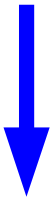
Optics + Semiconductors: How do we start?

1. Classical treatment of charge in an optical (electric) field – oscillator model
2. Quantum mechanical treatment of an atom in a classical field
3. Semiconductors: bands instead discrete levels
4. Nanostructures (quantum wells, quantum wires, quantum dots)



Rich optical properties due to many body environment

Role of lattice vibrations (phonons), Coulomb interactions, confinement, etc.

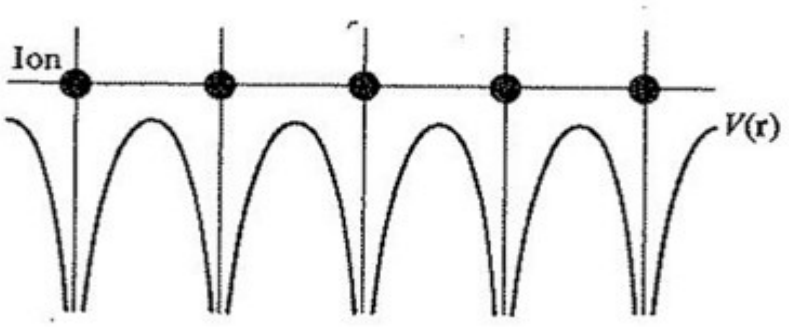
3. Solids: periodic lattice of atoms

Electron in a periodic potential

- In a crystal, $V_0(\mathbf{r}) = V_0(\mathbf{r} + \mathbf{R}_n)$

$$\mathbf{R}_n = \sum_i n_i \mathbf{a}_i \qquad n_i \in \mathbb{Z}$$

Lattice vector — Basis vectors



- Hamiltonian $H = \dfrac{p^2}{2m_0} + V_0(\mathbf{r})$ $\qquad H\psi_\lambda = E_\lambda \psi_\lambda$

- Translation operator $T_n f(\mathbf{r}) = f(\mathbf{r} + \mathbf{R}_n)$

$$T_n H \psi_\lambda(\mathbf{r}) = H(\mathbf{r} + \mathbf{R}_n)\psi_\lambda(\mathbf{r} + \mathbf{R}_n) = H(\mathbf{r})\psi_\lambda(\mathbf{r} + \mathbf{R}_n) = H T_n \psi_\lambda(\mathbf{r})$$

$$\Rightarrow \boxed{[H, T_n] = 0} \quad \Rightarrow \boxed{T_n \psi_\lambda(\mathbf{r}) = \psi_\lambda(\mathbf{r} + \mathbf{R}_n) = t_n \psi_\lambda(\mathbf{r})}$$

Also $|t_n| = 1$ and $t_n t_m = t_{n+m}$ $\qquad \rightarrow t_n = e^{i(\mathbf{k}\cdot\mathbf{R}_n + 2\pi N)}$

$$\boxed{\psi_\lambda(\mathbf{k}, \mathbf{r} + \mathbf{R}_n) = \psi_\lambda(\mathbf{k}, \mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{R}_n}}$$

Bloch Theorem

Real & reciprocal lattice

$$e^{i\mathbf{k}\cdot\mathbf{R}_n} \equiv e^{i(\mathbf{k}+\mathbf{g})\cdot\mathbf{R}_n} \Rightarrow \mathbf{g}\cdot\mathbf{R}_n = 2\pi N$$

- Real crystal lattice

$$\mathbf{R}_n = \sum_i n_i \mathbf{a}_i$$

- Reciprocal lattice

$$\mathbf{g} = \sum_j m_j \mathbf{b}_j$$

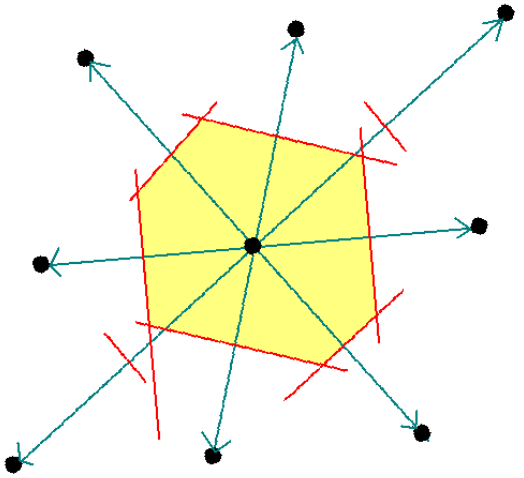
$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij} \Rightarrow \mathbf{b}_i = 2\pi \frac{\mathbf{a}_j \times \mathbf{a}_k}{\mathbf{a}_i \cdot (\mathbf{a}_j \times \mathbf{a}_k)}$$

