

Bandstructure in Low-Dimensional Structures

EE 698D, Advanced Semiconductor Physics

Debdeep Jena (djena@nd.edu)

Department of Electrical Engineering

University of Notre Dame

(Fall 2004)

Contents

1	Introduction	1
2	Bulk Bandstructure	2
2.1	Pure Semiconductors	2
2.2	Doped Semiconductors	3
3	Quantum Well	4
4	Quantum Wires	6
5	Quantum Dots	7

1 Introduction

With the explosion of usage of semiconductor heterostructures in a variety of applications, low-dimensional structures such a quantum wells, wires and dots have become important. They come in various avatars - these structures can be grown by compositional variations in epitaxially grown semiconductor layers by MBE/MOCVD techniques, or nanowires / nanotubes / nanocrystals can be grown by bottom-up approaches (by CVD techniques, or by solution chemistry). So, understanding bandstructure of these artificially engineered materials is of great interest.

The goal of many clever expitaxial/bottom-up techniques to create nanostructures amounts to modifying the bandstructure of the constituent bulk semiconductor material. Many of these designer materials have niche applications, and have a potential to perform functions that are difficult, if not impossible to achieve in bulk materials. An example is the semiconductor (diode) laser. The first semiconductor lasers were band-engineering by doping (i.e., they were p-n junctions).

We have derived the effective mass equation for carriers in bulk semiconductors in the envelope-function approximation. The three-dimensional effective mass equation is

$$\left[-\frac{\hbar^2}{2m^*}\nabla^2 + V(r)\right]C(r) = (E - E_c(r))C(r). \quad (1)$$

Here, $C(r)$ is the envelope function of carriers in the band under consideration. The Schrödinger equation is thus re-cast in a form which is identical to that of an electron in

a total potential $V(r) + E_c(r)$, determined by the band-edge behavior. It has mapped the complex problem of an electron moving through a crystal experiencing very complicated potentials to a textbook-type ‘particle in a well-defined potential’ problem, which is solvable. The particle mass is renormalized, absorbing the details of the crystal potential. The *real* wavefunction of the wavepacket that models the particle-like nature of the electrons is given by $\psi(r) \approx u_{n0}(r)C(r)$, where $u_{n0}(r)$ is the periodic part of the Bloch eigenstates of the crystal that result from the periodic crystal potential. However, the beauty of the effective mass approximation is that the envelope function is all that is needed to find the bandstructure of the low-dimensional structures¹! The envelope function concept is a powerful tool, as is demonstrated in its use in determining bandstructure modifications due to quantum confinement of carriers in low-dimensional structures.

2 Bulk Bandstructure

2.1 Pure Semiconductors

In a bulk semiconductor in the absence of external fields, $V(r) + E_c(r) = E_{c0}$ is a constant energy (flatband conditions), and thus the solution of the effective mass equation yields envelope functions

$$C(r) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}, \quad (2)$$

and energies

$$E(k) = E_{c0}(r) + \frac{\hbar^2 k^2}{2m^*} = E_{c0}(r) + \frac{\hbar^2}{2} \left(\frac{k_x^2}{m_{xx}^*} + \frac{k_y^2}{m_{yy}^*} + \frac{k_z^2}{m_{zz}^*} \right). \quad (3)$$

One should not forget that even though the k^s is written as a continuous variable, they are actually quantized, assuming values

$$k_x = k_y = k_z = \frac{2\pi}{L} m \quad (4)$$

where $m = 0, \pm 1, \pm 2, \dots$. Since L is a macroscopic length, the quantization is very fine, and for all practical purposes, k^s can be assumed continuous.

The density of states (DOS) is given by

$$g_{3D}(E) = \frac{1}{2\pi^2} \left(\frac{2m^*}{\hbar^2} \right)^{3/2} \sqrt{E - E_{c0}}, \quad (5)$$

from which one gets a carrier concentration in the conduction band

$$n = \int_0^\infty dE f_{FD}(E) g_{3D}(E) = N_C^{3D} F_{1/2} \left(\frac{E_C - E_F}{k_B T} \right) \approx N_C^{3D} e^{-\frac{E_C - E_F}{k_B T}}, \quad (6)$$

¹Note that the bulk bandstructure is assumed to be known. The effective mass contains information about the bulk bandstructure.

where $F_j(\dots)$ is the Fermi-Dirac integral function. The approximation holds only when Fermi-Dirac distribution can be approximated by a Maxwell-Boltzmann form. Here, it is easily shown that N_C^{3D} is a effective band-edge DOS is

$$N_C^{3D} = 2 \left(\frac{m^* k_B T}{2\pi \hbar^2} \right)^{\frac{3}{2}}. \quad (7)$$

Similar results hold for valence bands, where the contributions from the Light and Heavy hole bands add to give the total DOS. This is shown schematically in Figure 1.

