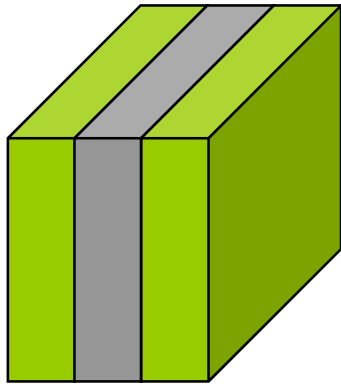


In This Lecture:

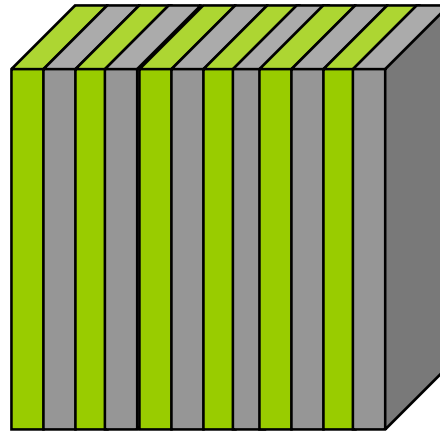
- Envelope Function Approximation for Low-dimensional Structures
- Block Diagonalization of PB Hamiltonian
- QW Band Structure with Strain

Low-Dimensional Structures

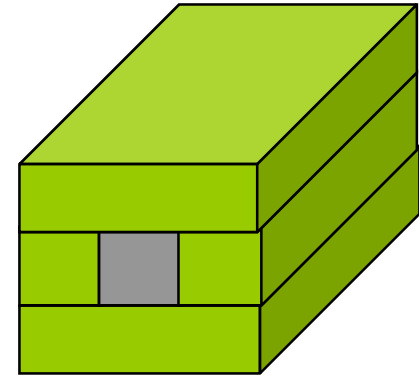
Quantum Well



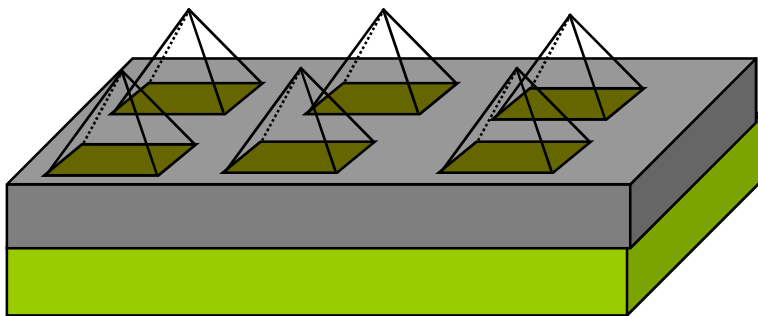
Superlattice



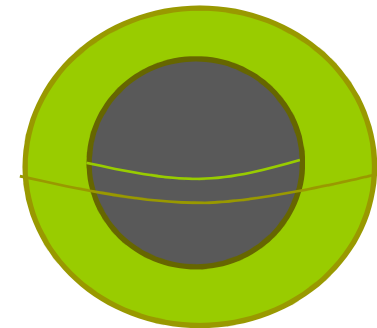
Quantum Wire



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.

A periodic crystal potential $V(\mathbf{r})$



Perfect bulk xtal

$$\underbrace{H_0 \psi_{n\mathbf{k}}(\mathbf{r}) = E_n(\mathbf{k}) \psi_{n\mathbf{k}}(\mathbf{r})}_{\text{use k.p, LK etc.}}$$

A periodic crystal potential $V(\mathbf{r})$ with an impurity potential $U(\mathbf{r})$



$$\underbrace{[H_0 + U(\mathbf{r})] \psi(\mathbf{r}) = E \psi(\mathbf{r})}_{\text{use EFA}}$$

An impurity potential $U(\mathbf{r})$



Ref: Chuang

EFA for a Single Band

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

So, one can expand the solution including the perturbation as

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

for infinite xtal

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

The perturbed equation can easily be converted to:

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

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

$$\langle n\mathbf{k}|U|n'\mathbf{k}'\rangle = \int d^3\mathbf{r} e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} \boxed{u_{n\mathbf{k}}^*(\mathbf{r})u_{n'\mathbf{k}'}(\mathbf{r})} \boxed{U(\mathbf{r})}$$

periodic in \mathbf{r}

$$u_{n\mathbf{k}}^*(\mathbf{r})u_{n'\mathbf{k}'}(\mathbf{r}) = \sum_{\mathbf{G}} \underbrace{C(n\mathbf{k}, n'\mathbf{k}', \mathbf{G})}_{\text{over all RLVs}} e^{i\mathbf{G}\cdot\mathbf{r}}$$

Fourier xform

$$\tilde{U}_{\mathbf{k}} = \int U(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} d^3\mathbf{r}$$

Inverse Fourier xform

$$U(\mathbf{r}) = \int \tilde{U}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \frac{d^3\mathbf{k}}{(2\pi)^3}$$

$$\langle n\mathbf{k}|U|n'\mathbf{k}'\rangle = \sum_{\mathbf{G}} C(n\mathbf{k}, n'\mathbf{k}', \mathbf{G}) \tilde{U}_{\mathbf{k}-\mathbf{k}'-\mathbf{G}}$$

Approximations:

$$\langle n\mathbf{k}|U|n'\mathbf{k}'\rangle \propto \delta_{nn'} \quad U(r) \text{ small; causes no band mixing}$$

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

The resultant equation for $a_n(\mathbf{k})$ becomes

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

inverse
Fourier
xform

Convolution of U & F in k -space

$$[E_n(-i\nabla) + U(\mathbf{r})]F(\mathbf{r}) = EF(\mathbf{r})$$

Becomes multiplication in real space

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

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

The solution
including U
becomes

$$\begin{aligned} \psi(\mathbf{r}) &= \int a_n(\mathbf{k}') \psi_{n\mathbf{k}'}(\mathbf{r}) \frac{d^3\mathbf{k}'}{(2\pi)^3} \\ &\simeq \int a_n(\mathbf{k}') e^{i\mathbf{k}' \cdot \mathbf{r}} u_{n\mathbf{k}_0}(\mathbf{r}) \frac{d^3\mathbf{k}'}{(2\pi)^3} \\ &= F(\mathbf{r}) u_{n\mathbf{k}_0}(\mathbf{r}) \end{aligned}$$

$u_{n\mathbf{k}}(\mathbf{r})$ final approx.