Wigner-Seitz cell

- SC
- BCC
- FCC

Brillouin zone

- SC
- FCC
- BCC



Bloch wave function

- Bloch Theorem: $\psi_\lambda(\mathbf{k}, \mathbf{r} + \mathbf{R}_n) = \psi_\lambda(\mathbf{k}, \mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{R}_n}$

$$\psi_\lambda = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{L^{3/2}} u_\lambda(\mathbf{k}, \mathbf{r})$$

$$u_\lambda(\mathbf{k}, \mathbf{r}) = u_\lambda(\mathbf{k}, \mathbf{r} + \mathbf{R}_n)$$

Bloch function

- Using $\sum_j \frac{\partial^2}{\partial x_j^2} \psi_\lambda = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{L^{3/2}} (\nabla + i\mathbf{k})^2 u_\lambda$

  the Schrödinger equation becomes

$$\left[-\frac{\hbar^2}{2m_0} (\nabla + i\mathbf{k})^2 + V_0(\mathbf{r}) \right] u_\lambda(\mathbf{k}, \mathbf{r}) = E_\lambda(\mathbf{k}) u_\lambda(\mathbf{k}, \mathbf{r})$$

$$\left[-\frac{\hbar^2}{2m_0} \nabla^2 + \frac{\hbar}{m_0} \mathbf{k}\cdot\mathbf{p} + V_0(\mathbf{r}) \right] u_\lambda(\mathbf{k}, \mathbf{r}) = \left[E_\lambda(\mathbf{k}) - \frac{\hbar^2 k^2}{2m_0} \right] u_\lambda(\mathbf{k}, \mathbf{r})$$

Bloch wave function properties

- Normalization

$$\int_{L^3} d^3r \psi^*_\lambda(\mathbf{k},\mathbf{r})\psi_{\lambda'}(\mathbf{k}',\mathbf{r}) = \delta_{\lambda,\lambda'}\delta_{\mathbf{k},\mathbf{k}'}$$

$$\int_{L^3} d^3r |\psi_\lambda(\mathbf{k},\mathbf{r})|^2 = 1 = \frac{1}{L^3}\int_{L^3} d^3r |u_\lambda(\mathbf{k},\mathbf{r})|^2$$

Using $\int_{L^3} \rightarrow \sum_N \int_{l^3}$ we get $\boxed{\int_{l^3} d^3r |u_\lambda(\mathbf{k},\mathbf{r})|^2 = 1}$

$$\sum_\lambda u^*_\lambda(\mathbf{k},\mathbf{r})u_\lambda(\mathbf{k},\mathbf{r}') = l^3\delta(\mathbf{r}-\mathbf{r}')$$

- Surface effects avoided via *periodic boundary conditions*

$$\psi_\lambda(\mathbf{k},\mathbf{r}+N_i\mathbf{a}_i) = \psi_\lambda(\mathbf{k},\mathbf{r}) \Rightarrow e^{i\mathbf{k}\cdot(N_i\mathbf{a}_i)} = 1 \Rightarrow N_i\mathbf{k}_i\cdot\mathbf{a}_i = 2\pi M$$

For a cubic lattice $-\frac{\pi}{a_i} \le k_i \le \frac{\pi}{a_i} \Rightarrow -\frac{N_i}{2} \le M \le \frac{N_i}{2}$

