

## Heterostructures and sub-bands

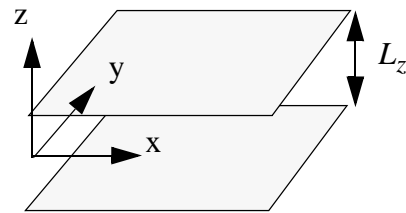
(Read Datta 6.1, 6.2; Davies 4.1-4.5)

### Quantum Wells

In a quantum well, electrons are confined in one of three dimensions to exist within a region of length  $L_z$ . If the barriers at  $z = \pm L_z$  have infinite height and the electrons are free in the x, y directions then



$$k_z = p \frac{\pi}{L_z} \quad p = 1, 2, 3, \dots$$



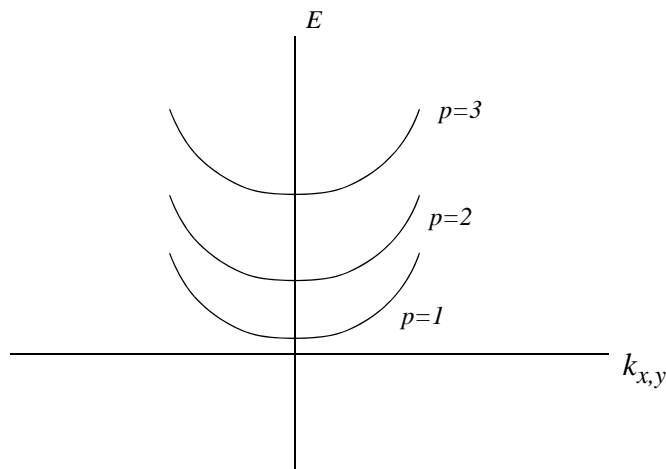
We still have freely propagating plane waves in the x-y directions

$$\phi_{x,y} = A_{x,y} \exp[i(k_x x + k_y y)] \quad k_{x,y} = \frac{2\pi n_{x,y}}{L_{x,y}}$$

with the energies given by:

$$E_p = \frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2) = \frac{\pi^2 \hbar^2 p^2}{2m L_z^2} + \frac{\hbar^2}{2m} (k_x^2 + k_y^2)$$

This gives us a series of 1D sub-bands (indexed by  $p$ ), each with a 2D dispersion relation



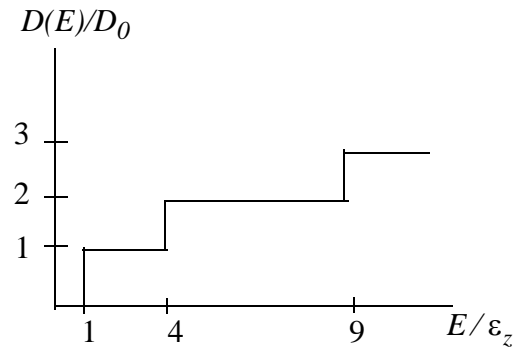
The sub-band energies are each shifted up by  $\epsilon_z p^2$  with

$$\epsilon_z = \frac{\hbar^2 \pi^2}{2mL_z^2} = \frac{m_0}{m^*} \left( \frac{10nm}{L_z} \right) \cdot 3.8\text{meV (with effective mass } m^* \text{)}.$$

2D density of states

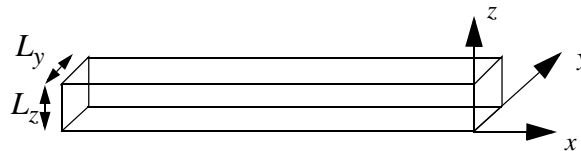


Where the sub-bands overlap, the density of states add.