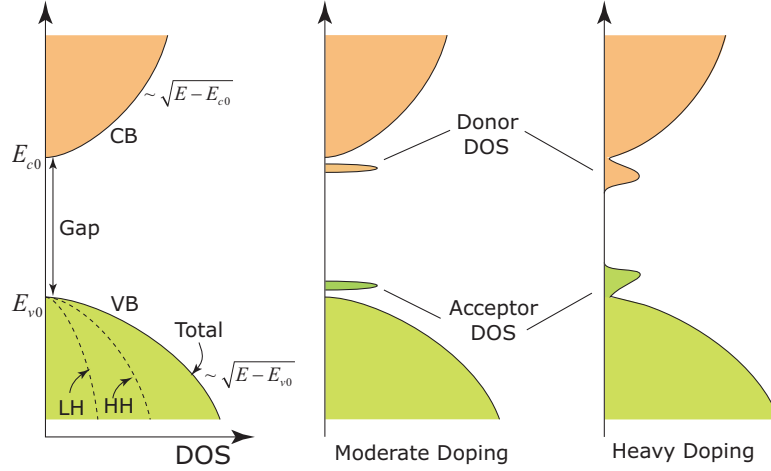


Figure 1: Density of States of bulk (undoped), moderately doped and heavily doped semiconductors.

2.2 Doped Semiconductors

Doping adds states in the bandgap of the semiconductor. A shallow dopant adds states close to the band-edges. Considering a shallow donor, the Hydrogenic-model solution from the effective mass equation

$$\left[-\frac{\hbar^2}{2m^*} \nabla^2 - \frac{e^2}{4\pi\epsilon r} \right] C(r) = (E - E_c) C(r) \quad (8)$$

showed that the eigenvalues were similar to that of a hydrogen atom, given by $E_n = E_{c0} - Ry^*/n^2$, where $Ry^* = 13.6 \times (m^*)/\epsilon_r^2$ is the modified Hydrogenic energy levels. The ground-state envelope functions around the donor atoms

$$C(r) \sim e^{-r/r_0} \quad (9)$$

is spread over many lattice constants ($r_0 = a_B(\epsilon_r/m^*) \gg a$); this implies that in k -space, the donor states are localized to $\Delta k \sim 1/r$. If the donor electron envelope function is spread over 1000 atoms in real space, in k -space it will be restricted to $\sim 1/1000$ of the volume

of the Brillouin zone. Thus, for all practical purposes, the donor states are assumed to be “atomic-like”. Energy separations between these individual atomic-like states is very small.

For heavy doping however, many changes can occur. The adjacent radii of electrons associated with adjacent donors can overlap, leading to formation of impurity bands. Then, the semiconductor acquires metal-like properties, since thermal activation of carriers into the bands is not necessary for transport. The effects of moderate and heavy doping on the DOS of bulk semiconductors is shown in Figure 1.

3 Quantum Well

Quantum wells are formed upon sandwiching a thin layer of semiconductor between wider bandgap barrier layers. The finite extent of the quantum well layer makes the conduction band profile mimic a one-dimensional quantum well in the direction of growth (z -direction), leaving motion in the $x - y$ plane free. Thus, the square-well potential (with reference to the conduction band edge E_{c0}) is written as

$$V(x, y, z) = 0, z < 0 \quad (10)$$

$$V(x, y, z) = 0, z > W \quad (11)$$

$$V(x, y, z) = -\Delta E_c, 0 \leq z \leq W. \quad (12)$$

Using the effective mass equation with this potential, it is evident that the envelope function should decompose as

$$C_{n_z}(x, y, z) = \phi(x, y)\chi_{n_z}(z) = \left[\frac{1}{\sqrt{A}}e^{i(k_x x + k_y y)}\right] \cdot [\chi_{n_z}(z)] \quad (13)$$

