\mathbf{r})=V(\mathbf{r}+\mathbf{R});\quad R=n_1\mathbf{a}+n_2\mathbf{b}+n_3\mathbf{c}$$




- 晶体中电子的Bloch波函数

Schrödinger方程： $H_0\psi_{n\mathbf{k}}(\mathbf{r})=E_n(\mathbf{k})\psi_{n\mathbf{k}}(\mathbf{r});\quad H_0=-\frac{\hbar^2}{2m_0}\nabla^2+V(\mathbf{r})$

Bloch定理： $\psi_{n\mathbf{k}}(\mathbf{r})=e^{j\mathbf{k}\cdot\mathbf{r}}u_{n\mathbf{k}}(\mathbf{r});\quad u_{n\mathbf{k}}(\mathbf{r}+\mathbf{R})=u_{n\mathbf{k}}(\mathbf{r})$

- 局域化波函数 $u_{n\mathbf{k}}(\mathbf{r})$的含义及其波动方程

$$\left[H_0+\frac{\hbar}{m_0}\mathbf{k}\cdot\mathbf{p}\right]u_{n\mathbf{k}}(\mathbf{r})=\left[E_n(k)-\frac{\hbar^2k^2}{2m_0}\right]u_{n\mathbf{k}}(\mathbf{r});\quad H_0u_{n0}(\mathbf{r})=E_{n0}u_{n0}(\mathbf{r})$$

# k·p 理论（单一能带）

- 紧束缚近似

在k＝0附近：

$$[H_0+H']u_{n\mathbf{k}}(\mathbf{r})=\left[E_n(\mathbf{k})-\frac{\hbar^2k^2}{2m_0}\right]u_{n\mathbf{k}}(\mathbf{r});\quad H'=\frac{\hbar}{m_0}\mathbf{k}\cdot\mathbf{p};\quad u_{n\mathbf{k}}(\mathbf{r})=u_{n0}(\mathbf{r})+\sum_{n'\neq n}a_n(\mathbf{k})u_{n'0}(\mathbf{r})$$

- 单一能带下的微扰解

$$E_n(\mathbf{k})=E_n(0)+\frac{\hbar^2k^2}{2m_0}+\frac{\hbar}{m_0}\mathbf{k}\cdot\mathbf{p}_{nn}+\frac{\hbar^2}{m_0^2}\sum_{n'\neq n}\frac{|\mathbf{k}\cdot\mathbf{p}_{nn'}|^2}{E_n(0)-E_{n'}(0)};\quad \mathbf{p}_{nn'}=\int_{\text{晶胞内}}u_{n0}^*(\mathbf{r})\mathbf{p}u_{n'0}(\mathbf{r})d^3\mathbf{r}$$

若k＝0为极值点，则 $\mathbf{p}_{nn}$＝0。

- 有效质量张量

$$E_n(\mathbf{k})=E_n(0)+\sum_{\alpha,\beta}D^{\alpha\beta}k_\alpha k_\beta=E_n(0)+\frac{\hbar^2}{2}\sum_{\alpha,\beta}\left(\frac{1}{m_n^*}\right)_{\alpha\beta}k_\alpha k_\beta$$

$$\left(\frac{1}{m_n^*}\right)_{\alpha\beta}=\frac{2}{\hbar^2}D^{\alpha\beta}=\frac{1}{m_0}\delta_{\alpha\beta}+\frac{1}{m_0^2}\sum_{n'\neq n}\frac{p_{nn'}^{\alpha}p_{n'n}^{\beta}+p_{nn'}^{\beta}p_{n'n}^{\alpha}}{E_n(0)-E_{n'}(0)}$$