So, EFA proceeds by replacing $\mathbf{k} \rightarrow -i\vec{\nabla}$ 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

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

So within EFA, the Hamiltonian including $U(r)$ is satisfied by

$$\psi(\mathbf{r}) = F(\mathbf{r}) u_{n\mathbf{k}_0}(\mathbf{r})$$

How about Degenerate Bands?

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

The main discrepancy is the free-xtal Hamiltonian:

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

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

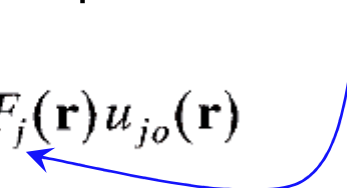
$$H_{\text{so}} = \frac{\hbar}{4m_0^2c^2} \nabla V \times \mathbf{p} \cdot \boldsymbol{\sigma}$$

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

Our aim is to solve in the presence of perturbation $U(r)$

$$[H + U(\mathbf{r})]\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

The envelope function now picks a band index:

$$\psi(\mathbf{r}) = \sum_{j=1}^6 F_j(\mathbf{r}) u_{j0}(\mathbf{r})$$


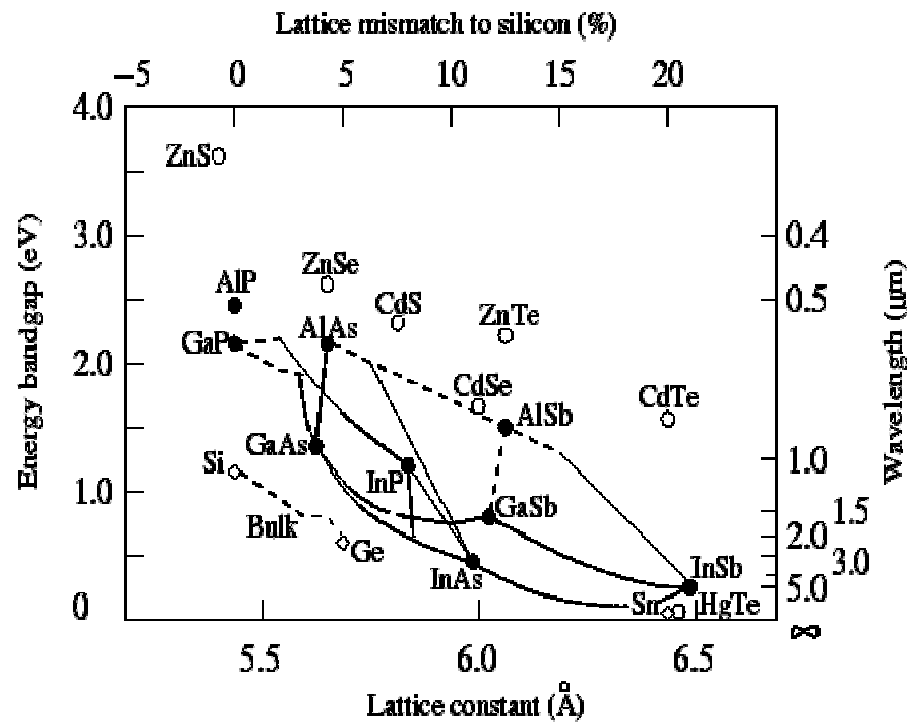
where, again we replace $\mathbf{k} \rightarrow -i\vec{\nabla}$ in the (LK) dispersion relation

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

Note that if $U(r) \equiv 0$, the solutions for the envelope functions reduce to $F_j(\mathbf{r}) = a_j(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}}$ i.e., back to plane waves

