In This Lecture:

- Envelope Function Approximation for Low-dimensional Structures
- Block Diagonalization of PB Hamiltonian
- QW Band Structure with Strain
Low-Dimensional Structures

Quantum Well

Superlattice

Quantum Wire

Self-assembled quantum dots

Nanocrystals
**Envelope Function Approximation (EFA)**
(a.k.a. Effective Mass Theory)

**What’s it for?**

- Treating an additional external (slowly-varying) potential
e.g., an impurity, quantum confinement (QW), excitonic potential etc.

**Perfect bulk xtal**

\[ H_0 \psi_{nk}(r) = E_n(k) \psi_{nk}(r) \]

use \( k.p \), LK etc.

**An impurity potential**

\[ [H_0 + U(r)] \psi(r) = E \psi(r) \]

use EFA

Ref: Chuang
EFA for a Single Band

Defining $H_0|n\ k\rangle = E_n(k)|n\ k\rangle$, therefore $|n\ k\rangle$ form a complete set.

So, one can expand the solution including the perturbation as

$$\psi(\vec{r}) = \langle \vec{r} | \sum_n \int_{BZ} \frac{d^3k}{(2\pi)^3} a_n(\vec{k}) | n\vec{k}\rangle$$

Using the orthonormality property $\langle n\ k | n'\ k' \rangle = \delta_{n, n'} \delta(k - k')$

The perturbed equation can easily be converted to:

$$(E_n(k) - E)a_n(k) + \sum_{n'} \int_{B.Z.} \frac{d^3k'}{(2\pi)^3} \langle n\ k | U | n'\ k' \rangle a_{n'}(k') = 0$$

$$\int d^3r \psi^*_{nk}(r) U(r) \psi_{n'k'}(r)$$

Ref: Chuang
\[ \langle n_k | U | n'_k' \rangle = \int \text{d}^3 r \ e^{-i(k-k') \cdot r} u^*_n(r) u_{n'_k}(r) U(r) \]

periodic in \( r \)

\[ u^*_n(r) u_{n'_k}(r) = \sum_{G} C(n_k, n'_k', G) e^{iG \cdot r} \]

over all RLVs

\[ \widetilde{U}_k = \int U(r) e^{-i k \cdot r} \text{d}^3 r \]

Inverse Fourier xform

\[ U(r) = \int \widetilde{U}_k e^{i k \cdot r} \frac{\text{d}^3 k}{(2\pi)^3} \]

Fourier xform

Approximations:

\[ \langle n_k | U | n'_k' \rangle \propto \delta_{nn'} \quad U(r) \text{ small; causes no band mixing} \]

\[ |\tilde{U}_{k-k'-G}|_{G \neq 0} \ll |\tilde{U}_{k-k'}| \quad U(r) \text{ slowly varying} \]

Ref: Chuang
The resultant equation for \( a_n(k) \) becomes

\[
(E_n(k) - E)a_n(k) + \int \frac{d^3k'}{(2\pi)^3} \tilde{U}_{k-k'}a_n(k') = 0
\]

Convolution of \( U \) & \( F \) in \( k \)-space

\[
[E_n(-i\nabla) + U(r)]F(r) = EF(r)
\]

Becomes multiplication in real space

if we define \( F(r) = \int a_n(k') e^{i k' \cdot r} \frac{d^3k'}{(2\pi)^3} \) (envelope function)

The solution including \( U \) becomes

\[
\psi(r) = \int a_n(k') \psi_{nk'}(r) \frac{d^3k'}{(2\pi)^3}
\]

\[
\simeq \int a_n(k') e^{i k' \cdot r} u_{nk_0}(r) \frac{d^3k'}{(2\pi)^3}
\]

\[
= F(r) u_{nk_0}(r)
\]

Ref: Chuang
So, EFA proceeds by replacing \( \mathbf{k} \rightarrow -i\mathbf{\nabla} \) in the dispersion relation

Recall that in the single-band k.p theory:

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

Hence, the envelope function is obtained by solving

\[
\left[ \sum_{\alpha, \beta} \frac{\hbar^2}{2} \left( \frac{1}{m^*} \right)_{\alpha\beta} \left( -i \frac{\partial}{\partial x_\alpha} \right) \left( -i \frac{\partial}{\partial x_\beta} \right) + U(\mathbf{r}) \right] F(\mathbf{r}) = \left[ E - E_n(0) \right] F(\mathbf{r})
\]

So within EFA, the Hamiltonian including \( U(\mathbf{r}) \) is satisfied by

\[
\psi(\mathbf{r}) = F(\mathbf{r}) u_{nk_0}(\mathbf{r})
\]

Ref: Chuang
How about Degenerate Bands?