If the quantum well is assumed to be infinitely deep, by simple wave-fitting procedure² the z -component of the electron quasi-momentum is quantized to

$$k_{n_z} = \frac{\pi}{W}n_z, \quad (14)$$

where $n_z = 1, 2, 3, \dots$. From simple particle-in-a-box model in quantum mechanics, the normalized z -component of the envelope function is

$$\chi_{n_z}(z) = \frac{2}{\sqrt{W}} \sin \frac{\pi n_z z}{W}. \quad (15)$$

The bandstructure is the set of energy eigenvalues is obtained from the effective mass equation, given by

$$E(k) = E_{c0} + \underbrace{\frac{\hbar^2}{2} \left(\frac{k_x^2}{m_{xx}^*} + \frac{k_y^2}{m_{yy}^*} \right)}_{E_{2D}(k_x, k_y)} + \underbrace{\frac{\hbar^2}{2m_{zz}^*} \left(\frac{\pi n_z}{W} \right)^2}_{E_{1D}(n_z)} \quad (16)$$

²Only waves that satisfy $n_z(\lambda/2) = W$ fit into the well of width W , leading to $k_{n_z} = 2\pi/\lambda = (\pi/W)n_z$.

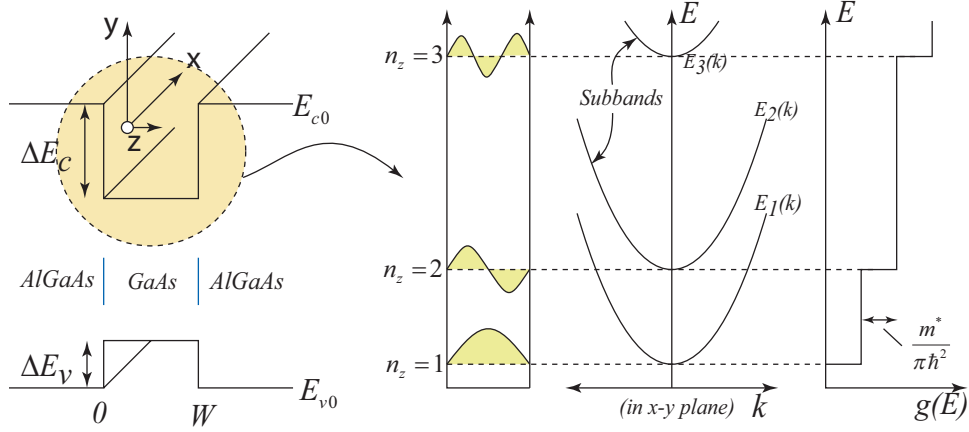


Figure 2: Bandstructure, and DOS of realistic heterostructure quantum wells.

which evidently decomposes to a free-electron component in the $x - y$ plane and a quantized component in the z - direction. The bandstructure consists of multiple bands $E_{2D}(k_x, k_y)$, each indexed by the quantum number n_z ; this is shown in Figure 2.

The DOS of electrons confined in an ideal 2-D plane is a constant, given by $g_{2D}(E) = m^*/\pi\hbar^2$. In the quantum well, each subband corresponding to an n_z is an ideal 2-D system, and each subband contributes $g_{2D}(E)$ to the total DOS. This is shown schematically in Figure 2. Thus, the DOS of the quantum well is

$$g_{QW}(E) = \frac{m^*}{\pi\hbar^2} \sum_{n_z} \theta(E - E_{n_z}), \quad (17)$$

where $\theta(\dots)$ is the unit step function. The carrier density of an ideal 2D electron system is thus given by

$$n_{2D} = \int_0^\infty dE f_{FD}(E) g_{2D}(E) = \underbrace{\frac{m^* k_B T}{\pi\hbar^2}}_{N_C^{2D}} \ln\left(1 + e^{\frac{E_F - E_1}{k_B T}}\right), \quad (18)$$

where E_1 is the ground state energy, E_F is the Fermi level, and N_C^{2D} is the effective band-edge DOS, the 2-dimensional counterpart of N_C^{3D} defined in Equation 7. (Verify the units of each!)

For the quantum well, which houses many subbands, the DOS becomes a sum of each subband (Figure 2), and the total carrier density is thus a sum of 2D-carriers housed in each subband -

$$n_{2D} = \sum_j n_j = N_c^{2D} \sum_j \ln\left(1 + e^{\frac{E_F - E_j}{k_B T}}\right). \quad (19)$$

Note that for a 2D system, no approximation of the Fermi-Dirac function is necessary to find the carrier density analytically.

It is important to note that if the confining potential in the z -direction can be engineered almost at will by modern epitaxial techniques by controlling the spatial changes in material composition. For example, a popular quantum well structure has a parabolic potential ($V(z) \sim z^2$), which leads to the E_{n_z} values spaced in equal energy intervals - this is a characteristic of a square, or Harmonic Oscillator potential. Another extremely important quantum well structure is the triangular well potential ($V(z) \sim z$), which appears in MOSFETs, HEMTs, and quantum wells under electric fields. The triangular well leads to E_{n_z} values given by Airy functions. Regardless of these details specific to the *shape* of the potential, the bandstructure and the DOS remain similar to the square well case; the only modification being the E_{n_z} values, and the corresponding subband separations.