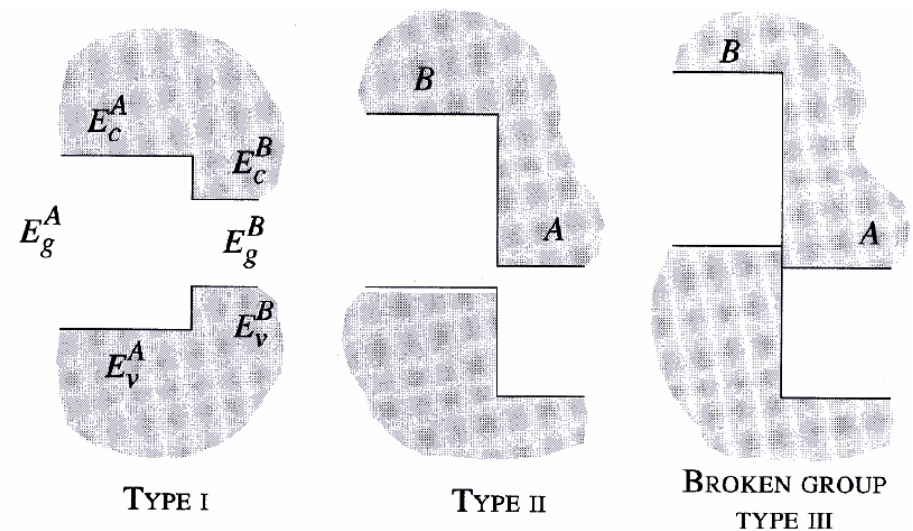
Quantum Wells

Confinement due to bandgap difference

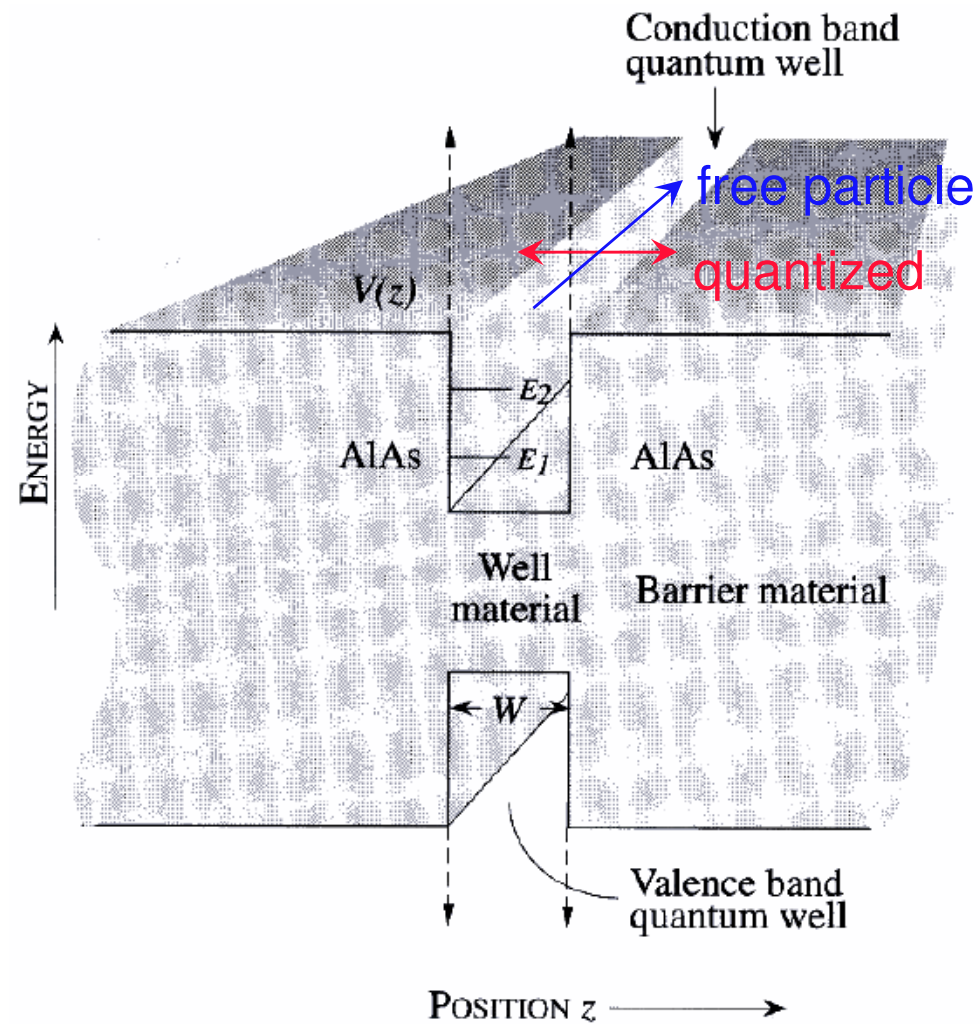


- ◊ = Elemental semiconductors
- = III - V semiconductors
- = II - VI semiconductors
- = Solid solution with direct bandgaps
- - - = Solid solution with indirect bandgaps

Various band edge line-ups

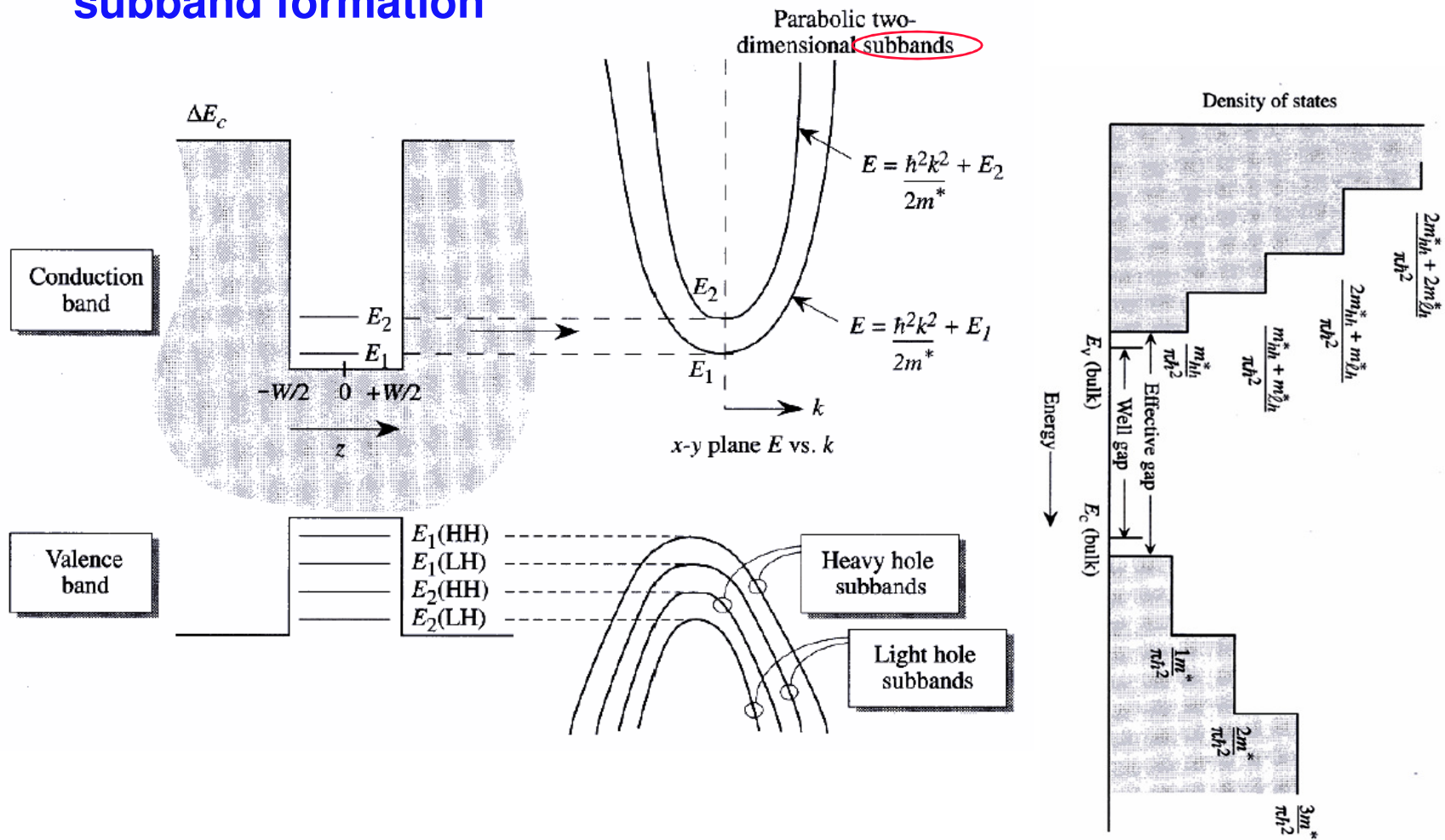


Consider a QW formed by two Type-I heterostructures (AlAs/GaAs/AlAs)