# M个能带的情况

$$u_{m\mathbf{k}}(\mathbf{r})=\sum_{n=1}^{M}a_n(\mathbf{k})u_{n0}(\mathbf{r}),\quad H_0u_{m\mathbf{k}}(\mathbf{r})=E_n(0)u_{n0}(\mathbf{r})$$

$$H=H_0+H';\quad Hu_{n\mathbf{k}}(\mathbf{r})=E_n(\mathbf{k})u_{n\mathbf{k}}(\mathbf{r})$$

$$\Rightarrow\quad \sum_{n=1}^{M}\left(H_{mn}-E_n(\mathbf{k})\delta_{mn}\right)a_n=0$$

$$H_{mn}=\left[E_m(0)+\frac{\hbar^2k^2}{2m_0}\right]\delta_{mn}+H'_{mn}$$

# 载流子的自旋—轨道相互作用

## ➢ 自旋算符与自旋—轨道相互作用能

自旋算符：$\mathbf{S}=\frac{\hbar}{2}\boldsymbol{\sigma};\quad \boldsymbol{\sigma}=\mathbf{e}_x\sigma_x+\mathbf{e}_y\sigma_y+\mathbf{e}_z\sigma_z;\quad \sigma_x=\begin{bmatrix}0&1\\1&0\end{bmatrix},\sigma_y=\begin{bmatrix}0&-j\\j&0\end{bmatrix},\sigma_z=\begin{bmatrix}1&0\\0&-1\end{bmatrix}$

自旋—轨道相互作用能：$H_{SL}=\frac{\hbar}{4m_0^2c^2}\boldsymbol{\sigma}\cdot\nabla V\times\mathbf{p}$

## ➢ 本征值方程

$$\left(H_0+\frac{\hbar}{m_0}\mathbf{k}\cdot\mathbf{p}+\frac{\hbar}{4m_0^2c^2}\nabla V\times\mathbf{p}\cdot\boldsymbol{\sigma}+\frac{\hbar}{4m_0^2c^2}\nabla V\times\mathbf{k}\cdot\boldsymbol{\sigma}\right)u_{n\mathbf{k}}(\mathbf{r})=\left(E_n(\mathbf{k})-\frac{\hbar^2k^2}{2m_0}\right)u_{n\mathbf{k}}(\mathbf{r})$$

在 $\mathbf{k}=0$ 极值点附近，则 $\hbar\mathbf{k}\ll\mathbf{p}$，Hamiltonian中末项可略去。

## ➢ 常见Ⅳ族和Ⅲ-Ⅴ族半导体材料内价电子的带边波函数

s电子：$|S\uparrow\rangle$，$|S\downarrow\rangle$ $H_0$的能量本征值 $E_s$。

p电子：$\left|\frac{X-iY}{\sqrt{2}}\uparrow\right\rangle,|Z\downarrow\rangle,\left|-\frac{X+iY}{\sqrt{2}}\uparrow\right\rangle,\left|\frac{X-iY}{\sqrt{2}}\downarrow\right\rangle,|Z\uparrow\rangle,\left|-\frac{X+iY}{\sqrt{2}}\downarrow\right\rangle$ 能量本征值 $E_p$。

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# 半导体能带结构的Kane模型（ 8×8 Hamiltonian ）

基函数：

$$\left|iS\downarrow\right\rangle,\left|\frac{X-iY}{\sqrt{2}}\uparrow\right\rangle,\left|Z\downarrow\right\rangle,\left|-\frac{X+iY}{\sqrt{2}}\uparrow\right\rangle,\ \text{和}\ \left|iS\uparrow\right\rangle,\left|\frac{X-iY}{\sqrt{2}}\downarrow\right\rangle,\left|Z\uparrow\right\rangle,\left|-\frac{X+iY}{\sqrt{2}}\downarrow\right\rangle$$

在 $\mathbf{k}=k\mathbf{e}_z$ 并选择 $E_p=-\Delta/3$ 情况下的 8×8 Hamiltonian矩阵：

$$H_{8\times8}=\begin{bmatrix} H_{4\times4} & 0 \\ 0 & H_{4\times4} \end{bmatrix};\qquad H_{4\times4}=\begin{bmatrix} E_s & 0 & kP & 0 \\ 0 & -\frac{2\Delta}{3} & \frac{\sqrt{2}\Delta}{3} & 0 \\ kP & \frac{\sqrt{2}\Delta}{3} & -\frac{\Delta}{3} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Kane参数： $P=-i\frac{\hbar}{m_0}\left\langle S\right|p_z\left|Z\right\rangle$

自旋一轨道分裂能： $\Delta=i\frac{3\hbar}{4m_0^2c^2}\left\langle X\right|\frac{\partial V}{\partial x}p_y-\frac{\partial V}{\partial y}p_x\left|Y\right\rangle$