Quantum wires

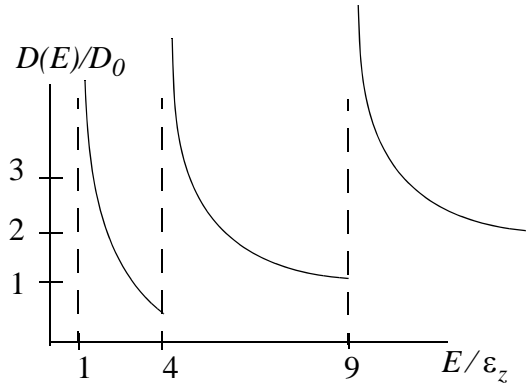
In this case we have 2D confinement and free propagation in 1D



$$E_{n,p} = (n^2 \epsilon_y + p^2 \epsilon_z) + \frac{\hbar^2}{2m} k_x^2$$

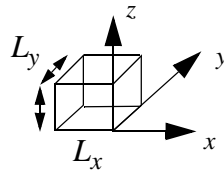
Now we have 2D sub-bands with a 1D dispersion. The 1D density of states is:





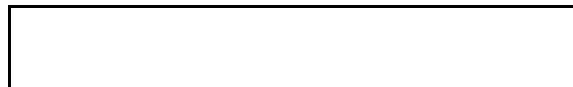
Quantum dots

3D confinement



$$E_{m,n,p} = m^2 \epsilon_x + n^2 \epsilon_y + p^2 \epsilon_z$$

Density of states is a delta function



Other confining potentials

Square well, finite depth. This is the actual situation for heterostructured quantum wells (more on this later). In this case, we have a finite number of sub-bands. States above the top of the barrier merge into 3D states. The solution for the wavefunctions and energy states is given in many standard textbooks.

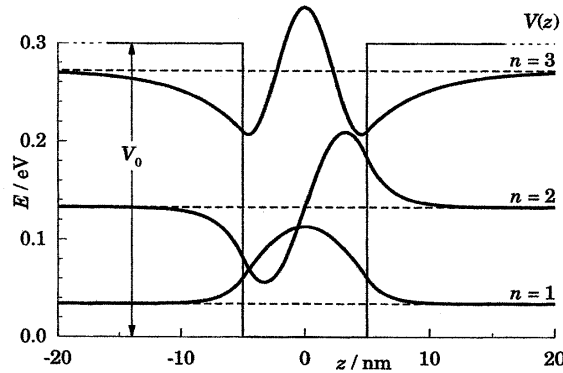


FIGURE 4.1. Finite square well in GaAs of depth  $V_0 = 0.3 \text{ eV}$  and width  $a = 10 \text{ nm}$ , showing three bound states.

Infinite triangular well. This case is approximated in doped quantum wells and in a MOSFET channel.

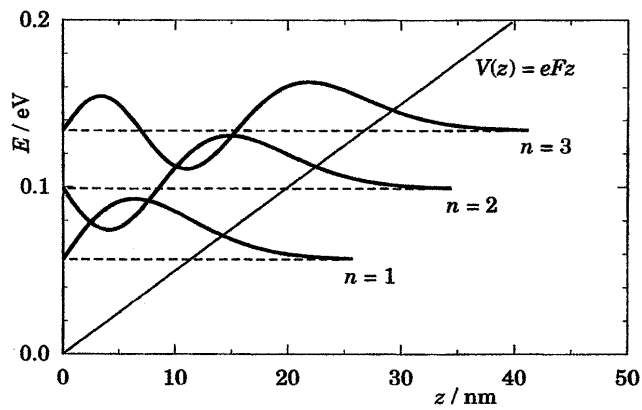


FIGURE 4.6. Triangular potential well  $V(z) = eFz$ , showing the energy levels and wave functions. The scales are for electrons in GaAs and a field of  $5 \text{ MV m}^{-1}$ .