QW: a sketch of what to expect

subband formation



Application of EFA to QWs

Conduction Band: (single band EFA)

$$E(k) = \frac{\hbar^2 k^2}{2m^*} \quad \text{dispersion relation}$$

use corresponding well/barrier effective mass

The task for EFA is to incorporate the confinement potential

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

energy ref set to well region CB edge

Single band EFA reads

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

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: $\psi(\mathbf{r}) = \frac{e^{i\mathbf{k}_t \cdot \mathbf{r}}}{\sqrt{A}} \psi(z)$

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

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

Valence Band: (SO band will be neglected)

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

1st 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:

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

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

$$m_{\text{hh}}^z \equiv \frac{m_0}{\gamma_1 - 2\gamma_2}$$

$$m_{\text{lh}}^z \equiv \frac{m_0}{\gamma_1 + 2\gamma_2}$$

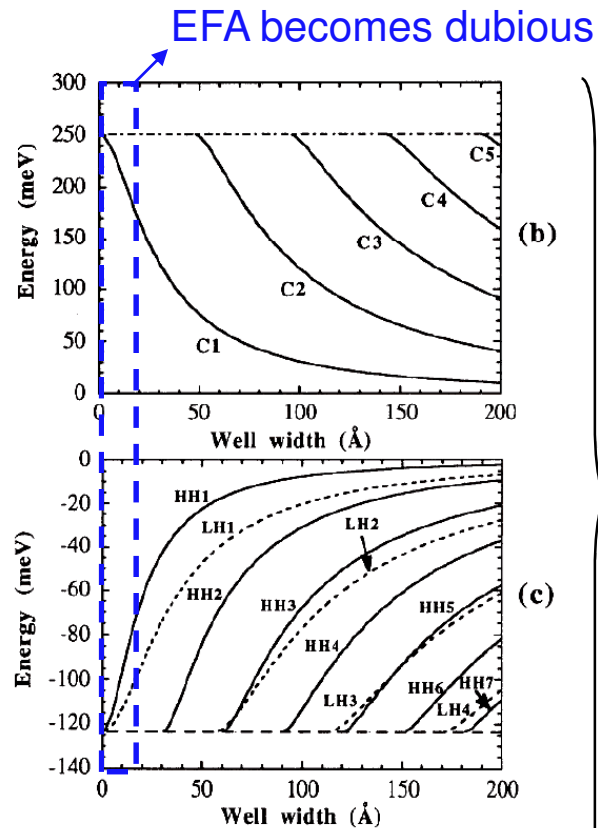
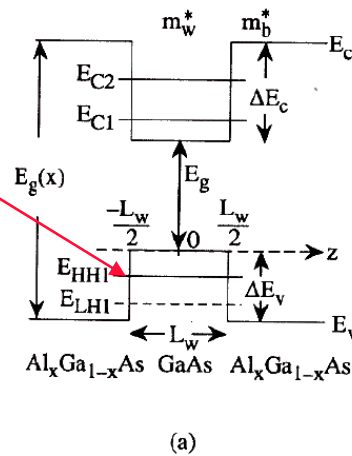
} use well / barrier values

So for the valence band-edge energies solve:

$$\left[+ \frac{\hbar^2}{2} \frac{\partial}{\partial z} \frac{1}{m_{(m)}^z} \frac{\partial}{\partial z} + V_h(z) \right] g_{(m)}(z) = E g_{(m)}(z)$$

m_{hh} OR m_{lh}

solution yields valence band-edge energies



variation of band-edge energies with well width

Figure 4.18. (a) Quantum-well profiles for the conduction and valence bands of a GaAs/Al_xGa_{1-x}As system. (b) Conduction subband energies, E_{C1}, E_{C2}, \dots , and (c) valence subband energies E_{HH1}, E_{HH2}, \dots , and E_{LH1}, E_{LH2}, \dots vs. the well width L_w .

Now comes valence subband dispersion relations

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

SO bands are neglected

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

Envelope functions in vector form: $\mathbf{F}_{\mathbf{k}}(\mathbf{r}) = \begin{bmatrix} F_1 \\ F_2 \\ F_3 \\ F_4 \end{bmatrix} = \begin{bmatrix} g_{3/2}(k_x, k_y, z) \\ g_{1/2}(k_x, k_y, z) \\ g_{-1/2}(k_x, k_y, z) \\ g_{-3/2}(k_x, k_y, z) \end{bmatrix} \frac{e^{ik_x x + ik_y y}}{\sqrt{A}}$

QW wavefunctions

$$\left\{ \begin{aligned} \psi_{\mathbf{k}}(\mathbf{r}) &= F_1 \left| \frac{3}{2}, \frac{3}{2} \right\rangle + F_2 \left| \frac{3}{2}, \frac{1}{2} \right\rangle + F_3 \left| \frac{3}{2}, -\frac{1}{2} \right\rangle + F_4 \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \\ &= \frac{e^{ik_x x + ik_y y}}{\sqrt{A}} \sum_{\nu} g_{\nu}(k_x, k_y, z) \left| \frac{3}{2}, \nu \right\rangle \end{aligned} \right.$$

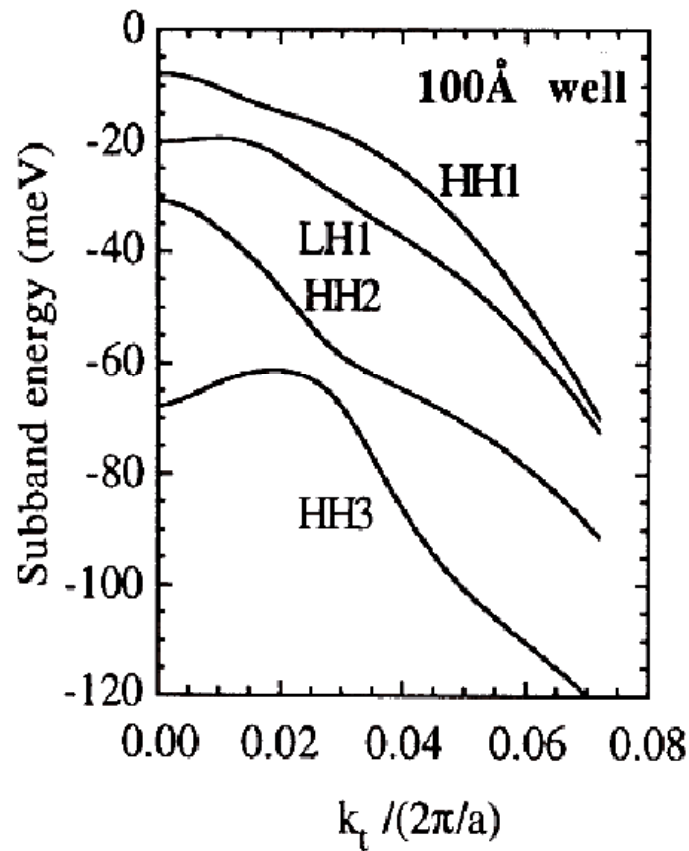
where $\nu = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2},$ and $-\frac{3}{2}$. Denote