# 半导体能带结构的Kane模型（本征值和带边波函数）

- 本征值

$$E_1(k)=E_s+\frac{\hbar^2k^2}{2m_0}+\frac{k^2P^2(E_s+2\Delta/3)}{E_s(E_s+\Delta)}$$

导带C　$(E_s=E_g)$

$$E_2(k)=\frac{\hbar^2k^2}{2m_0}$$

重空穴带HH　（与实验不符）

$$E_3(k)=\frac{\hbar^2k^2}{2m_0}-\frac{2k^2P^2}{3E_s}$$

轻空穴带LH

$$E_4(k)=-\Delta+\frac{\hbar^2k^2}{2m_0}-\frac{k^2P^2}{3(E_s+\Delta)}$$

自旋一轨道分裂带SO

- **$k\to 0$** 时的带边函数

$$u_{c1,0}(\mathbf{r})=\left|iS\downarrow\right\rangle,\ u_{c2,0}(\mathbf{r})=\left|iS\uparrow\right\rangle;\quad u_{hh1,0}(\mathbf{r})=-\left|\frac{X+iY}{\sqrt{2}}\uparrow\right\rangle=\left|\frac{3}{2},\frac{3}{2}\right\rangle,\ u_{hh2,0}(\mathbf{r})=\left|\frac{X-iY}{\sqrt{2}}\downarrow\right\rangle=\left|\frac{3}{2},-\frac{3}{2}\right\rangle$$

$$u_{lh1,0}(\mathbf{r})=\frac{1}{\sqrt{3}}\left|\frac{X-iY}{\sqrt{2}}\uparrow\right\rangle+\sqrt{\frac{2}{3}}\left|Z\downarrow\right\rangle=\left|\frac{3}{2},-\frac{1}{2}\right\rangle,\ u_{lh2,0}(\mathbf{r})=-\frac{1}{\sqrt{3}}\left|\frac{X+iY}{\sqrt{2}}\downarrow\right\rangle+\sqrt{\frac{2}{3}}\left|Z\uparrow\right\rangle=\left|\frac{3}{2},\frac{1}{2}\right\rangle$$

$$u_{so1,0}(\mathbf{r})=\sqrt{\frac{2}{3}}\left|\frac{X-iY}{\sqrt{2}}\uparrow\right\rangle-\frac{1}{\sqrt{3}}\left|Z\downarrow\right\rangle=\left|\frac{1}{2},-\frac{1}{2}\right\rangle,\ u_{so2,0}(\mathbf{r})=\sqrt{\frac{2}{3}}\left|\frac{X+iY}{\sqrt{2}}\downarrow\right\rangle+\frac{1}{\sqrt{3}}\left|Z\uparrow\right\rangle=\left|\frac{1}{2},\frac{1}{2}\right\rangle$$

# 微扰理论中的Löwdin重整化方法

## ➢ 基本理论

$$H\psi = E\psi;\quad \psi = \sum_n a_n |n\rangle \Longrightarrow (E - H_{mm})a_m = \sum_{n\neq m} H_{mn}a_n = \sum_{n\neq m}^{A} H_{mn}a_n + \sum_{\alpha\neq m}^{B} H_{m\alpha}a_\alpha;\quad H_{mn} = \langle m|H|n\rangle$$

$$\Longrightarrow a_m = \sum_{n\neq m}^{A}\frac{H_{mn}a_n}{E - H_{mm}} + \sum_{\alpha\neq m}^{B}\frac{H_{m\alpha}a_\alpha}{E - H_{mm}} \Longrightarrow a_m = \sum_n^{A}\frac{U_{mn}^{A} - H_{mn}\delta_{mn}}{E - H_{mm}}a_n \Longrightarrow \sum_n^{A}\left(U_{mn}^{A} - E\delta_{mn}\right)a_n = 0$$

$$U_{mn}^{A} = H_{mn} + \sum_{\alpha\neq m}^{B}\frac{H_{m\alpha}H_{\alpha n}}{E - H_{\alpha\alpha}} + \sum_{\substack{\alpha,\beta\neq m,n\\ \alpha\neq\beta}}^{B}\frac{H_{m\alpha}H_{\alpha\beta}H_{\beta n}}{(E - H_{\alpha\alpha})(E - H_{\beta\beta})} + \cdots$$