Wannier Functions

- Localized functions

$$w_\lambda(\mathbf{r}-\mathbf{R}_n) = \frac{1}{\sqrt{L^3 N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{R}_n)} u_\lambda(\mathbf{k},\mathbf{r})$$

$$u_\lambda(\mathbf{k},\mathbf{r}) = \sqrt{\frac{L^3}{N}} \sum_{n} e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{R}_n)} w_\lambda(\mathbf{r}-\mathbf{R}_n)$$

$$\int d^3 r w_\lambda^*(\mathbf{r}) w_{\lambda'}(\mathbf{r}-\mathbf{R}_n) = \delta_{\lambda,\lambda'}\delta_{n,0}$$

- Electron wavefunction

$$\psi_\lambda(\mathbf{k},\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{n} e^{i\mathbf{k}\cdot\mathbf{R}_n} w_\lambda(\mathbf{r}-\mathbf{R}_n)$$

Tight Binding Approximation

- Assumption: electrons remain close to atomic sites, i.e. electronic wave functions between neighboring atoms have small overlap

$$H_0\phi_\lambda(\mathbf{r}-\mathbf{R}_l)=\varepsilon_\lambda\phi_\lambda(\mathbf{r}-\mathbf{R}_l) \qquad H_0=-\frac{\hbar^2\nabla^2}{2m_0}+V_0(\mathbf{r}-\mathbf{R}_l)$$

$$\left[-\frac{\hbar^2\nabla^2}{2m_0}+\sum_l V_0(\mathbf{r}-\mathbf{R}_l)-E_\lambda(\mathbf{k})\right]\psi_\lambda(\mathbf{k},\mathbf{r})=0$$

- Ansatz:

$$\psi_\lambda(\mathbf{k},\mathbf{r})=\sum_n \frac{e^{i\mathbf{k}\cdot\mathbf{R}_n}}{L^{3/2}}\phi_\lambda(\mathbf{r}-\mathbf{R}_n)$$

Tight Binding Wave function

- Energy

$$E_\lambda(\mathbf{k})=\frac{\int d^3r\psi^*_\lambda(\mathbf{k},\mathbf{r})H\psi_\lambda(\mathbf{k},\mathbf{r})}{\int d^3r\psi^*_\lambda(\mathbf{k},\mathbf{r})\psi_\lambda(\mathbf{k},\mathbf{r})}=\frac{N}{D}$$

Tight Binding Approximation

- Assuming localized electrons

$$D = \frac{1}{L^3}\sum_{n,m} e^{i\mathbf{k}\cdot(\mathbf{R}_n-\mathbf{R}_m)} \underbrace{\int d^3r \phi^*_\lambda(\mathbf{r}-\mathbf{R}_m)\phi_\lambda(\mathbf{r}-\mathbf{R}_n)}_{\approx\delta_{n,m}} \Rightarrow D \approx \frac{N}{L^3}$$

$$N = \frac{1}{L^3}\sum_{n,m} e^{i\mathbf{k}\cdot(\mathbf{R}_n-\mathbf{R}_m)} \int d^3r \phi^*_\lambda(\mathbf{r}-\mathbf{R}_m) H \phi_\lambda(\mathbf{r}-\mathbf{R}_n)$$

$$I = \int d^3r \phi^*_\lambda(\mathbf{r}-\mathbf{R_m}) \left[-\frac{\hbar^2\nabla^2}{2m_0} + \sum_l V_0(\mathbf{r}-\mathbf{R}_l)\right] \phi_\lambda(\mathbf{r}-\mathbf{R}_n)$$

$$I = \delta_{n,m}\left[\varepsilon_\lambda + \sum_{l\neq n}\int d^3r \phi^*_\lambda(\mathbf{r}-\mathbf{R_m}) V_0(\mathbf{r}-\mathbf{R}_l)\phi_\lambda(\mathbf{r}-\mathbf{R}_n)\right]$$

$$+\delta_{n\pm1,m}\sum_l \int d^3r \phi^*_\lambda(\mathbf{r}-\mathbf{R_{n\pm1}}) V_0(\mathbf{r}-\mathbf{R}_l)\phi_\lambda(\mathbf{r}-\mathbf{R}_n) + \ldots$$