$$\mathbf{k}_t = \hat{x}k_x + \hat{y}k_y$$

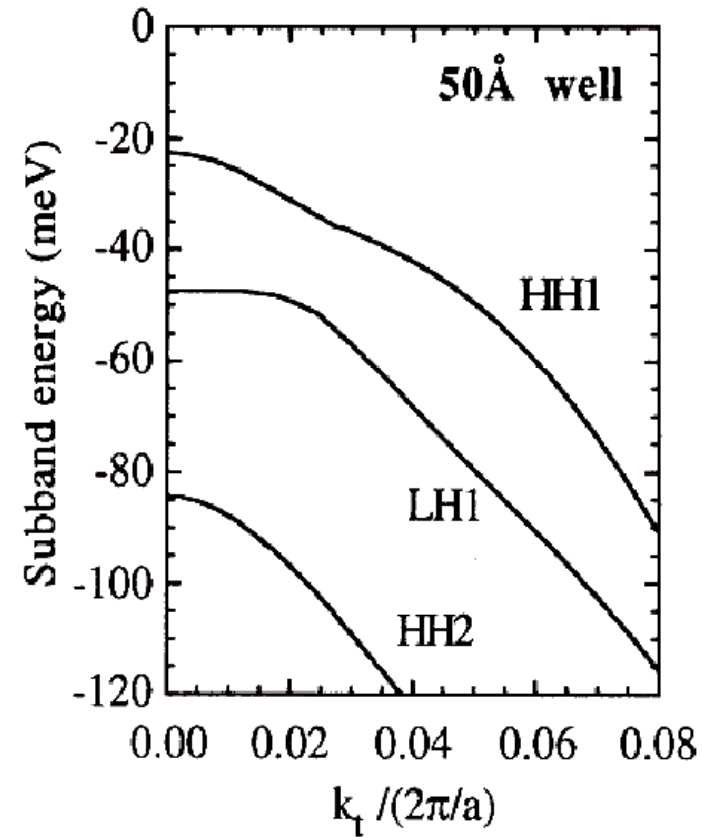
We write

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

Typical VB Dispersion with LK+EFA



(a)



(b)

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

$$\bar{\bar{\mathbf{H}}} = - \begin{bmatrix} P + Q & -S & R & 0 \\ -S^+ & P - Q & 0 & R \\ R^+ & 0 & P - Q & S \\ 0 & R^+ & S^+ & P + Q \end{bmatrix} \begin{bmatrix} |\frac{3}{2}, \frac{3}{2}\rangle \\ |\frac{3}{2}, \frac{1}{2}\rangle \\ |\frac{3}{2}, -\frac{1}{2}\rangle \\ |\frac{3}{2}, -\frac{3}{2}\rangle \end{bmatrix} \rightarrow \text{old bases}$$

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

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

$$\bar{\bar{\mathbf{H}}} = \bar{\bar{\mathbf{U}}}\bar{\bar{\mathbf{H}}}\text{LK}\bar{\bar{\mathbf{U}}}^{\dagger} = - \begin{bmatrix} P+Q & \tilde{R} & 0 & 0 \\ \tilde{R}^{\dagger} & P-Q & 0 & 0 \\ 0 & 0 & P-Q & \tilde{R} \\ 0 & 0 & \tilde{R}^{\dagger} & P+Q \end{bmatrix} \begin{matrix} |1\rangle \\ |2\rangle \\ |3\rangle \\ |4\rangle \end{matrix}$$

where $\tilde{R} = |R| - i|S|$ $\tilde{R}^{\dagger} = |R| + i|S|$ new bases

The transformation
bet. old and new bases:

$$\begin{aligned} |1\rangle &= \alpha \left| \frac{3}{2}, \frac{3}{2} \right\rangle - \alpha^* \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \\ |2\rangle &= -\beta^* \left| \frac{3}{2}, \frac{1}{2} \right\rangle + \beta \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \\ |3\rangle &= \beta^* \left| \frac{3}{2}, \frac{1}{2} \right\rangle + \beta \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \\ |4\rangle &= \alpha \left| \frac{3}{2}, \frac{3}{2} \right\rangle + \alpha^* \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \end{aligned}$$

$$\alpha = \frac{1}{\sqrt{2}} e^{i[(\theta_S + \theta_R)/2 + \pi/4]}$$

where

$$\beta = \frac{1}{\sqrt{2}} e^{i[(\theta_S - \theta_R)/2 + \pi/4]}$$

$$\bar{\bar{\mathbf{U}}} = \begin{bmatrix} \alpha^* & 0 & 0 & -\alpha \\ 0 & -\beta & \beta^* & 0 \\ 0 & \beta & \beta^* & 0 \\ \alpha^* & 0 & 0 & \alpha \end{bmatrix}$$