## ➢ 单态微扰解

微扰形式：$H = H_0 + H';\quad H_0|n\rangle = E_n|n\rangle;\quad H_{mn} = E_m\delta_{mn} + H'_{mn}$

$$E = U_{nn}^{A} = E_n + H'_{nn} + \sum_{\alpha\neq n}^{B}\frac{H'_{n\alpha}H'_{\alpha n}}{E_n - E_\alpha} + \cdots$$

## ➢ 简并态微扰解

$$E_m \approx E_A \quad \text{for } m\in A \Longrightarrow U_{mn}^{A} = H_{mn} + \sum_{\alpha}^{B}\frac{H'_{m\alpha}H'_{\alpha n}}{E_A - E_\alpha} + \cdots$$

# Luttinger-Kohn 的能带结构模型

➢ A类基矢量

$$u_{10}(\mathbf{r})=\left|\frac{3}{2},\frac{3}{2}\right\rangle,\ u_{20}(\mathbf{r})=\left|\frac{3}{2},\frac{1}{2}\right\rangle,\ u_{30}(\mathbf{r})=\left|\frac{3}{2},-\frac{1}{2}\right\rangle,\ u_{40}(\mathbf{r})=\left|\frac{3}{2},-\frac{3}{2}\right\rangle,\ u_{50}(\mathbf{r})=\left|\frac{1}{2},\frac{1}{2}\right\rangle,\ u_{60}(\mathbf{r})=\left|\frac{1}{2},-\frac{1}{2}\right\rangle$$

➢ 本征值方程

$$\sum_{n}^{A}\left(U_{mn}^{A}-E\delta_{mn}\right)a_n=0$$

$$U_{mn}^{A}=H_{mn}+\sum_{\gamma\neq m,n}^{B}\frac{H_{m\gamma}H_{\gamma n}}{E_{av}-H_{\gamma\gamma}}=\left[E_m(0)+\frac{\hbar^2k^2}{2m_0}\right]\delta_{mn}+\frac{\hbar^2}{m_0^2}\sum_{\alpha,\beta}\sum_{\gamma}^{B}\frac{k_\alpha k_\beta p_{m\gamma}^{\alpha}p_{\gamma n}^{\beta}}{E_{av}-E_\gamma}$$

➢ 有效质量张量

$$U_{mn}^{A}=E_m(0)\delta_{mn}+\sum_{\alpha,\beta}D_{mn}^{\alpha\beta}k_\alpha k_\beta$$

$$D_{mn}^{\alpha\beta}=\frac{\hbar^2}{2m_0}\left(\delta_{mn}\delta_{ij}+\frac{1}{m_0}\sum_{\gamma}^{B}\frac{p_{m\gamma}^{\alpha}p_{\gamma n}^{\beta}+p_{m\gamma}^{\beta}p_{\gamma n}^{\alpha}}{E_{av}-E_\gamma}\right)$$

# Luttinger-Kohn 的 6×6 Hamiltonian

$$H^{\mathrm{LK}} = -\begin{bmatrix} P+Q & -S & R & 0 & -S/\sqrt{2} & \sqrt{2}R \\ -S^{+} & P-Q & 0 & R & -\sqrt{2}Q & \sqrt{3/2}S \\ R^{+} & 0 & P-Q & S & \sqrt{3/2}S^{+} & \sqrt{2}Q \\ 0 & R^{+} & S^{+} & P+Q & -\sqrt{2}R^{+} & -S^{+}/\sqrt{2} \\ -S^{+}/\sqrt{2} & -\sqrt{2}Q^{+} & \sqrt{3/2}S & -\sqrt{2}R & P+\Delta & 0 \\ \sqrt{2}R^{+} & \sqrt{3/2}S^{+} & \sqrt{2}Q^{+} & -S/\sqrt{2} & 0 & P+\Delta \end{bmatrix}$$