Here, the potential is given by:



The Schrodinger equation for the z-dependent part of the wavefunction for this potential is:

$$\left[ \frac{-\hbar^2}{2m} \frac{d}{dz^2} + eFz \right] \psi(z) = \epsilon \psi(z)$$

Define

$$z_0 = \left( \frac{\hbar^2}{2meF} \right)^{1/3} \quad \epsilon_0 = \left[ \frac{(eF\hbar)^2}{2m} \right]^{1/3} = eFz_0$$

and

$$\bar{z} = \frac{z}{z_0} \quad \bar{\epsilon} = \frac{\epsilon}{\epsilon_0}$$

Then, with  $s \equiv \bar{z} - \bar{\epsilon}$ ,

“Airy equation”

The solutions are “Airy” functions, a special function related to Bessel functions of order 1/3. See Handbook of Mathematical Functions, M. Abramowitz and I. A. Stegun, (Dover, 1972). The boundary conditions are  $\psi(z=0) = \psi(s=-\bar{\epsilon}) = 0$ , and  $\psi \rightarrow 0$  as  $s \rightarrow \infty$ . The un-normalized wavefunctions are then

The energies are:

$$\epsilon_n = c_n \left[ \frac{(eF\hbar)^2}{2m} \right]^{1/3}$$

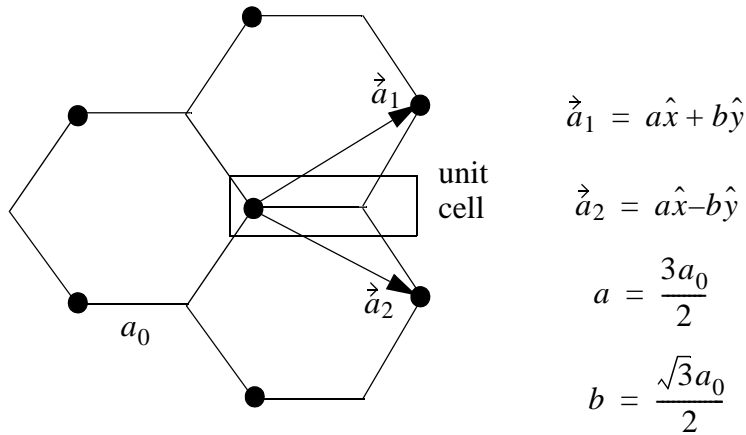
where  $c_n$  is a constant.  $c_1 = 2.338$ . An approximate expression for  $c_n$  is:

The energy levels get closer together as n increases, unlike the square well, where they get farther apart. The parabolic well is the ‘middle’ case, with equal spacing.

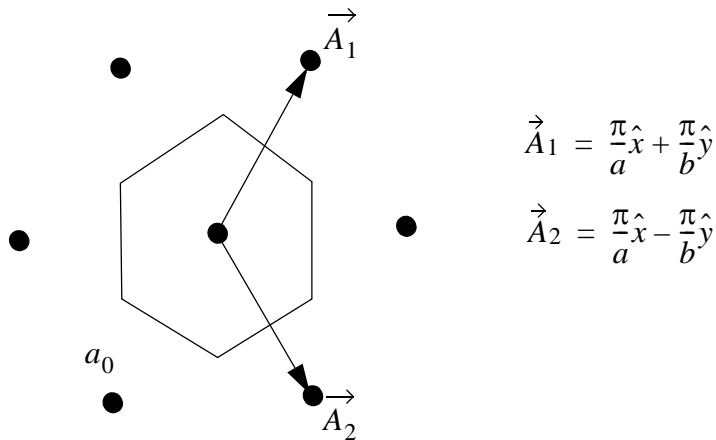
## Graphene and carbon nanotubes

(read Datta 5.2 and 6.1)

The graphene lattice is hexagonal with a 2-atom basis.



The reciprocal lattice is also hexagonal



### Graphene bandstructure near $E_F$

We should have 8 atomic basis functions per cell (2s, 2p<sub>x,y,z</sub> on each atom). However, the 2s, 2p<sub>x,y</sub> interactions are so strong, the resulting levels are well above and below  $E_F$ . Thus the only interactions that contribute are the p<sub>z</sub> orbitals forming what is called a  $\pi$  band (very common in organic molecules). The band structure is well approximated here by a simple 2X2 matrix and the resulting bandstructure is simply given by:

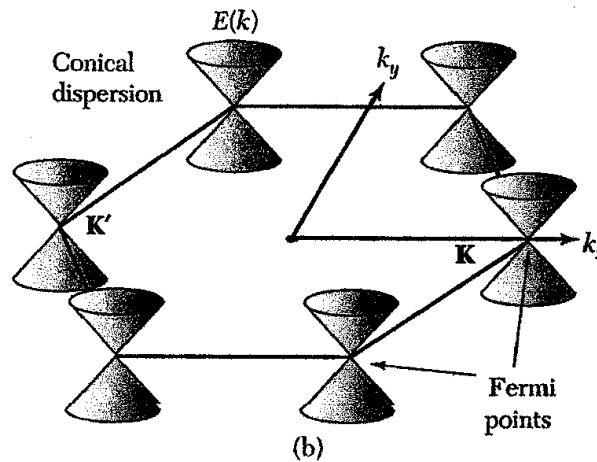


There are  $2N$  states due to 2 basis atoms per cell ( $\times 2$  for spin) =  $4N$ , where  $N$  is the number of cells. Each carbon atom contributes 1  $p_z$  electron so there are  $2N$  electrons filling exactly half the states. The bands are symmetric about  $E = 0$ , so  $E_F$  is located exactly at  $E = 0$ . Where does this occur in the zone? There are 6 such points at each of the corners of the 1st Brillouin zone. These occur at:

$$k_x a = 0 \quad k_y b = \pm \frac{2\pi}{3}$$

$$k_x a = \pm \pi \quad k_y b = \pm \frac{\pi}{3}$$

Near these “Fermi points”, the band dispersion is approximately linear, a highly unusual situation implying zero effective mass. (Can you explain that?)



Carbon nanotubes

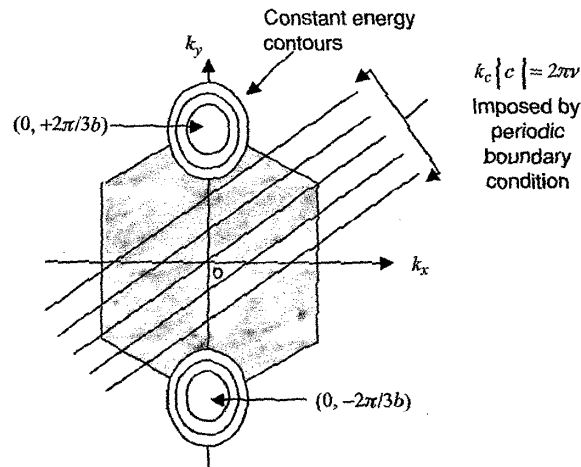
Nanotubes can be thought of as rolled up graphene. We get true periodic boundary conditions in this case that constrain the allowed values of  $k$ . Define the circumferential, or chirality vector:



This vector joins two equivalent points of the graphene sheet that connect when it is rolled up. The periodic boundary condition then requires:

$$\vec{k} \cdot \vec{c} = k_x a(m+n) + k_y b(m-n) = 2\pi v$$

with  $v$  an integer. For a given chirality  $(m, n)$ , we get a series of parallel lines in  $k$ -space that define the allowed values of  $k$ .



**Fig. 6.1.4** Reciprocal lattice of graphite showing straight lines  $k_c |c| = 2\pi v$  representing the constraint imposed by the nanotube periodic boundary conditions.

We then get a series of sub-bands that are formed by where each allowed  $k$ -line cuts through the graphene bandstructure. If one of these lines passes through one of the Fermi points, then there will be no bandgap in the nanotube bandstructure and it will be metallic. Otherwise a gap is formed and the nanotube is semiconducting. Clearly the bandgap for semiconducting nanotubes becomes a function of the chirality. If one of the lines specified by the equation:

$$k_c |c| = 2\pi v$$

passes exactly through the point  $(k_x a, k_y b) = (0, \pm 2\pi/3)$ , the condition is met and the tube is metallic. This is satisfied if and only if  $(m-n) = 3v$ . If you examine the condition to have one of the lines pass through any of the other Fermi points, you will find the identical condition.