$$\equiv \delta_{n,m}\varepsilon'_\lambda + \delta_{n\pm1,m}B_\lambda + \ldots$$

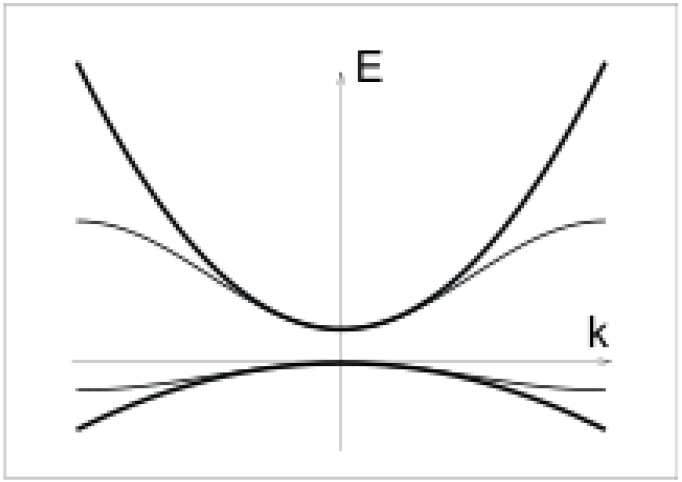
Tight Binding Approximation

- Up to nearest neighbors $N \approx \frac{1}{L^3}\sum_{n,m} e^{i\mathbf{k}\cdot(\mathbf{R}_n-\mathbf{R}_m)}(\delta_{n,m}\varepsilon'_\lambda + \delta_{n\pm1,m}B_\lambda)$

$$E_\lambda(\mathbf{k}) = \varepsilon'_\lambda + \frac{B_\lambda}{N}\sum_{n,m}\delta_{m,n\pm1}e^{i\mathbf{k}\cdot(\mathbf{R}_n-\mathbf{R}_m)}$$

- For a cubic lattice $\mathbf{R}_{n\pm1} = \mathbf{R}_n \pm \mathbf{a}$

$$e^{i\mathbf{k}\cdot\mathbf{a}} + e^{-i\mathbf{k}\cdot\mathbf{a}} = 2\cos(\mathbf{k}\cdot\mathbf{a}) \qquad E_\lambda(\mathbf{k}) = \varepsilon'_\lambda + 2B_\lambda\cos(\mathbf{k}\cdot\mathbf{a})$$



- Bands formed; Energy gaps possible
- Typically B>0 for s-type and B<0 for p-type φ
- Near band min/max: parabolic band approximation

$$E_\lambda(\mathbf{k}) \approx E_{\lambda,0} + \frac{\hbar^2k^2}{2m_{\lambda,eff}} \qquad m_{\lambda,eff} = \frac{\hbar^2}{\frac{\partial^2 E_\lambda(\mathbf{k})}{\partial k^2}\Big|_{k=0}}$$

k·p Theory

- Assume the band structure is known at some point of high symmetry
- Compute energy eigenvalues & Bloch functions around that point

Consider Γ point of Brillouin zone: $\mathbf{k}_0 = 0$

$$\left[-\frac{\hbar^2}{2m_0}\nabla^2 + \frac{\hbar}{m_0}\mathbf{k}\cdot\mathbf{p} + V_0(\mathbf{r})\right] u_\lambda(\mathbf{k},\mathbf{r}) = \left[E_\lambda(\mathbf{k}) - \frac{\hbar^2 k^2}{2m_0}\right] u_\lambda(\mathbf{k},\mathbf{r})$$

or $$\left[H_0 + \frac{\hbar}{m_0}\mathbf{k}\cdot\mathbf{p}\right] u_\lambda(\mathbf{k},\mathbf{r}) = \bar{E}_\lambda(\mathbf{k}) u_\lambda(\mathbf{k},\mathbf{r})$$