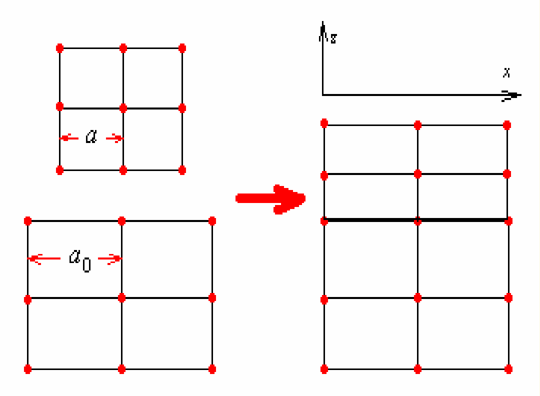
$$P = \frac{\hbar^2\gamma_1}{2m_0}\left(k_x^2 + k_y^2 + k_z^2\right); \qquad Q = \frac{\hbar^2\gamma_2}{2m_0}\left(k_x^2 + k_y^2 - 2k_z^2\right)$$

$$R = \frac{\hbar^2}{2m_0}\left(-\sqrt{3}\gamma_2\left(k_x^2 - k_y^2\right) + i2\sqrt{3}\gamma_3 k_x k_y\right); \qquad S = \frac{\hbar^2\gamma_3}{m_0}\sqrt{3}\left(k_x - ik_y\right)k_z$$

$$\sum_{n=1}^{6} H_{mn}^{\mathrm{LK}} a_n(\mathbf{k}) = E(\mathbf{k}) a_m(\mathbf{k})$$

# 应变效应和形变势

➢ 应变层中的双轴应变




$$\varepsilon_{xx}=\varepsilon_{yy}=\frac{a_0-a}{a};\ \ \varepsilon_{zz}=-\frac{2C_{12}}{C_{11}}\varepsilon_{xx};\ \ \varepsilon_{xy}=\varepsilon_{yz}=\varepsilon_{zx}=0$$

$C_{11},C_{12}$为闪锌矿材料的刚性系数张量矩阵元。

➢ 应变势能

$$(H_\varepsilon)_{mn}=\sum_{\alpha,\beta}\hat{D}_{mn}^{\alpha\beta}\,\varepsilon_{\alpha\beta}$$

Pikus和Bir证明上述应变势能可通过在L-K Hamiltonian中作如下替换得到：

$$\frac{\hbar^2}{2m_e^*}\to a_c;\ \ \frac{\hbar^2\gamma_1}{2m_0}\to -a_v;\ \ \frac{\hbar^2\gamma_2}{2m_0}\to -\frac{b}{2};\ \ \frac{\hbar^2\gamma_3}{2m_0}\to -\frac{d}{2\sqrt{3}};\ \ k_\alpha k_\beta=\varepsilon_{\alpha\beta}$$

➢ 导带应变Hamiltonian

$$E_c(\mathbf{k})=E_c(0)+\frac{\hbar^2k^2}{2m_e^*}+a_c\left(\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz}\right)$$

# 价带 6×6 Pikus-Bir Hamiltonian

$$H^{\mathrm{PB}}=-\begin{bmatrix} P+Q & -S & R & 0 & -S/\sqrt{2} & \sqrt{2}R \\ -S^{+} & P-Q & 0 & R & -\sqrt{2}Q & \sqrt{3/2}S \\ R^{+} & 0 & P-Q & S & \sqrt{3/2}S^{+} & \sqrt{2}Q \\ 0 & R^{+} & S^{+} & P+Q & -\sqrt{2}R^{+} & -S^{+}/\sqrt{2} \\ -S^{+}/\sqrt{2} & -\sqrt{2}Q^{+} & \sqrt{3/2}S & -\sqrt{2}R & P+\Delta & 0 \\ \sqrt{2}R^{+} & \sqrt{3/2}S^{+} & \sqrt{2}Q^{+} & -S/\sqrt{2} & 0 & P+\Delta \end{bmatrix}$$

$$P=P_k+P_\varepsilon;\quad Q=Q_k+Q_\varepsilon;\quad R=R_k+R_\varepsilon;\quad S=S_k+S_\varepsilon$$

$$P_k=\frac{\hbar^2\gamma_1}{2m_0}\left(k_x^2+k_y^2+k_z^2\right);\qquad Q_k=\frac{\hbar^2\gamma_2}{2m_0}\left(k_x^2+k_y^2-2k_z^2\right)$$