4 Quantum Wires

Artificial quantum wires are formed either lithographically (top-down approach), or by direct growth in the form of semiconductor nanowires or nanotubes (bottom-up approach). In a quantum well, out of the three degrees of freedom for real space motion, carriers were confined in one, and were free to move in the other two. In a quantum wire, electrons are free to move freely in one dimension only (hence the name ‘wire’), and the other two degrees of freedom are quantum-confined. Assume that the length of the wire (total length L_z) is along the z -direction (see Figure 3), and the wire is quantum-confined in the $x - y$ plane ($L_x, L_y \ll L_z$). Then, the envelope function naturally decomposes into

$$C(x, y, z) = \chi_{n_x}(x) \cdot \chi_{n_y}(y) \cdot \left(\frac{1}{\sqrt{L_z}} e^{ik_x x}\right), \quad (20)$$

and the energy eigenvalues are given by

$$E(n_x, n_y, k_z) = E(n_x, n_y) + \frac{\hbar^2 k_k^2}{2m_{z^*}^*}. \quad (21)$$

If the confinement in the $x - y$ directions is by infinite potentials (a useful model applicable in many quantum wires), then similar to the quantum well situation, a wave-fitting procedure gives

$$k_{n_x} = \frac{\pi}{L_x} n_x, \quad (22)$$

$$k_{n_y} = \frac{\pi}{L_y} n_y, \quad (23)$$

where $n_x, n_y = 1, 2, 3, \dots$ independently.

The eigenfunctions assume the form

$$C_{n_x, n_y}(x, y, z) = \left[\sqrt{\frac{2}{L_x}} \sin\left(\frac{\pi n_x}{L_x} x\right)\right] \cdot \left[\sqrt{\frac{2}{L_y}} \sin\left(\frac{\pi n_y}{L_y} y\right)\right] \cdot \left[\frac{1}{\sqrt{L_z}} e^{ik_x x}\right], \quad (24)$$

and the corresponding bandstructure is given by

$$E(n_x, n_y, k_z) = \underbrace{\left[\frac{\hbar^2}{2m_{xx}} \left(\frac{\pi n_x}{L_x} \right)^2 + \frac{\hbar^2}{2m_{yy}} \left(\frac{\pi n_y}{L_y} \right)^2 \right]}_{E(n_x, n_y)} + \frac{\hbar^2 k_z^2}{2m_{zz}^*}. \quad (25)$$

Multiple subbands are formed, similar to the quantum well structure. A new subband forms at each eigenvalue $E(n_x, n_y)$, and each subband has a dispersion $E(k_z) = \hbar^2 k_z^2 / 2m_{zz}$ (Figure 3).

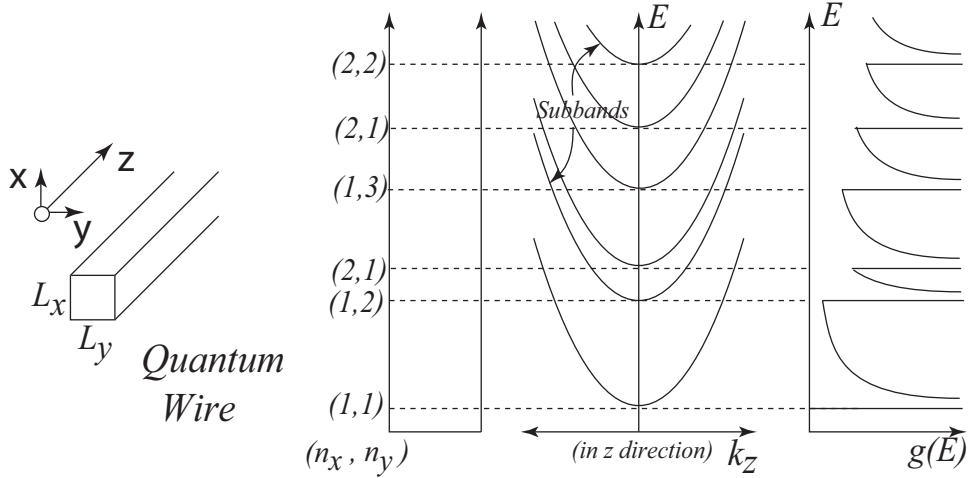


Figure 3: Bandstructure, and DOS of realistic quantum wires.