- Perturbation theory

parity

$$\bar{E}_\lambda(\mathbf{k}) = E_\lambda(0) + \mathbf{k}\cdot\langle\lambda|\mathbf{p}|\lambda\rangle + \sum_{\eta\neq\lambda}\frac{\hbar^2}{m_0^2}\frac{(\mathbf{k}\cdot\langle\lambda|\mathbf{p}|\eta\rangle)(\mathbf{k}\cdot\langle\eta|\mathbf{p}|\lambda\rangle)}{E_\lambda(0) - E_\eta(0)}$$

$$|\mathbf{k},\lambda\rangle = |\lambda\rangle + \frac{\hbar}{m_0}\sum_{\eta\neq\lambda}\frac{|\eta\rangle\mathbf{k}\cdot\langle\eta|\mathbf{p}|\lambda\rangle}{E_\lambda(0) - E_\eta(0)}$$

Conduction & valence band effective mass

- Assume 2 bands only, 0 and 1, with $E_0 = E_g$ and $E_1 = 0$

$$E_{0,1}(k) = E_{0,1} + \frac{\hbar^2 k^2}{2m_0} \pm \sum_{ij} \frac{\hbar^2 k_i k_j}{2m_0} \frac{2p_i^* p_j}{m_0 E_g}$$

$$= \langle 0|\hat{p}_j|1\rangle$$

- Effective mass tensor

$$\left(\frac{1}{m_{eff}}\right)_{ij} = \frac{1}{\hbar^2} \left.\frac{\partial^2 E(k)}{\partial k_i \partial k_j}\right|_{k=0} = \frac{1}{m_0}\left(\delta_{ij} \pm \frac{2p_i^* p_j}{m_0 E_g}\right)$$

- Isotropic:

$$m_i = \frac{m_0}{1 \pm \frac{2p^2}{m_0 E_g}}$$

l = c,v
The effective mass for the lower (valence) band can be negative

- Reduce e-h effective mass

$$\frac{1}{m_r} = \frac{1}{m_e} + \frac{1}{m_h} = \frac{4p^2}{m_0^2 E_g}$$

Degenerate Valence Bands

- Valence band originates from p orbitals
- 4 states $|l=0, m_l=0\rangle = |0,0\rangle,\ |1,\pm 1\rangle,\ |1,0\rangle$

$$\langle l, m_l | H_0 + \frac{\hbar}{m_0}(\mathbf{k}\cdot\mathbf{p} - \bar{E}(k)|\psi(\mathbf{k})\rangle = 0$$

$$|\psi(\mathbf{k})\rangle = \sum_{l',m'_{l'}} c_{l',m'_{l'}}(\mathbf{k})|l', m'_{l'}\rangle \qquad \langle l, m_l|\mathbf{k}\cdot\mathbf{p}|l', m'_{l'}\rangle = kp\delta_{l,l'\pm 1}\delta_{m_l,m'_{l'}}$$

$$A = \hbar p/m_0 \qquad \begin{pmatrix} E_0 - \bar{E} & 0 & Ak & 0 \\ 0 & E_1 - \bar{E} & 0 & 0 \\ Ak & 0 & E_1 - \bar{E} & 0 \\ 0 & 0 & 0 & E_1 - \bar{E} \end{pmatrix} = 0$$

$$E = E_1 + \frac{\hbar^2 k^2}{2m_0} \qquad E = \frac{\hbar^2 k^2}{2m_0} + \frac{E_g}{2}\left(1 \pm \sqrt{1 + \frac{4A^2k^2}{Eg^2}}\right)$$

2 bands unaffected

One band with positive curvature

Degenerate Valence Bands

- In the presence of spin, we need to consider total angular momentum

$$\mathbf{J} = \mathbf{L} + \mathbf{s}$$

- 6 states:

$$|3/2, \pm 3/2\rangle = \begin{cases} |m_l = +1, m_s = \uparrow\rangle \\ |m_l = -1, m_s = \downarrow\rangle \end{cases}$$

$$|3/2, \pm 1/2\rangle = \frac{1}{\sqrt{3}} \begin{cases} \sqrt{2}|0, \uparrow\rangle + |1, \downarrow\rangle \\ \sqrt{2}|0, \downarrow\rangle + |-1, \uparrow\rangle \end{cases}$$

$$|1/2, \pm 1/2\rangle = \frac{1}{\sqrt{3}} \begin{cases} -|0, \uparrow\rangle + \sqrt{2}|1, \downarrow\rangle \\ -|0, \downarrow\rangle + \sqrt{2}|-1, \uparrow\rangle \end{cases}$$