Effect of Strain on the Band Structure

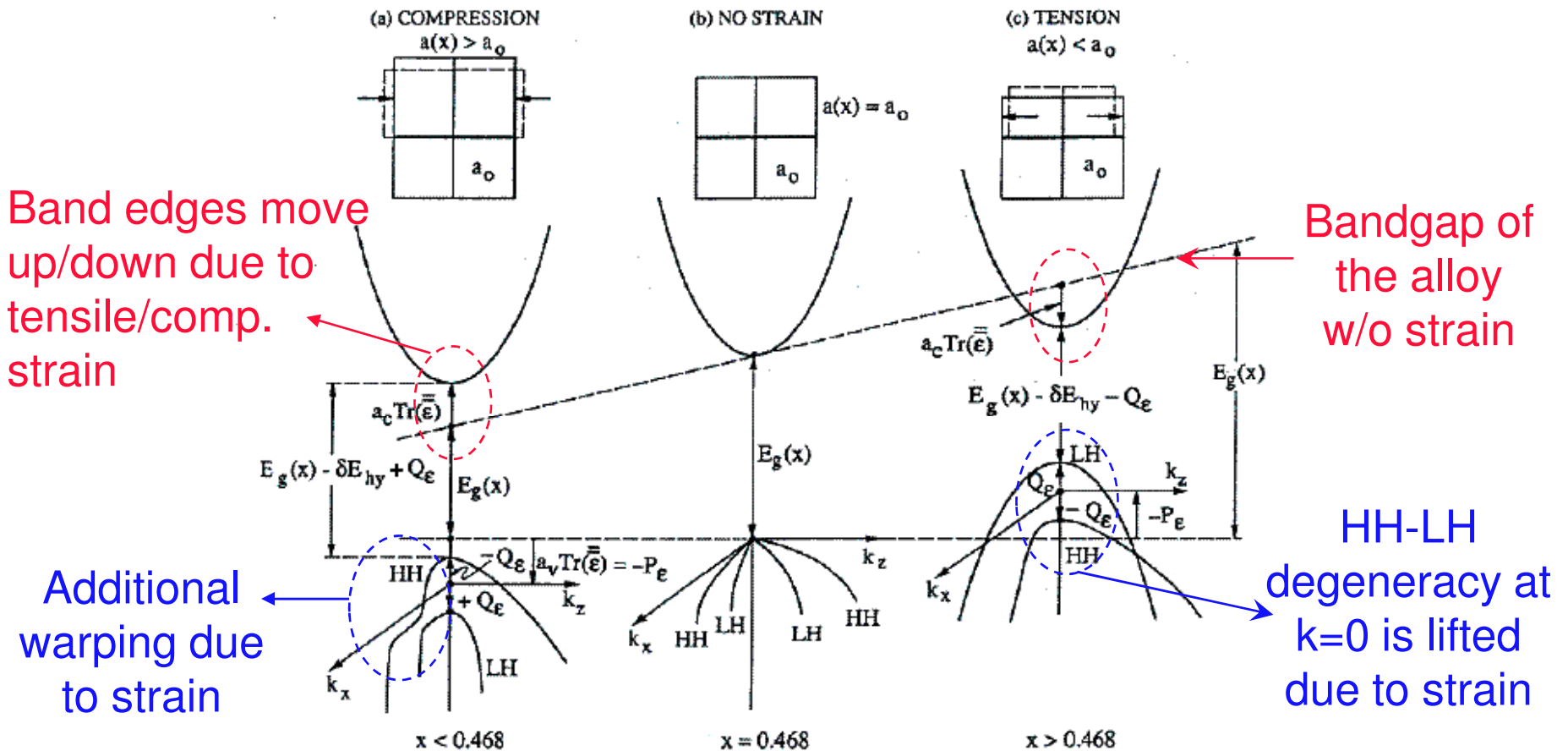
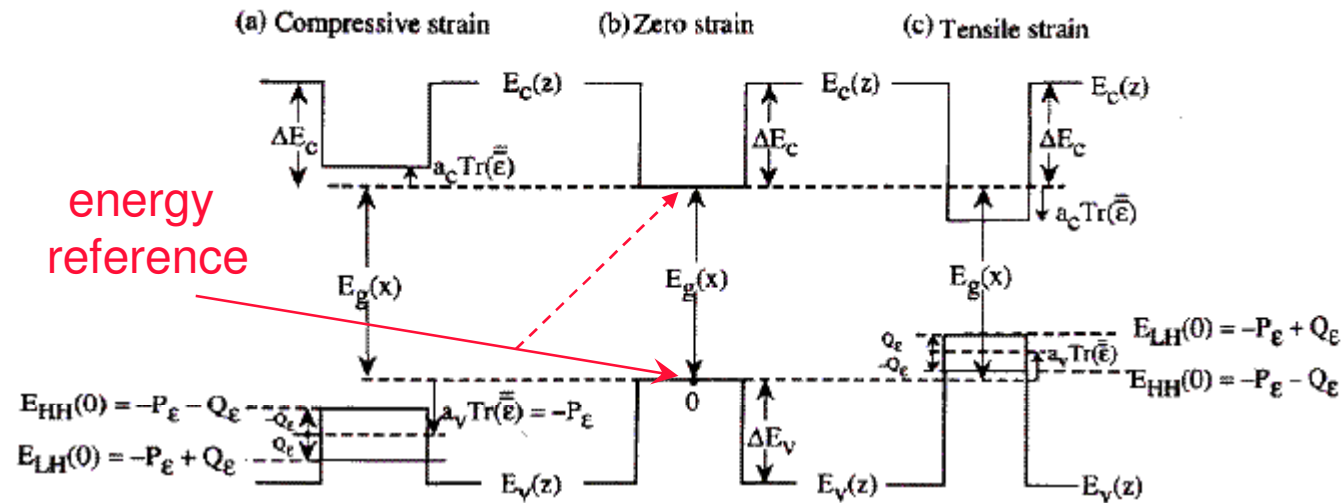


Figure 4.8. The energy-band structure in the momentum space for a bulk $\text{Ga}_x\text{In}_{1-x}\text{As}$ material under (a) biaxial compression, (b) lattice-matched condition, and (c) biaxial tension for different Ga mole fractions x . The heavy-hole band is above the light-hole band and its effective 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.)

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

Subband Energies in a Strained QW

Conduction Subbands

$$E_c(z) = \left\{ \begin{array}{ll} a_c(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) & |z| \leq \frac{L_w}{2} \\ \Delta E_c & |z| > \frac{L_w}{2} \end{array} \right\} \text{Conduction band edge (}\mathbf{k}=0\text{)}$$

where $\varepsilon_{xx} = \varepsilon_{yy} = (a_0 - a)/a$ and $\varepsilon_{zz} = -2(C_{12}/C_{11})\varepsilon_{xx}$

↑ ↑
barrier/well region lattice constants

Conduction subbands can be obtained using single-band EFA

What we need are the dispersion relation and the confinement potential

$$m_e^* = \left\{ \begin{array}{ll} m_w^* & |z| \leq \frac{L_w}{2} \\ m_b^* & |z| > \frac{L_w}{2} \end{array} \right.$$

Valence Subband Energies (w/o SO bands)