The procedure to obtain EFA is just like the single-band case.

The main discrepancy is the free-xtal Hamiltonian:

$$H\psi_{nk}(\mathbf{r}) = E(\mathbf{k})\psi_{nk}(\mathbf{r})$$

$$H = \frac{p^2}{2m_0} + V(\mathbf{r}) + H_{so}$$

$$H_{so} = \frac{\hbar}{4m_0c^2} \nabla V \times \mathbf{p} \cdot \mathbf{\sigma}$$

$$\sum_{j' = 1}^{6} H_{j' j}^{LK} a_{j'}(\mathbf{k}) = \sum_{j' = 1}^{6} \left[ E_j(0) \delta_{jj'} + \sum_{\alpha, \beta} D_{jj'}^{\alpha \beta} k_\alpha k_\beta \right] a_{j'}(\mathbf{k}) = E(\mathbf{k}) a_j(\mathbf{k})$$

Ref: Chuang
Our aim is to solve in the presence of perturbation \( U(r) \)

\[
[H + U(r)]\psi(r) = E\psi(r)
\]

The envelope function now picks a band index:

\[
\psi(r) = \sum_{j=1}^{6} F_j(r) u_{\beta j}(r)
\]

where, again we replace \( k \rightarrow -i\hat{\nabla} \) in the (LK) dispersion relation

\[
\sum_{j'=1}^{6} \left[ E_j(0) \delta_{jj'} + \sum_{\alpha, \beta} D_{j'j}^{\alpha\beta} \left( -i \frac{\partial}{\partial x_\alpha} \right) \left( -i \frac{\partial}{\partial x_\beta} \right) + U(r) \delta_{jj'} \right] F_j(r) = EF_j(r)
\]

Note that if \( U(r) \equiv 0 \), the solutions for the envelope functions reduce to

\[
F_j(r) = a_j(k) e^{i k \cdot r} \quad \text{i.e., back to plane waves}
\]

Ref: Chuang
Quantum Wells

Confinement due to bandgap difference

Various band edge line-ups

Ref: Singh
Consider a QW formed by two Type-I heterostructures (AlAs/GaAs/AlAs)
QW: a sketch of what to expect

**subband formation**

\[ E = \frac{\hbar^2 k^2}{2m^*} + E_1 \]

\[ E = \frac{\hbar^2 k^2}{2m^*} + E_2 \]

**Parabolic two-dimensional subbands**

Ref: Singh
Application of EFA to QWs

Conduction Band: (single band EFA)

\[ E(k) = \frac{\hbar^2 k^2}{2m^*} \]

Dispersion relation

use corresponding well/barrier effective mass

The task for EFA is to incorporate the confinement potential

\[ V(z) = \begin{cases} 
V_0 = \Delta E_c & |z| > \frac{L_w}{2} \\
0 & |z| \leq \frac{L_w}{2}
\end{cases} \]

corresponding well region CB edge

Ref: Chuang
Single band EFA reads

\[
\left[-\frac{\hbar^2}{2} \frac{\partial}{\partial z} \frac{1}{m(z)} \frac{\partial}{\partial z} + \frac{\hbar^2}{2m(z)} \nabla_z^2 + V(z)\right] \psi(r) = E \psi(r)
\]

This ordering is to ensure the Hermiticity and the continuity of \(j_z\) across the heterojunction (controversial, more later...)

\[j_z(z) \sim \frac{1}{m(z)} \left[ \psi^* \frac{\partial}{\partial z} \psi - \psi \frac{\partial \psi^*}{\partial z} \right] \]

Since there is no confinement on the \(xy\) plane:

\[\psi(r) = \frac{e^{i \mathbf{k} \cdot \mathbf{r}}}{\sqrt{A}} \psi(z)\]

\[-\frac{\hbar^2}{2} \frac{\partial}{\partial z} \frac{1}{m(z)} \frac{\partial}{\partial z} \psi(z) + V(z)\psi(z) = \left(E(k_z) - \frac{\hbar^2 k_z^2}{2m(z)}\right) \psi(z)\]

To solve, use finite difference, finite element or transfer matrix method ...