Split to lower energies due to spin-orbit interaction

Can be ignored

Degenerate Valence Bands

- 4 degenerate valence bands described by spherical symmetric H

$$H = \frac{\hbar^2}{2m_0}\left[\left(\gamma_1 + \frac{5}{2}\gamma_2\right)k^2 - 2\gamma_2(\mathbf{k}\cdot\mathbf{J})^2\right]$$

$$E = \frac{\hbar^2 k^2}{2m_0}\left(\gamma_1 + \frac{5}{2}\gamma_2 - 2\gamma_2 m_j^2\right)$$

$$E_{hh} = (\gamma_1 - 2\gamma_2)\frac{\hbar^2 k^2}{2m_0} \qquad m_j = \pm\frac{3}{2}$$

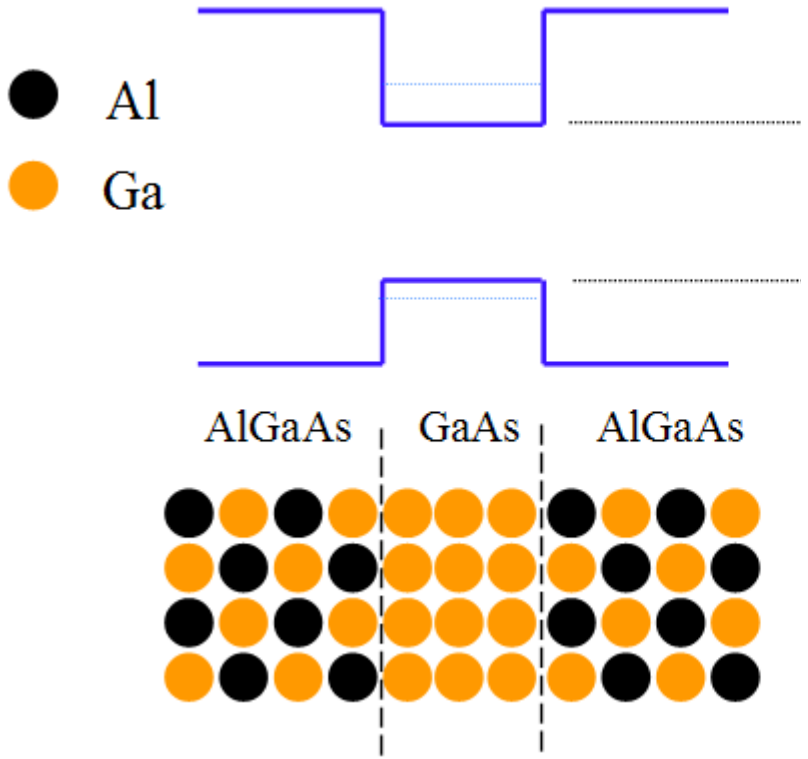
$$E_{lh} = (\gamma_1 + 2\gamma_2)\frac{\hbar^2 k^2}{2m_0} \qquad m_j = \pm\frac{1}{2}$$

$$\frac{1}{m_{hh}} = \frac{1}{m_0}(\gamma_1 - 2\gamma_2) \qquad \frac{1}{m_{lh}} = \frac{1}{m_0}(\gamma_1 + 2\gamma_2)$$