- Without SO bands, HH and LH bands are uncoupled at $\mathbf{k}=0$
- So the subband energies are determined as in **single-band** EFA

confinement potentials

$$E_{\text{HH}}(z) = \begin{cases} -P_\varepsilon - Q_\varepsilon & |z| \leq \frac{L_w}{2} \\ -\Delta E_v & |z| > \frac{L_w}{2} \end{cases}$$

$$E_{\text{LH}}(z) = \begin{cases} -P_\varepsilon + Q_\varepsilon & |z| \leq \frac{L_w}{2} \\ -\Delta E_v & |z| > \frac{L_w}{2} \end{cases}$$

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

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

where

$$P_\varepsilon = -a_v(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz})$$

$$Q_\varepsilon = \frac{-b}{2}(\varepsilon_{xx} + \varepsilon_{yy} - 2\varepsilon_{zz})$$

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

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

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

All strain-related band edge shifts are here
envelope functions
dispersion relation

use the unstrained band edge confinement
 $V_h(z) = E_v^0(z) = \begin{cases} 0 & |z| \leq \frac{L_w}{2} \\ -\Delta E_v & |z| > \frac{L_w}{2} \end{cases}$

Results for Valence Subband Dispersion w/o SO

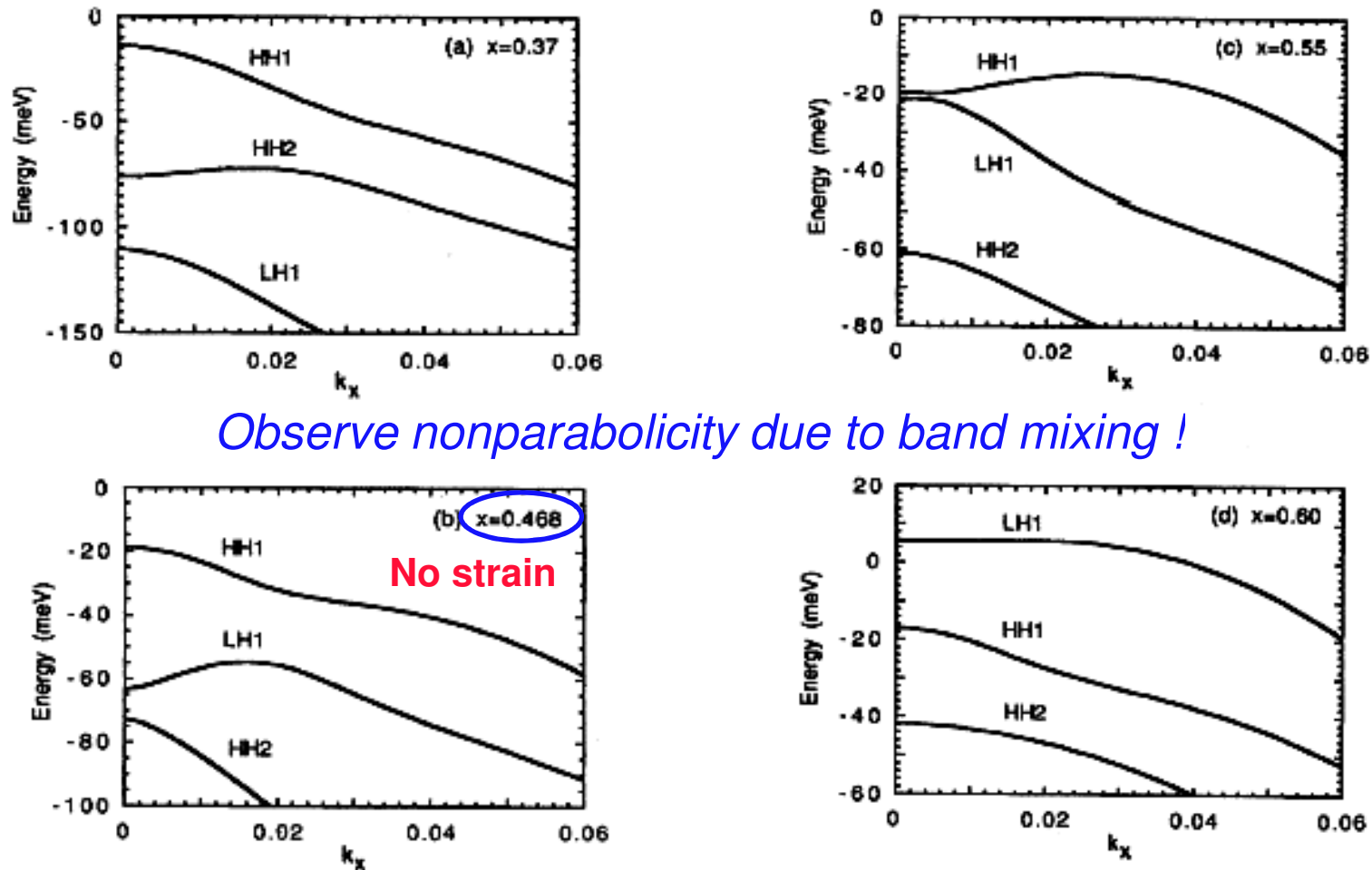
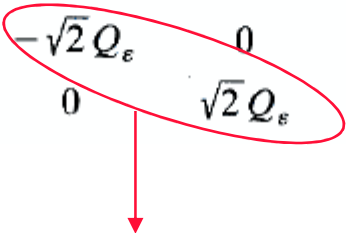


FIG. 5. The valence-band structures for $\text{Ga}_x\text{In}_{1-x}\text{As}$ grown on an $\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$ (band-gap wavelength is $1.3 \mu\text{m}$) lattice matched to InP for (a) compression ($x=0.37$), (b) lattice-matched case ($x=0.468$), (c) small tension ($x=0.55$),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

Cray X-MP
acknowledged!