The DOS of electrons confined to an ideal 1-D potential is given by

$$g_{1D}(E) = \frac{1}{\pi} \sqrt{\frac{2m^*}{\hbar^2}} \frac{1}{\sqrt{E - E_1}}, \quad (26)$$

where E_1 is the lowest allowed energy (ground state). Due to multiple subbands, the DOS acquires peaks at every eigenvalue $E(n_x, n_y)$. Since there are two quantum numbers involved, some eigenvalues can be degenerate, and the peaks can occur at irregular intervals as opposed to the quantum well case. The general DOS for a quantum wire can thus be written as

$$g_{QWire}(E) = \frac{1}{\pi} \sqrt{\frac{2m^*}{\hbar^2}} \sum_{n_x, n_y} \frac{1}{\sqrt{E - E(n_x, n_y)}}, \quad (27)$$

which is shown schematically in Figure 3.

5 Quantum Dots

The quantum dot is the ultimate nanostructure. All three degrees of freedom are quantum confined; therefore there is no plane-wave component of electron wavefunctions. The

envelope function for a “quantum box” of sides L_x, L_y, L_z (see Figure 4) is thus written as

$$C(x, y, z) = \chi_{n_x}(x)\chi_{n_y}(y)\chi_{n_z}(z), \quad (28)$$

and if the confining potential is infinitely strong, we have $k_{n_i} = (\pi/L_i)n_i$ for $i = x, y, z$. The envelope functions are thus given by

$$C(x, y, z) = \left[\sqrt{\frac{2}{L_x}} \sin\left(\frac{\pi n_x}{L_x}\right)\right] \cdot \left[\sqrt{\frac{2}{L_y}} \sin\left(\frac{\pi n_y}{L_y}\right)\right] \cdot \left[\sqrt{\frac{2}{L_z}} \sin\left(\frac{\pi n_z}{L_z}\right)\right], \quad (29)$$

and the energy eigenvalues are given by

$$E(n_x, n_y, n_z) = \frac{\hbar^2}{2m_{xx}}\left(\frac{\pi n_x}{L_x}\right)^2 + \frac{\hbar^2}{2m_{yy}}\left(\frac{\pi n_y}{L_y}\right)^2 + \frac{\hbar^2}{2m_{zz}}\left(\frac{\pi n_z}{L_z}\right)^2. \quad (30)$$

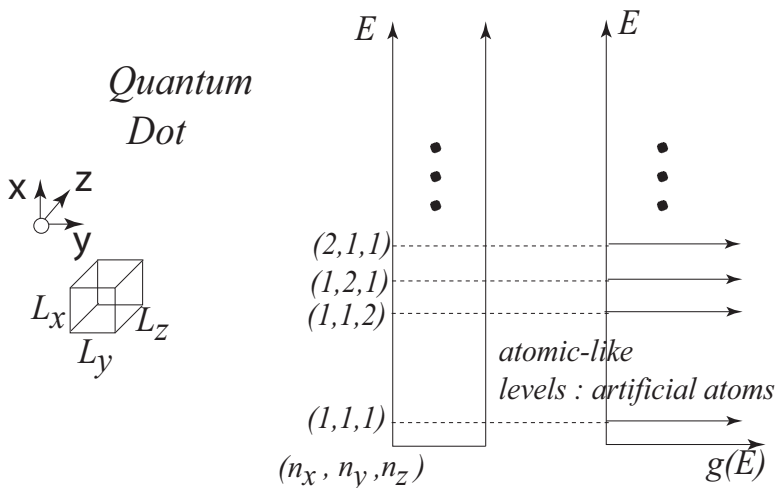


Figure 4: Energy levels and DOS of quantum dots.

Note that the the energy eigenvalues are no more quasi-continuous, and are indexed by three quantum numbers (n_x, n_y, n_z) . Thus, it does not make sense to talk about “bandstructure” of quantum dots; the DOS is a sum of delta functions, written as

$$g_{QDot} = \sum_{n_x, n_y, n_z} \delta(E - E_{n_x, n_y, n_z}). \quad (31)$$

This is shown schematically in Figure 4. Since there is no direction of free motion, there is no transport *within* a quantum dot, and there is no quasi-continuous momentum components. Fabricating quantum dots by lithographic techniques is pushing the limits of top-down approach to the problem. On the other hand, epitaxial techniques can coax quantum dots to self-assemble by cleverly exploiting the strain in lattice-mismatched semiconductors. On the other hand, bottom-up techniques of growing nanocrystals in solution by chemical synthetic routes is becoming increasingly popular.