Ref: Chuang
Valence Band: (SO band will be neglected)

Confinement potential: \( V_h(z) = \begin{cases} 
0 & |z| \leq \frac{L_w}{2} \\
-\Delta E_v & |z| > \frac{L_w}{2} 
\end{cases} \)

1\textsuperscript{st} destination is band-edge energies:

Note that at \( k_x = k_y = 0 \) LK Hamiltonian is diagonal, i.e., HH LH do not mix!

Define:

\[
E_{\text{HH}}(k_z) = -\frac{\hbar^2}{2m_0} (\gamma_1 - 2\gamma_2) k_z^2
\]

\[
E_{\text{LH}}(k_z) = -\frac{\hbar^2}{2m_0} (\gamma_1 + 2\gamma_2) k_z^2
\]

\[
m_{\text{hh}}^z = \frac{m_0}{\gamma_1 - 2\gamma_2}
\]

\[
m_{\text{lh}}^z = \frac{m_0}{\gamma_1 + 2\gamma_2}
\]

Ref: Chuang
So for the valence band-edge energies solve:

\[
\begin{bmatrix}
\frac{\hbar^2}{2} \frac{\partial}{\partial z} + \frac{1}{m^*(m)} \frac{\partial}{\partial z} + V_h(z)
\end{bmatrix} g_{(m)}(z) = E_{g(m)}(z)
\]

solution yields valence band-edge energies

\[
m_{hh} \quad \text{or} \quad m_{lh}
\]

EFA becomes dubious

variation of band-edge energies with well width

Ref: Chuang
Now comes valence subband dispersion relations

\[
\begin{bmatrix}
\mathbf{H}^{LK}(k_x, k_y, k_z) - i \frac{\partial}{\partial z} + V_k(z) \mathbf{I}
\end{bmatrix} \cdot 
\begin{bmatrix}
F_1 \\
F_2 \\
F_3 \\
F_4
\end{bmatrix} = E 
\begin{bmatrix}
F_1 \\
F_2 \\
F_3 \\
F_4
\end{bmatrix}
\]

SO bands are neglected

\[
\mathbf{H}^{LK}_{6 \times 6} = 
\begin{bmatrix}
P + Q & -S & R & 0 & -S/\sqrt{2} & \sqrt{2} R \\
-S^+ & P - Q & 0 & R & -\sqrt{2} Q & \sqrt{3}/2 S \\
R^+ & 0 & P - Q & S & \sqrt{3}/2 S^+ & \sqrt{2} Q \\
0 & R^+ & S^+ & P + Q & -\sqrt{2} R^+ & -S^+ / \sqrt{2} \\
-S^+ / \sqrt{2} & -\sqrt{2} Q^+ & \sqrt{3}/2 S^+ & -\sqrt{2} R & P + \Delta & 0 \\
\sqrt{2} R^+ & \sqrt{3}/2 S^+ & \sqrt{2} Q^+ & -S/\sqrt{2} & 0 & P + \Delta
\end{bmatrix}
\]

Envelope functions in vector form: \( \mathbf{F}_k(\mathbf{r}) = \frac{\mathbf{g}_3/2(k_x, k_y, z)}{\sqrt{A}} \frac{\mathbf{g}_1/2(k_x, k_y, z)}{\sqrt{A}} \frac{\mathbf{g}_{-1/2}(k_x, k_y, z)}{\sqrt{A}} \frac{\mathbf{g}_{-3/2}(k_x, k_y, z)}{\sqrt{A}} \)