Valence Band Energies (with SO bands)

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

$$\bar{\bar{H}}(\mathbf{k}=0) = - \begin{bmatrix} P_\varepsilon + Q_\varepsilon & 0 & 0 & 0 & 0 & 0 \\ 0 & P_\varepsilon - Q_\varepsilon & 0 & 0 & -\sqrt{2}Q_\varepsilon & 0 \\ 0 & 0 & P_\varepsilon - Q_\varepsilon & 0 & 0 & \sqrt{2}Q_\varepsilon \\ 0 & 0 & 0 & P_\varepsilon + Q_\varepsilon & 0 & 0 \\ 0 & -\sqrt{2}Q_\varepsilon & 0 & 0 & P_\varepsilon + \Delta & 0 \\ 0 & 0 & \sqrt{2}Q_\varepsilon & 0 & 0 & P_\varepsilon + \Delta \end{bmatrix} \begin{matrix} \text{HH} \\ \text{LH} \\ \text{LH} \\ \text{HH} \\ \text{SO} \\ \text{SO} \end{matrix}$$


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:

$$\begin{bmatrix} -P_\varepsilon + Q_\varepsilon & \pm\sqrt{2}Q_\varepsilon \\ \pm\sqrt{2}Q_\varepsilon & -P_\varepsilon - \Delta \end{bmatrix} \begin{bmatrix} F_{3/2, \pm 1/2} \\ F_{1/2, \pm 1/2} \end{bmatrix} = E(0) \begin{bmatrix} F_{3/2, \pm 1/2} \\ F_{1/2, \pm 1/2} \end{bmatrix}$$

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

Effect of SO bands on bulk band energies

Solution for band edge energies yields

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

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

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

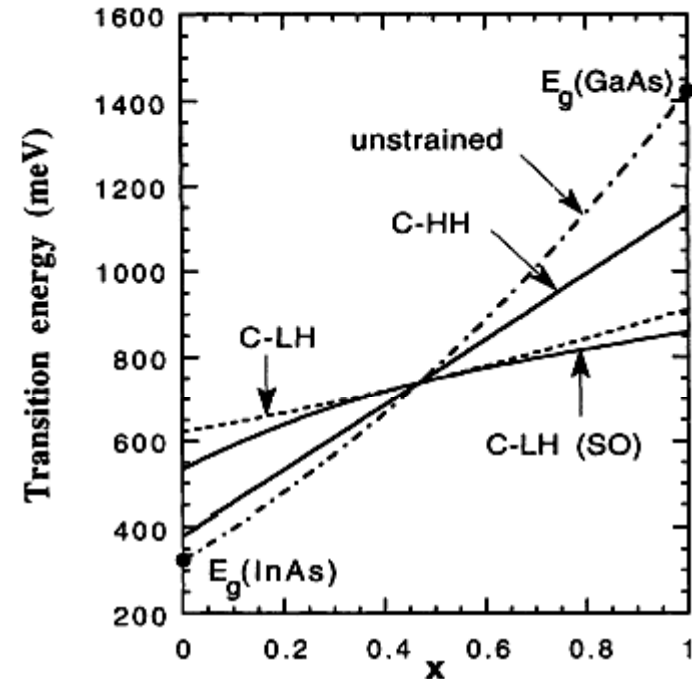


FIG. 1. The energy band gap of a **bulk** $\text{In}_{1-x}\text{Ga}_x\text{As}$ vs the Ga mole fraction x . The dotted-dashed curve: unstrained $\text{In}_{1-x}\text{Ga}_x\text{As}$; the solid curves: transition energies from the conduction band (C) to the heavy-hole (HH) and light-hole (LH) bands for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

Effect of including SO bands on valence subband energies

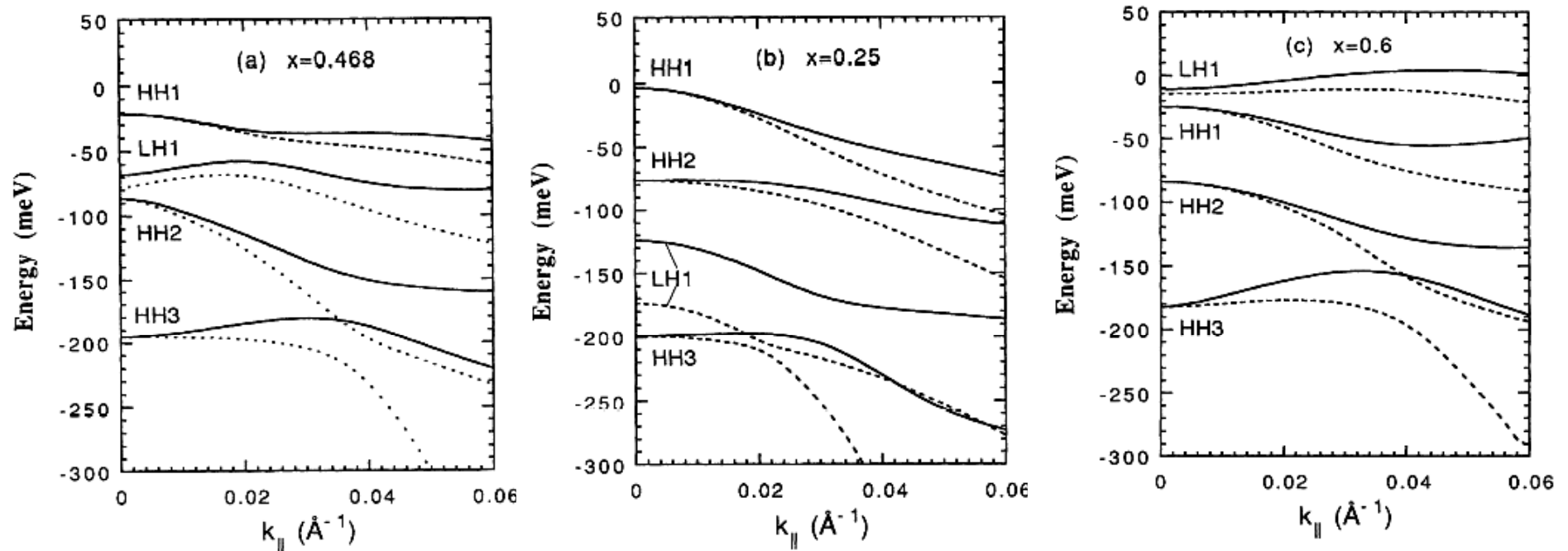


FIG. 7. The valence subband structure for a 60-Å $\text{In}_{1-x}\text{Ga}_x\text{As}$ quantum well sandwiched between InP barriers for (a) $x = 0.468$ (lattice-matched), (b) $x = 0.25$ (compressive strain), and (c) $x = 0.6$ (tensile strain). The solid curves: including the SO coupling, the dashed curves: 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:

B. A. Foreman, Phys. Rev. B 56, R12748 (1997).

B. A. Foreman, Phys. Rev. B 75, 235331 (2007).