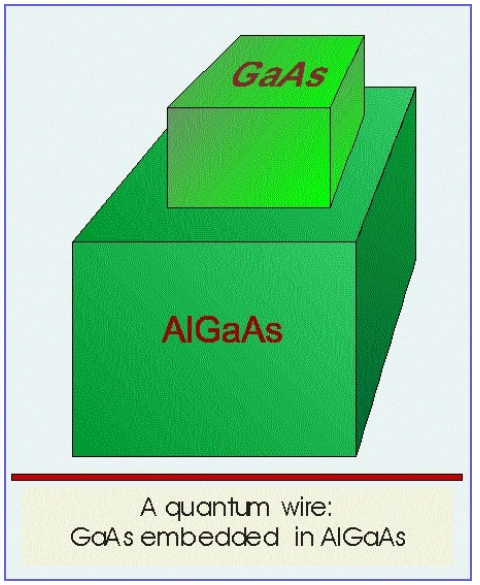
4. Nanostructures

Nanostructures

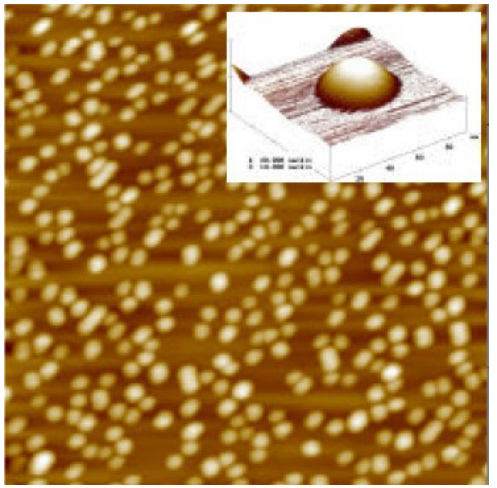
Quantum Well



Quantum Wire



Quantum Dot



Electrons confined in 1, 2 or 3 dimensions

Envelope function approximation

- Quantum well

$$\psi(\mathbf{r}) = \zeta_n(z)\frac{e^{i(k_x x + k_y y)}}{L}u_\lambda(\mathbf{k} \approx 0, \mathbf{r})$$

- Quantum wire

$$\psi(\mathbf{r}) = \zeta_n(x)\zeta_m(y)\frac{e^{ik_z z}}{\sqrt{L}}u_\lambda(\mathbf{k} \approx 0, \mathbf{r})$$

- Quantum dot

$$\psi(\mathbf{r}) = \zeta_n(x)\zeta_m(y)\zeta_p(z)u_\lambda(\mathbf{k} \approx 0, \mathbf{r})$$

- Density of states changes with dimensionality

$$N_3(E) \sim E^{3/2} \Rightarrow D_3(E) \sim \sqrt{E}$$

$$N_2(E) \sim E \Rightarrow D_2(E) \sim const.$$

$$N_1(E) \sim E^{1/2} \Rightarrow D_3(E) \sim 1/\sqrt{E}$$

Quantum Wells (I)

- Assuming infinitely deep walls

$$V(z) = \begin{cases} 0 & \text{for} -L_c/2 < z < L_c/2 \\ \infty & \text{for} |z| > L_c/2 \end{cases}$$

$$\left[-\frac{\hbar^2}{2m_0}\frac{\partial^2}{\partial z^2} + V(z) \right] \zeta(z) = E_z \zeta(z) \qquad \zeta(\pm L_c/2) = 0$$

$$\zeta(z) = A\sin(k_z z) + B\cos(k_z z) \qquad k_z^2 = \frac{2m_0}{\hbar^2} E_z$$

Even & odd solutions

$$\zeta_{even}(z) = \sqrt{\frac{2}{L_c}}\cos(k_z z) \qquad \zeta_{odd}(z) = \sqrt{\frac{2}{L_c}}\sin(k_z z)$$

$$k_{z,even} = \frac{\pi}{L_c}(2n-1) \qquad k_{z,odd} = \frac{\pi}{L_c}2n \qquad \text{n=1,2,3,...}$$

$$E_z = \frac{\pi^2\hbar^2}{2m_0 L_c^2}\bar{n}^2$$

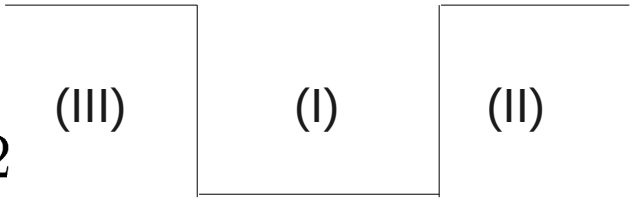
$$\boxed{E = \frac{\hbar^2}{2m_0}\left(\frac{\bar{n}^2\pi^2}{L_c^2} + k_\perp^2\right)}$$

Quantum Wells (II)