$$R_k=\frac{\hbar^2}{2m_0}\left(-\sqrt{3}\gamma_2\left(k_x^2-k_y^2\right)+i2\sqrt{3}\gamma_3k_xk_y\right);\qquad S_k=\frac{\hbar^2\gamma_3}{m_0}\sqrt{3}\left(k_x-ik_y\right)k_z$$

$$P_\varepsilon=-a_v\left(\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz}\right);\qquad Q_\varepsilon=-\frac{b}{2}\left(\varepsilon_{xx}+\varepsilon_{yy}-2\varepsilon_{zz}\right)$$

$$R_\varepsilon=\frac{\sqrt{3}}{2}b\left(\varepsilon_{xx}-\varepsilon_{yy}\right)-id\varepsilon_{xy};\qquad S_\varepsilon=-d\left(\varepsilon_{xz}-i\varepsilon_{yz}\right)$$

$$\sum_{n=1}^{6}H_{mn}^{\mathrm{PB}}a_n(\mathbf{k})=E(\mathbf{k})a_m(\mathbf{k})$$

# k→0附近的价带近似解

$$E_{HH}(\mathbf{k}) \approx E_{HH}(0) - \frac{\hbar^2}{2m_0}\left[(\gamma_1+\gamma_2)k_t^2 + (\gamma_1 - 2\gamma_2)k_z^2\right]$$

$$E_{LH}(\mathbf{k}) \approx E_{LH}(0) - \frac{\hbar^2}{2m_0}\left[(\gamma_1 - f_+\gamma_2)k_t^2 + (\gamma_1 + 2f_+\gamma_2)k_z^2\right]$$

$$E_{SO}(\mathbf{k}) \approx E_{SO}(0) - \frac{\hbar^2}{2m_0}\left[(\gamma_1 - f_-\gamma_2)k_t^2 + (\gamma_1 + 2f_-\gamma_2)k_z^2\right]$$

$$E_{HH}(0) = -P_\varepsilon - Q_\varepsilon$$

$$E_{LH}(0) = -P_\varepsilon + \frac{1}{2}\left(Q_\varepsilon - \Delta + \sqrt{\Delta^2 + 2\Delta Q_\varepsilon + 9Q_\varepsilon^2}\right)$$

$$E_{SO}(0) = -P_\varepsilon + \frac{1}{2}\left(Q_\varepsilon - \Delta - \sqrt{\Delta^2 + 2\Delta Q_\varepsilon + 9Q_\varepsilon^2}\right)$$

$$f_\pm(x) = \frac{2x\left[1 + \frac{3}{2}\left(x - 1 \pm \sqrt{1+2x+9x^2}\right)\right] + 6x^2}{\frac{3}{4}\left(x - 1 \pm \sqrt{1+2x+9x^2}\right)^2 + x - 1 \pm \sqrt{1+2x+9x^2} - 3x^2}; \qquad x = \frac{Q_\varepsilon}{\Delta}$$

# 各能带的横向和纵向有效质量

$$m_{hh}^{z}=\frac{m_0}{\gamma_1-2\gamma_2};\qquad m_{hh}^{t}=\frac{m_0}{\gamma_1+\gamma_2}$$

$$m_{lh}^{z}=\frac{m_0}{\gamma_1+2f_{+}\gamma_2};\qquad m_{lh}^{t}=\frac{m_0}{\gamma_1-f_{+}\gamma_2}$$

$$m_{so}^{z}=\frac{m_0}{\gamma_1+2f_{-}\gamma_2};\qquad m_{so}^{t}=\frac{m_0}{\gamma_1-f_{-}\gamma_2}$$

无应变情况下：

$$Q_\varepsilon=0,\quad x=0\quad\rightarrow\quad f_{+}=1,\quad f_{-}=0$$

# 应变层量子阱中的子带和包络函数

➢ 导带

$$V_e(z)=\begin{cases}\Delta E_c & \text{for } |z|\ge L/2\\ 0 & \text{for } |z|<L/2\end{cases}\qquad \left[-\frac{\hbar^2}{2m_e^*}\frac{d^2}{dz^2}+V_e(z)\right]f(z)=\left[E_{cn}(\mathbf{k}_t)-E_c(0)-\frac{\hbar^2k_t^2}{2m_e^*}\right]f(z)$$