Ref: Chuang
QW wavefunctions

\[ \psi_k(r) = F_1 \left( \frac{3}{2}, \frac{3}{2} \right) + F_2 \left( \frac{3}{2}, \frac{1}{2} \right) + F_3 \left( \frac{3}{2}, -\frac{1}{2} \right) + F_4 \left( \frac{3}{2}, -\frac{3}{2} \right) \]

\[ \text{e}^{i k_x x + i k_y y} \]

\[ = \frac{1}{\sqrt{A}} \sum_{\nu} g_{\nu}(k_x, k_y, z) \left| \frac{3}{2}, \nu \right> \]

where \( \nu = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, \) and \(-\frac{3}{2}\). Denote

\[ k_t = \hat{x} k_x + \hat{y} k_y \]

We write

\[ \left[ \overline{H}^{LK} \left( k_t, k_z = -i \frac{\partial}{\partial z} \right) + V_h(z) \right] \cdot \begin{bmatrix} g_{3/2}(k_t, z) \\ g_{1/2}(k_t, z) \\ g_{-1/2}(k_t, z) \\ g_{-3/2}(k_t, z) \end{bmatrix} = E(k_t) \begin{bmatrix} g_{3/2}(k_t, z) \\ g_{1/2}(k_t, z) \\ g_{-1/2}(k_t, z) \\ g_{-3/2}(k_t, z) \end{bmatrix} \]

Ref: Chuang
Typical VB Dispersion with LK+EFA

Ref: Chuang
Include Strain: Pikus-Bir Hamiltonian

A technical trick: Block Diagonalization of PB

Introduced by Broido-Sham (1985)

Start with the PB (including strain) Hamiltonian for HH-LH bands

\[
\begin{pmatrix}
P + Q & -S & R & 0 \\
-S^+ & P - Q & 0 & R \\
R^+ & 0 & P - Q & S \\
0 & R^+ & S^+ & P + Q
\end{pmatrix} \begin{pmatrix}
|\frac{3}{2}, \frac{3}{2}\rangle \\
|\frac{3}{2}, \frac{1}{2}\rangle \\
|\frac{3}{2}, -\frac{1}{2}\rangle \\
|\frac{3}{2}, -\frac{3}{2}\rangle
\end{pmatrix}
\]

Define the phase angles as: \( R = |R| e^{i\theta_R} \) \( S = |S| e^{i\theta_S} \)

Ref: Chuang
This 4x4 Hamiltonian can be transformed into two 2x2 blocks as:

\[
\begin{bmatrix}
P + Q & \tilde{R} & 0 & 0 \\
\tilde{R}^+ & P - Q & 0 & 0 \\
0 & 0 & P - Q & \tilde{R} \\
0 & 0 & \tilde{R}^+ & P + Q \\
\end{bmatrix}
\]

where \( \tilde{R} = \langle R \rangle - i |S| \) \( \tilde{R}^+ = \langle R \rangle + i |S| \)

The transformation bet. old and new bases:

\[
\begin{align*}
|1\rangle &= \alpha \frac{3}{2}, \frac{3}{2} \rangle - \alpha^* \frac{3}{2}, -\frac{3}{2} \rangle \\
|2\rangle &= -\beta^* \frac{3}{2}, \frac{1}{2} \rangle + \beta \frac{3}{2}, -\frac{1}{2} \rangle \\
|3\rangle &= \beta^* \frac{3}{2}, \frac{1}{2} \rangle + \beta \frac{3}{2}, -\frac{1}{2} \rangle \\
|4\rangle &= \alpha \frac{3}{2}, \frac{3}{2} \rangle + \alpha^* \frac{3}{2}, -\frac{3}{2} \rangle
\end{align*}
\]

where

\[
\begin{align*}
\alpha &= \frac{1}{\sqrt{2}} e^{i[(\theta_S + \theta_R)/2] + \pi/4} \\
\beta &= \frac{1}{\sqrt{2}} e^{i[(\theta_S - \theta_R)/2] + \pi/4}
\end{align*}
\]

\[
\begin{bmatrix}
\alpha^* & 0 & 0 & -\alpha \\
0 & -\beta & \beta^* & 0 \\
0 & \beta & \beta^* & 0 \\
\alpha^* & 0 & 0 & \alpha
\end{bmatrix}
\]