- Assuming finite potential walls

$$V(z) = \begin{cases} 0 & \text{for} -L_c/2 < z < L_c/2 \\ V_c & \text{for} |z| > L_c/2 \end{cases}$$

- 3 regions



$$\zeta_{even}(z) = \begin{cases} B\cos k_z z \text{for} -L_c/2 < z < L_c/2 \\ Ce^{-K_z z} \text{for} z > L_c/2 \\ Ce^{K_z z} \text{for} z < -L_c/2 \end{cases}$$

$$K_z^2 = \frac{2m_0}{\hbar^2}(V_c - E)$$

$$\pm\sqrt{E_z}\tan\left(\sqrt{m_0\frac{E_z}{2\hbar^2}}L_c\right) = \sqrt{V_c - E_z}$$

$$\zeta_{odd}(z) = \begin{cases} B\sin k_z z \text{for} -L_c/2 < z < L_c/2 \\ Ce^{-K_z z} \text{for} z > L_c/2 \\ Ce^{K_z z} \text{for} z < -L_c/2 \end{cases}$$

Quantum Wells (III)

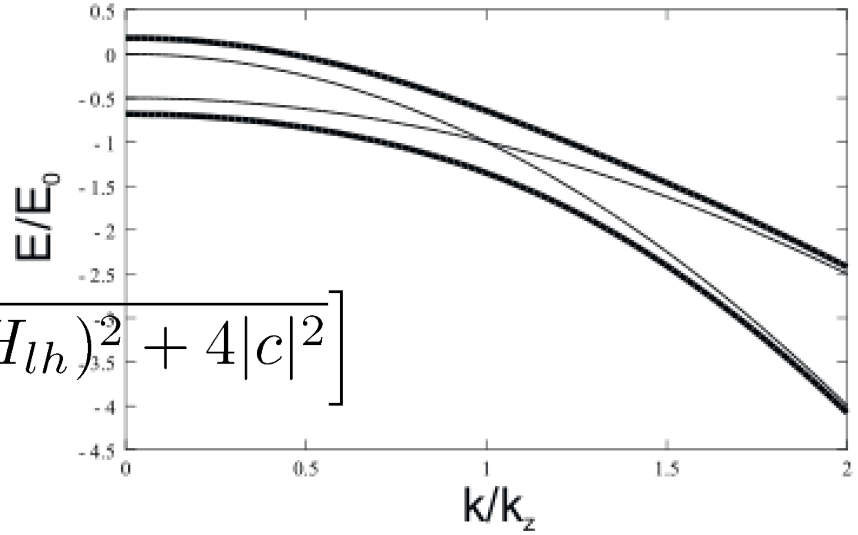
- Valence bands

$$\langle m_j'|H|m_j\rangle = \begin{pmatrix} H_{hh} & b & c & 0 \\ b^* & H_{lh} & 0 & c \\ c^* & 0 & H_{lh} & -b \\ 0 & c^* & -b^* & H_{hh} \end{pmatrix} = 0 \qquad b \propto \langle p_z \rangle = 0$$

$$H_{hh} = \frac{1}{2m_0}\langle p_z^2\rangle(\gamma_1 - 2\gamma_2) + \frac{\hbar^2(k_x^2+k_y^2)}{2m_0}(\gamma_1+\gamma_2)$$

$$H_{lh} = \frac{1}{2m_0}\langle p_z^2\rangle(\gamma_1 + 2\gamma_2) + \frac{\hbar^2(k_x^2+k_y^2)}{2m_0}(\gamma_1-\gamma_2)$$

$$E_{1,2} = \frac{1}{2}\left[(H_{hh}+H_{lh}) \pm \sqrt{(H_{hh}-H_{lh})^2 + 4|c|^2}\right]$$



Summary

- Electron in periodic potential described by Bloch function
- Description possible with Wannier (localized) or Bloch(delocalized) functions
- Tight binding approximation: electron wavefunction can be approximated as a sum of atomic orbitals
  - Conduction & valence bands formed; energy gaps created
- k.p theory: treats k dependence as a perturbation around k=0 point
  - Valence bands: HH, LH and SO split off band
- Dimensionality matters: HH-LH degeneracy is lifted at k=0 in nanostructures