## Semiconductor Alloys and Heterostructures

Three important phenomena for band tailoring:

1. Alloying 2 or more semiconductors
2. Use of heterostructures to cause quantum confinement
3. Use of strain via lattice mismatched epitaxy (pseudomorphic growth).

### Alloys

Object: alter bandgap and/or lattice constant

Mix materials A&B. Usually they have the same crystal structure as pure materials.

We may desire either a random, or an ordered arrangement of A-B.

If like - atom bonding (A-A and B-B) is much stronger than unlike atom bonding (A-B) we can get phase separation (clustering).

In most cases of interest, we observe random alloys. Ordering is extremely rare.

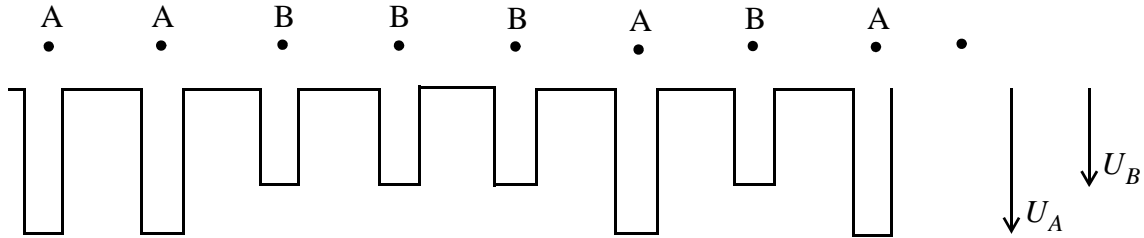
If the crystal is grown under near-equilibrium conditions, thermodynamics determines the structure. However, MBE, MOCVD, sputtering deposition are non-equilibrium growth processes. Kinetics determines the structure (i.e.: surface diffusion, impingement rate, sticking ... )

Mixture is denoted as:  $A_xB_{1-x}$        $0 < x < 1$

The lattice constant of the alloy is a weighted average of the two lattice constants:

$$\boxed{\phantom{a_{alloy} = xa_A + (1-x)a_B}}$$

Bandstructure of alloy:



Due to disorder, the Bloch theorem not strictly true in the alloy. At low T, the electrons localize in the deeper wells. But in practical cases  $|U_A - U_B| \ll U_A, U_B$ , and the random potential is a small perturbation

Virtual crystal approx:

$$U_{AV}(r) = xU_A(r) + (1-x)U_B(r)$$

Then, to 1st approx.  $E_g^{alloy} = xE_g^A + (1-x)E_g^B$

Disorder introduces correction:

$$E_g^{alloy} = a + bx + cx^2$$

$c$  is called the bowing parameter and is often significant.

Effective masses also scale:

$$\left[ \text{Empty box} \right],$$

since  $E^{alloy} = \frac{\hbar^2 k^2}{2m_{alloy}^*}$

GaAs - AlAs alloy

$a_{GaAs} = 5.653 \text{ \AA}$ .  $a_{AlAs} = 5.660 \text{ \AA}$ .

$\frac{\Delta a}{a}$  only 0.13%. Full range of composition can be grown on GaAs substrates.

AlAs is indirect gap.  $\text{Al}_x\text{As}_{1-x}$  is indirect for  $x \geq 0.35$

InGaAs - InAlAs - InP

$\text{In}_{.53}\text{Ga}_{.47}\text{As}$  lattice matches to InP.  $E_g = 0.8\text{eV}$ .

So does  $\text{In}_{.52}\text{Al}_{.48}\text{As}$ . ( $E_g = 1.45\text{eV}$ ).

“Strained” layers:

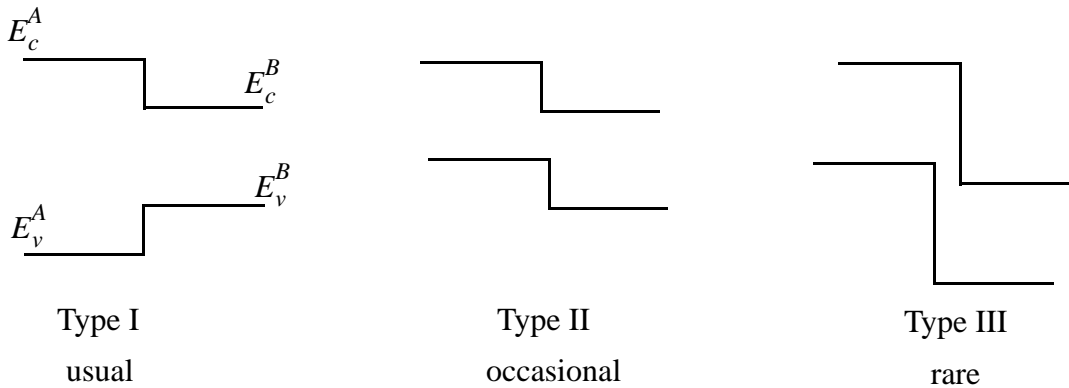
$\text{In}_x\text{Ga}_{1-x}\text{As}$  on GaAs, or

$\text{In}_{.53+x}\text{Ga}_{.47-x}\text{As}$  on InP

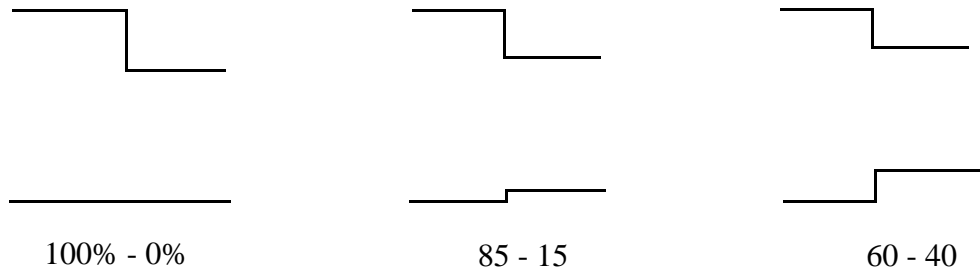
(recall critical thickness for strained layers)

Strain produces additional change in bandstructure due to deformation potential. Can even produce permanent built in polarization field via piezoelectric coefficient.

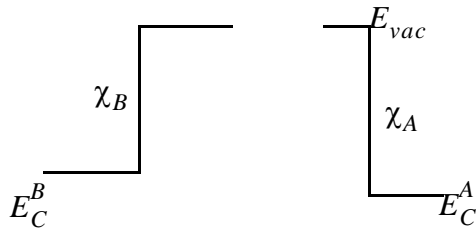
Band edge line-up at heterojunctions



Type I discontinuity distribution



It's somewhat tricky to measure this. Simple theory: electron affinity rule. Assume vacuum levels should line-up.  $EA = E_{vac} - E_C$

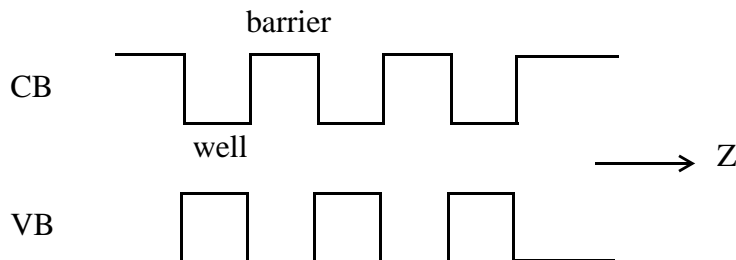


So

Based on this, then GaAlAs was thought to be 85-15 for almost 6 years while many devices were made and successfully operated! around 1985-1986, better experiments settled 60-40. (see Wang 11.3)

Quantum Wells

Layered structure - alternating band-gap

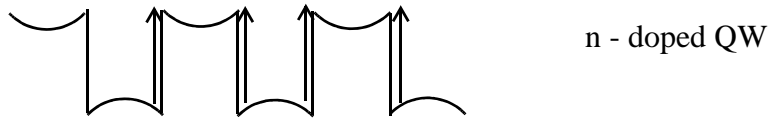


if barriers thick - wells uncoupled and act independently

if barriers thin - wells coupled --> band structure ==> "superlattice"

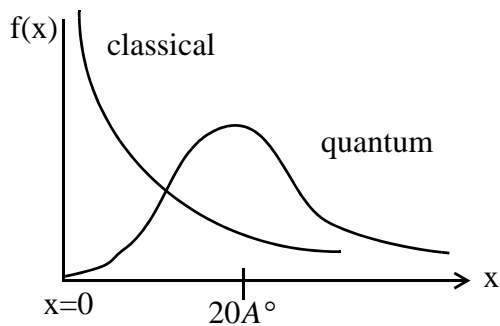
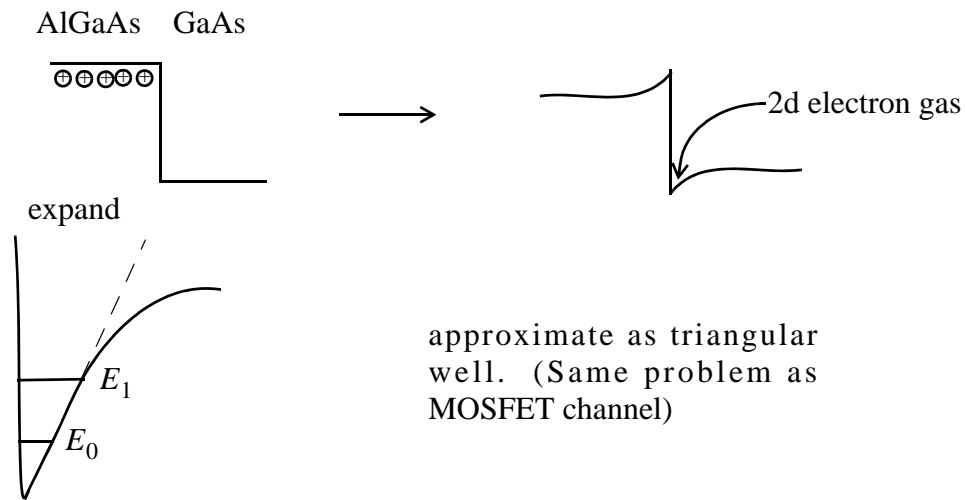
"minibands"

Very clean method: internal photoemission



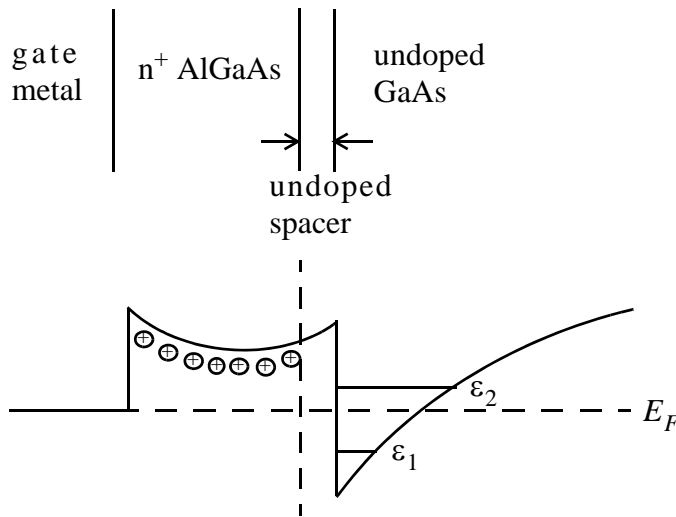
shine IR photon  $\hbar\omega_{IR} \geq E_c^A - E_c^B$  photoionize QW --> photocurrent spectrum gives band offset

2D electron gas



Modulation doping

Doping placed in barrier (wide-gap) only. Undoped spacer in barrier to separate doping and 2 DEG



- 1) ionized impurity scattering dramatically reduced
- 2) No freeze out at low temperature.