Ref: Chuang
Effect of Strain on the Band Structure

Figure 4.8. The energy-band structure in the momentum space for a bulk Ga$_x$In$_{1-x}$As material under (a) biaxial compression, (b) lattice-matched condition, and (c) biaxial tension for different Ga mole fractions $x$. The heavy-hole band is above the light-hole band and its effective mass in the transverse plane (the $k_x$ or $k_y$ direction) is lighter than that of the light-hole band in the compressive strain case in (a). The light-hole band shifts above the heavy-hole band in the case of tension in (c). (After Ref. 37.)

Ref: Chuang
QW Bandstructure: Now with the strain included

- Assume the barrier regions to be under no strain
  (same/lattice-matched substrate)
- Set the energy reference to band edge of unstrained crystal

Ref: Chuang
Subband Energies in a Strained QW

Conduction Subbands

\[ E_c(z) = \begin{cases} 
  a_c(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) & |z| \leq \frac{L_w}{2} \\
  \Delta E_c & |z| > \frac{L_w}{2}
\end{cases} \]

where

\[ \varepsilon_{xx} = \varepsilon_{yy} = (a_0 - a)/a \quad \text{and} \quad \varepsilon_{zz} = -2(C_{12}/C_{11})\varepsilon_{xx} \]

Conduction subbands can be obtained using single-band EFA

What we need are the dispersion relation and the confinement potential

Ref: Chuang
Valence Subband Energies (w/o SO bands)

> Without SO bands, HH and LH bands are uncoupled at $k=0$

> So the subband energies are determined as in single-band EFA

\[
E_{\text{HH}}(z) = \begin{cases} 
-P_e - Q_e & |z| \leq \frac{L_w}{2} \\
-\Delta E_v & |z| > \frac{L_w}{2}
\end{cases}
\]

\[
m_{\text{hh}}^{\bar{r}} = \begin{cases} 
\frac{m_0}{\gamma_{1w} - 2\gamma_{2w}} & |z| \leq \frac{L_w}{2} \\
\frac{m_0}{\gamma_{1b} - 2\gamma_{2b}} & |z| > \frac{L_w}{2}
\end{cases}
\]

\[
E_{\text{LH}}(z) = \begin{cases} 
-P_e + Q_e & |z| \leq \frac{L_w}{2} \\
-\Delta E_v & |z| > \frac{L_w}{2}
\end{cases}
\]

\[
m_{\text{lh}}^{\bar{r}} = \begin{cases} 
\frac{m_0}{\gamma_{1w} + 2\gamma_{2w}} & |z| \leq \frac{L_w}{2} \\
\frac{m_0}{\gamma_{1b} + 2\gamma_{2b}} & |z| > \frac{L_w}{2}
\end{cases}
\]

where

\[
P_e = -a_v(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz})
\]

\[
Q_e = \frac{-b}{2}(\epsilon_{xx} + \epsilon_{yy} - 2\epsilon_{zz})
\]

Ref: Chuang
Valence Subband Dispersions in a Strained QW (w/o SO bands)

Use the 4x4 upper block of the (bulk) LK matrix with $k_z \rightarrow -i \frac{\partial}{\partial z}$

\[
\begin{bmatrix}
\bar{H}\left(k_z = -i \frac{\partial}{\partial z}\right) + V_h(z)I
\end{bmatrix}
\cdot
\begin{bmatrix}
g_{3/2}(k_t, z) \\
g_{1/2}(k_t, z) \\
g_{-1/2}(k_t, z) \\
g_{-3/2}(k_t, z)
\end{bmatrix}
= E(k_t)
\begin{bmatrix}
g_{3/2}(k_t, z) \\
g_{1/2}(k_t, z) \\
g_{-1/2}(k_t, z) \\
g_{-3/2}(k_t, z)
\end{bmatrix}
\]

All strain-related band edge shifts are here

envelope functions

dispersion relation

use the unstrained band edge confinement

\[V_h(z) = E_v^0(z) = \begin{cases} 
0 & |z| \leq \frac{L_w}{2} \\
-\Delta E_v & |z| > \frac{L_w}{2}
\end{cases}\]

Ref: Chuang
Results for Valence Subband Dispersion w/o SO

Observe nonparabolicity due to band mixing!