$$E_{cn}(\mathbf{k}_t)=E_{cn}(0)+\frac{\hbar^2k_t^2}{2m_e^*}\qquad \hat{\psi}_{n\mathbf{k}_t}(\mathbf{r})=\frac{e^{i\mathbf{k}_t\cdot\mathbf{r}_t}}{\sqrt{A}}f_n(z)\left|S\uparrow\right\rangle,\quad \breve{\psi}_{n\mathbf{k}_t}(\mathbf{r})=\frac{e^{i\mathbf{k}_t\cdot\mathbf{r}_t}}{\sqrt{A}}f_n(z)\left|S\uparrow\right\rangle$$

➢ 价带

$$V_h(z)=\begin{cases}-\Delta E_v & \text{for } |z|\ge L/2\\ 0 & \text{for } |z|<L/2\end{cases}\qquad \left[\mathbf{H}^{PB}\left(\mathbf{k}_t,k_z=-i\frac{\partial}{\partial z}\right)+V_h(z)\right]\mathbf{g}(\mathbf{k}_t,z)=E_h(\mathbf{k}_t)\mathbf{g}(\mathbf{k}_t,z)$$

$$\mathbf{g}(\mathbf{k}_t,z)=\begin{bmatrix}g_1(\mathbf{k}_t,z)\\ g_2(\mathbf{k}_t,z)\\ g_3(\mathbf{k}_t,z)\\ g_4(\mathbf{k}_t,z)\\ g_5(\mathbf{k}_t,z)\\ g_6(\mathbf{k}_t,z)\end{bmatrix}$$

$$\psi_{m\mathbf{k}_t}(\mathbf{r})=\frac{e^{i\mathbf{k}_t\cdot\mathbf{r}_t}}{\sqrt{A}}\left[g_{m1}\left|\frac{3}{2},\frac{3}{2}\right\rangle+g_{m2}\left|\frac{3}{2},\frac{1}{2}\right\rangle+g_{m3}\left|\frac{3}{2},-\frac{1}{2}\right\rangle+g_{m4}\left|\frac{3}{2},-\frac{3}{2}\right\rangle+g_{m5}\left|\frac{1}{2},\frac{1}{2}\right\rangle+g_{m6}\left|\frac{1}{2},-\frac{1}{2}\right\rangle\right]$$

一般情况下，可略去SO带，仅考虑HH与LH带之间的耦合即可。此时$H^{PB}$退化为4×4矩阵。

# 4×4 Hamiltonian 的块对角化

- **4×4 Hamiltonian**

$$H=-\begin{bmatrix} P+Q & -S & R & 0 \\ -S^{+} & P-Q & 0 & R \\ R^{+} & 0 & P-Q & S \\ 0 & R^{+} & S^{+} & P+Q \end{bmatrix}$$

在一般双轴应变情况下： $R_\varepsilon=S_\varepsilon=0$

$$R=\frac{\hbar^2}{2m_0}\left(-\sqrt{3}\gamma_2\left(k_x^2-k_y^2\right)+i2\sqrt{3}\gamma_3k_xk_y\right)=|R|e^{i\theta_R}$$

$$S=\frac{\hbar^2\gamma_3}{m_0}\sqrt{3}\left(k_x-ik_y\right)k_z=|S|e^{i\theta_S}$$

- **块对角化**

作么正变换：

$$U=\begin{bmatrix} \alpha^* & 0 & 0 & -\alpha \\ 0 & -\beta & \beta^* & 0 \\ 0 & \beta & \beta^* & 0 \\ \alpha^* & 0 & 0 & \alpha \end{bmatrix} \Rightarrow H=-\begin{bmatrix} P+Q & \tilde{R} & 0 & 0 \\ \tilde{R}^{+} & P-Q & 0 & 0 \\ 0 & 0 & P-Q & \tilde{R} \\ 0 & 0 & \tilde{R}^{+} & P+Q \end{bmatrix}$$

$$\begin{cases} \alpha=\dfrac{1}{\sqrt{2}}e^{i[(\theta_S+\theta_R)/2+\pi/4]} \\ \beta=\dfrac{1}{\sqrt{2}}e^{i[(\theta_S-\theta_R)/2+\pi/4]} \\ \tilde{R}=|R|-i|S| \end{cases}$$

新的基矢量为：

$$\begin{bmatrix} |1\rangle \\ |2\rangle \\ |3\rangle \\ |4\rangle \end{bmatrix}=U\begin{bmatrix} |3/2,3/2\rangle \\ |3/2,1/2\rangle \\ |3/2,-1/2\rangle \\ |3/2,-3/2\rangle \end{bmatrix}$$

# 轴向近似

在一般双轴应变情况下： $R_\varepsilon = S_\varepsilon = 0$

$$R = -\frac{\hbar^2\sqrt{3}}{2m_0}\left(\frac{\gamma_2+\gamma_3}{2}\left(k_x - ik_y\right)^2 + \frac{\gamma_2-\gamma_3}{2}\left(k_x+ik_y\right)^2\right)$$

$$\approx -\frac{\hbar^2\sqrt{3}}{2m_0}\bar{\gamma}\left(k_x - ik_y\right)^2 = \frac{\hbar^2\sqrt{3}}{2m_0}\bar{\gamma}k_t^2 e^{-i(\pi-2\phi)} \qquad \left(\bar{\gamma} = \frac{\gamma_2+\gamma_3}{2}\right)$$

$$S = \frac{\hbar^2\gamma_3}{m_0}\sqrt{3}\left(k_x - ik_y\right)k_z = \frac{\hbar^2\sqrt{3}}{m_0}\gamma_3 k_t k_z e^{-i\phi}$$

$$\theta_S = -\phi,\ \ \theta_R = \pi - 2\phi,\ \ \phi = \tan^{-1}\left(k_y/k_x\right)$$

$$\alpha = \frac{1}{\sqrt{2}}e^{i(3\pi/4-3\phi/2)} \qquad \beta = \frac{1}{\sqrt{2}}e^{i(\phi/2-\pi/4)}$$

$$\tilde{R} = |R| - i|S| = \frac{\hbar^2\sqrt{3}}{2m_0}\bar{\gamma}k_t^2 - i\frac{\hbar^2\sqrt{3}}{m_0}\gamma_3 k_t k_z$$

此时，体系Hamiltonian仅与 $\mathbf{k}_t$ 的大小有关，而与其方向无关。

# 轴向近似下对称量子阱的子带和波函数

## ➢ 对称量子阱的简并性

对于对称量子阱：$V_h(z)=V_h(-z)$ 则上下块对角矩阵简并，仅需求解其一则可得出量子阱的能带结构和波函数。

## ➢ 有效质量方程

$$-\begin{bmatrix} P+Q-V_h(z) & \tilde{R} \\ \tilde{R}^{+} & P-Q-V_h(z) \end{bmatrix}\begin{bmatrix} g^{(1)}(k_t,z) \\ g^{(2)}(k_t,z) \end{bmatrix}=E(k_t)\begin{bmatrix} g^{(1)}(k_t,z) \\ g^{(2)}(k_t,z) \end{bmatrix}$$

$$P=P_\varepsilon+\frac{\hbar^2\gamma_1}{2m_0}\left(k_t^2-\frac{\partial^2}{\partial z^2}\right); \qquad Q=Q_\varepsilon+\frac{\hbar^2\gamma_2}{2m_0}\left(k_t^2+2\frac{\partial^2}{\partial z^2}\right)$$

$$\tilde{R}=\frac{\hbar^2\sqrt{3}}{2m_0}\bar{\gamma}k_t^2-\frac{\hbar^2\sqrt{3}}{m_0}\gamma_3 k_t\frac{\partial}{\partial z}; \qquad \tilde{R}^{+}=\frac{\hbar^2\sqrt{3}}{2m_0}\bar{\gamma}k_t^2+\frac{\hbar^2\sqrt{3}}{m_0}\gamma_3 k_t\frac{\partial}{\partial z}$$

## ➢ 波函数

$$\psi(\mathbf{k}_t,\mathbf{r})=\frac{e^{i\mathbf{k}_t\cdot\mathbf{r}}}{\sqrt{A}}\left[g^{(1)}(k_t,z)|1\rangle+g^{(2)}(k_t,z)|2\rangle\right]$$

# 存在的问题