No strain

FIG. 5. The valence-band structures for Ga$_x$In$_{1-x}$As grown on an In$_{1-x}$Ga$_x$As$_y$P$_{1-y}$ (band-gap wavelength is 1.3 μm) lattice matched to InP for (a) compression (x = 0.37), (b) lattice-matched case (x = 0.468), (c) small tension (x = 0.55), and (d) large tension (x = 0.60). The wave vector $k_x$ along the horizontal axis is normalized by $2\pi/a_0$.

Ref: Chuang, PRB 1991
Valence Band Energies (with SO bands)

Recall the 6x6 LK Hamiltonian at the band edge (k=0):

\[
\mathbf{H}(k = 0) = -\begin{bmatrix}
P_e + Q_e & 0 & 0 & 0 & 0 & 0 \\
0 & P_e - Q_e & 0 & 0 & -\sqrt{2} Q_s & 0 \\
0 & 0 & P_e - Q_e & 0 & 0 & \sqrt{2} Q_s \\
0 & 0 & 0 & P_e + Q_e & 0 & 0 \\
0 & -\sqrt{2} Q_s & 0 & 0 & P_e + \Delta & 0 \\
0 & 0 & \sqrt{2} Q_s & 0 & 0 & P_e + \Delta \\
\end{bmatrix}
\]

LH and SO bands are coupled even at k=0 due to strain
So they are not pure states (even at k=0); for the subband energies solve:

\[
\begin{bmatrix}
-P_e + Q_e & \pm \sqrt{2} Q_e \\
\pm \sqrt{2} Q_e & -P_e - \Delta
\end{bmatrix}
\begin{bmatrix}
F_{3/2, \pm 1/2} \\
F_{1/2, \pm 1/2}
\end{bmatrix}
= E(0)
\begin{bmatrix}
F_{3/2, \pm 1/2} \\
F_{1/2, \pm 1/2}
\end{bmatrix}
\]

\[
|F_{3/2, \pm 1/2}|^2 + |F_{1/2, \pm 1/2}|^2 = 1
\]

Ref: Chuang
Effect of SO bands on bulk band energies

Solution for band edge energies yields

\[ E_{HH}(0) = -P_{\varepsilon} - Q_{e} \]
\[ E_{LH}(0) = -P_{\varepsilon} + \frac{1}{2} \left( Q_{e} - \Delta + \sqrt{\Delta^2 + 2\Delta Q_{e} + 9Q_{e}^2} \right) \]
\[ E_{SO}(0) = -P_{\varepsilon} + \frac{1}{2} \left( Q_{e} - \Delta - \sqrt{\Delta^2 + 2\Delta Q_{e} + 9Q_{e}^2} \right) \]

FIG. 1. The energy band gap of a bulk In\textsubscript{1-x}Ga\textsubscript{x}As vs the Ga mole fraction \(x\). The dotted-dashed curve: unstrained In\textsubscript{1-x}Ga\textsubscript{x}As; the solid curves: transition energies from the conduction band (C) to the heavy-hole (HH) and light-hole (LH) bands for a bulk In\textsubscript{1-x}Ga\textsubscript{x}As pseudomorphically grown on InP; the dashed curve: the conduction to light-hole transition energy calculated without the SO coupling.

Ref: Chuang, PRB 1992
Effect of including SO bands on valence subband energies

Ref: Chuang, PRB 1992

**FIG. 7.** The valence subband structure for a 60-Å In$_{1-x}$Ga$_x$As quantum well sandwiched between InP barriers for (a) $x = 0.468$ (lattice-matched), (b) $x = 0.25$ (compressive strain), and (c) $x = 0.6$ (tensile strain). The solid curves: including the SO coupling; the dashed curves: ignoring the SO coupling.
Caveat: The k.p + EFA has some complications.

Such as:

- **Unphysical solutions:** particularly appearing within the gap making the systems seemingly metallic.

- **Dependence on operator orderings:** particularly in the case of heterostructures

For remedies, see:
