# Semiconductor heterostructures – quantum wells



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"FACE IT - ANECDOTAL EVIDENCE JUST DOESN'T CARRY ANY WEIGHT IN MATH." anecdotal evidence = niepotwierdzony dowód



## Bandgap engineering

The presence of the well changes the symmetry of the crystal (eg. quantum wells in the direction of [001] corresponds to an uniaxial pressure applied perpendicular to the layer). You have to solve the kp perturbation theory (Chemla 1983):

Effects of biaxial strain: decrease of the degeneracy of the valence band and change of the effective masses in the  $Ga_xIn_{1-x}As / Ga_xIn_{1-x}As_yyP_{1-y}$  material system.

S.L. Chuang, Phys. Rev. B 43, p. 9649 (1991). 9, 10



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





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Transformation:

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$$\frac{d^2}{dz^2}\psi(z) = \frac{2m}{\hbar^2}(eFz - \varepsilon)\psi(z)$$
Substituting:  $z_0 = \left(\frac{\hbar^2}{2meF}\right)^{1/3}$ ,  $\bar{z} = \frac{z}{z_0}$ ,  $\bar{\varepsilon} = \frac{\varepsilon}{\varepsilon_0}$ 

$$\frac{d^2}{dz^2}\psi(z) = \frac{2m}{\hbar^2}(eFz - \varepsilon)\psi(z)$$
The equation reduces to Stokes or Airy equation:

1.00

$$\frac{d^2}{dz^2}f(z) = zf(z)$$

Its two independent solutions the Airy functions Ai(z) and Bi(z). The solutions of the equation are the zeros of a function Ai(z) (after some rearrangements).



**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 MV m<sup>-1</sup>.

WKB approximation (Wentzel – Krammers – Brillouin) – for slowly changing potential

It is also known as the **LG** or **Liouville–Green** method or **JWKB** and **WKBJ**, where the "J" stands for Jeffreys or *phase integral method* **or** *semi-classical approximation*.

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x)$$

What is slowly varing potential? It is for sure  $V(x) = V_0 = const$ . The solution for this potential is a plane wave  $\psi(x) = e^{ikx}$  - phase of the wavefunction k(x) = k = const is constant in the whole space  $k^2 = \frac{2m}{\hbar} [E - V_0]$ 

Let's define  $k^2(x) = \frac{2m}{\hbar} [E - V(x)]$  - we want the phase k(x) to be slowly varying in space, i.e.  $\left| \frac{dk}{dx} \right| \ll k^2$ 

(such condition).

We are looking for the solution  $\psi(x) = e^{i\chi(x)}$  where  $\chi(x)$  is the phase of the wavefunction.

WKB approximation (Wentzel – Krammers – Brillouin) – for slowly changing potential

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x)$$

Let's define  $k^2(x) = \frac{2m}{\hbar} [E - V(x)]$  - slowly varing in real space k(x).

We are looking for the solution  $\psi(x) = e^{i\chi(x)}$  where  $\chi(x)$  its the phase of the wavefunction. Inserting into Schrodinger equation:

$$[\chi'(x)]^2 - i\chi''(x) = \frac{2m}{\hbar} [E - V(x)] \equiv k^2(x)$$
 - this is rigorous.

Zero-order WKB approximation assumes  $[\chi'(x)]^2 \gg |\chi''(x)| \operatorname{czyli} \chi''(x) pprox 0$ 

$$[\chi'(x)]^2 = k^2(x) \text{ czyli} \qquad \qquad \chi(x) = \pm \int^x k(x') dx'$$

Usually we expand more

$$[\chi'(x)]^2 = k^2(x) + i\chi''(x) = k^2(x) + i[\chi'(x)]' \approx k^2(x) \pm i[k(x)]'$$

Thus:

$$\chi'(x) \approx \pm k(x) \sqrt{1 + \frac{ik'(x)}{k^2(x)}} \approx \pm k(x) + \frac{ik'(x)}{2k(x)}$$

WKB approximation (Wentzel – Krammers – Brillouin) – for slowly changing potential Typically, the WKB method continues into

$$[\chi'(x)]^2 = k^2(x) + i\chi''(x) = k^2(x) + i[\chi'(x)]' \approx k^2(x) \pm i[k(x)]'$$

Thus:

$$\chi'(x) \approx \pm k(x) \sqrt{1 + \frac{ik'(x)}{k^2(x)}} \approx \pm k(x) + \frac{ik'(x)}{2k(x)}$$

therefore:

$$\chi(x) = \pm \int^x k(x')dx' + \frac{i}{2}\ln k(x)$$

We get:

$$\psi(x) \approx \frac{1}{\sqrt{k(x)}} \exp\left[\pm i \int^x k(x') dx'\right]$$

The term  $1/\sqrt{k(x)}$  - the density of probability of fast-moving particles is small for large k - OK!

WKB approximation (Wentzel – Krammers – Brillouin) – for slowly varying potential



In the case of turning points (ie. the edges of the barriers well) potential changes rapidly compared with the wavelength k(x) - WKB approximation is not valid (a rigorous approach avoids it by moving into the complex plane). Another way is to note that the potential is linear for a small region around the turning point  $\Delta x_L$  - and the Airy functions are the exact solutions. Then the solution must match on both regions near  $x_L$ . The problem sounds complicated but fortunately the results are simple (we got additional

phase).

WKB approximation (Wentzel – Krammers – Brillouin) – for slowly varying potential



WKB approximation (Wentzel – Krammers – Brillouin) – for slowly varying potential

$$\psi(x) \sim \frac{2}{\sqrt{k(x)}} \cos\left[\int_{x_L}^x k(x')dx' - \frac{\pi}{4}\right], \qquad x \gg x_L$$

Examples:

1. "Hard" (infinitely steep) wall – the wave function goes to zero at the boundaries, so an exact number of half-wavelengths must fit between them  $\int x_R$ 

$$\int_{x_L}^{x_R} k(x') dx' = n\pi$$

For : k(x) = const we have  $k_n = \frac{n\pi}{L}$ 

2. "Soft wall" – an allowed state must obey the matching conditions ( $x \gg x_L$ , above) and at  $x_L$  it has additional phase  $\left(-\frac{\pi}{4}\right)$  and similarly at  $x_R$  - next  $\left(-\frac{\pi}{4}\right)$ . Altogether:

$$\int_{x_L}^{x_R} k(x') dx' = \left(n - \frac{1}{2}\right)\pi$$

WKB approximation (Wentzel – Krammers – Brillouin) – for slowly varying potential

$$\psi(x) \sim \frac{2}{\sqrt{k(x)}} \cos\left[\int_{x_L}^x k(x')dx' - \frac{\pi}{4}\right], \qquad x \gg x_L$$

3. Triangular well of "hard" and "soft" well:

$$x \gg x_L$$

$$\int_{x_L}^{x_R} k(x') dx' = \left(n - \frac{1}{4}\right)\pi$$

Eg. Triangular well: 
$$V(x) = eFx$$
 then  $k_n(x) = \frac{1}{\hbar} \sqrt{2m(E_n - V(x))} = \frac{1}{\hbar} \sqrt{2m(E_n - eFx)}$   
$$\int_{x_L}^{x_R} k_n(x') dx' = \int_0^{E_n/eF} \frac{1}{\hbar} \sqrt{2m(E_n - eFx')} dx' = \left[\frac{2mE_n}{\hbar^2}\right]^{1/2} \frac{E_n}{eF} \int_0^1 \sqrt{1 - s} \, ds =$$

$$\left[\frac{2mE_n}{\hbar^2}\right]^{1/2} \frac{E_n}{eF} \int_0^1 \sqrt{1-s} \, ds = \frac{2}{3} \left[\frac{2mE_n}{\hbar^2}\right]^{1/2} \frac{E_n}{eF}$$
$$\int \sqrt{1-x} \, dx = -\frac{2}{3} \left(1-x\right)^{3/2} + \text{constant}$$
$$E_n = \left[\frac{3}{2}\pi \left(n-\frac{1}{4}\right)\right]^{2/3} \left[\frac{(eF\hbar)^2}{2m}\right]^{1/3}$$



WKB approximation (Wentzel – Krammers – Brillouin) – for slowly varying potential

**TABLE 7.1** A comparison of various approximate methods for energy levels in a triangular potential, in units of  $\varepsilon_0 = [(eF\hbar)^2/(2m)]^{1/3}$ , and the exact results from the Airy function.

	n	Airy function (exact)	WKB	Variational (Fang–Howard)	Variational (Gaussian)	
	1 2 3	2.3381 4.0879 5.5206	2.3203 4.0818 5.5172	2.4764	2.3448	-
	: 10	: 12.8288	: 12.8281		0.2	V(z) = eFz
						n = 3 n = 2
$E_n = \left[\frac{3}{2}\pi\right(r)$	$n-\frac{1}{4}$	$\left[\frac{1}{4}\right]^{2/3} \left[\frac{(eF\hbar)}{2m}\right]^{2/3}$	$\left[\frac{2}{-}\right]^{1/3}$		0.0 0 10	n = 1 20 30 $z/nm$ 40 50

WKB approximation (Wentzel – Krammers – Brillouin) – for slowly varying potential



http://www.phys.unsw.edu.au/QED/research/2D\_scattering.htm

$$E_n = \left[\frac{3}{2}\pi\left(n - \frac{1}{4}\right)\right]^{2/3} \left[\frac{(eF\hbar)^2}{2m}\right]^{1/3}$$

 $V(x) = V_b \left[ 1 - \left(\frac{x}{d}\right)^2 \right]$ 



**FIGURE 7.7.** Schottky barrier in the conduction band  $E_c(x)$  between a metal and n-GaAs. The potential is parabolic with height  $V_b$  and thickness d.



#### Praca domowa:

Prosiłbym o narysowanie funkcji Airy w przestrzeni nie w jednostkach niemianowanych, ale metrycznych - czyli rysunek w nanometrach. Proszę przyjąć wartość pola elektrycznego dla dwóch przypadków: taką, żeby zmiana o 20 nm zwiększała potencjał o 250 meV, oraz zmiana o 20 nm zwiększała potencjał o 100 meV. Proszę podać wartości pola elektrycznego (w jednostkach SI). Obliczenia przeprowadzić dla pasma przewodnictwa i pasma walencyjnego GaAs (masy efektywne znajdziecie sami).



$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + V(z)\right]\psi(z) = E\psi(z) \qquad V(z) = \frac{1}{2}Kz^2 = \frac{1}{2}m\omega_0^2 z^2 \qquad E_n = \left(n - \frac{1}{2}\right)\hbar\omega_0$$



FIGURE 4.4. Potential well V(z), energy levels, and wave functions of a harmonic oscillator. The potential is generated by a magnetic field of 1 T acting on electrons in GaAs.

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + \frac{1}{2}m\omega_0^2 z^2\right]\psi(z) = E\psi(z) \qquad \qquad \varepsilon = \frac{E}{\hbar\omega_0} \qquad \xi = \sqrt{\frac{m\omega_0}{\hbar}}z$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + \frac{1}{2}m\omega_0^2 z^2\right]\psi(z) = E\psi(z) \qquad \qquad \varepsilon = \frac{E}{\hbar\omega_0} \qquad \xi = \sqrt{\frac{m\omega_0}{\hbar}}z$$

$$\left[-\frac{\hbar^2}{2m}\frac{m\omega_0}{\hbar}\frac{d^2}{d\xi^2} + \frac{1}{2}m\omega_0^2\frac{\hbar}{m\omega_0}\xi^2\right]\psi(\xi) = \hbar\omega_0\varepsilon\,\psi(\xi)$$

$$\left[-\frac{\hbar^2}{2m}\frac{m\omega_0}{\hbar}\frac{d^2}{d\xi^2} + \frac{1}{2}m\omega_0^2\frac{\hbar}{m\omega_0}\xi^2\right]\psi(\xi) = \hbar\omega_0\varepsilon\,\psi(\xi) \quad \Rightarrow \quad \left[\frac{d^2}{d\xi^2} - \xi^2\right]\psi(\xi) = -2\varepsilon\,\psi(\xi)$$

#### Tożsamości:

$$\left[ \left( \frac{d}{d\xi} - \xi \right) \left( \frac{d}{d\xi} + \xi \right) \right] \psi_0(\xi) = \dots$$
$$\left[ \left( \frac{d}{d\xi} - \xi \right) \left( \frac{d}{d\xi} + \xi \right) - \left( \frac{d}{d\xi} + \xi \right) \left( \frac{d}{d\xi} - \xi \right) \right] \psi_0(\xi) = \dots$$



$$\left[-\frac{\hbar^2}{2m}\frac{m\omega_0}{\hbar}\frac{d^2}{d\xi^2} + \frac{1}{2}m\omega_0^2\frac{\hbar}{m\omega_0}\xi^2\right]\psi(\xi) = \hbar\omega_0\varepsilon\,\psi(\xi) \quad \Rightarrow \quad \left[\frac{d^2}{d\xi^2} - \xi^2\right]\psi(\xi) = -2\varepsilon\,\psi(\xi)$$

Tożsamości:

$$\left[\left(\frac{d}{d\xi} - \xi\right)\left(\frac{d}{d\xi} + \xi\right)\right]\psi_0(\xi) = (-2\varepsilon_0 + 1)\psi_0(\xi)$$

$$\left[\left(\frac{d}{d\xi} - \xi\right)\left(\frac{d}{d\xi} + \xi\right) - \left(\frac{d}{d\xi} + \xi\right)\left(\frac{d}{d\xi} - \xi\right)\right]\psi_0(\xi) = 2\psi_0(\xi)$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + \frac{1}{2}m\omega_0^2 z^2\right]\psi(z) = E\psi(z) \qquad \qquad \varepsilon = \frac{E}{\hbar\omega_0} \qquad \xi = \sqrt{\frac{m\omega_0}{\hbar}} z$$

$$\left[-\frac{\hbar^2}{2m}\frac{m\omega_0}{\hbar}\frac{d^2}{d\xi^2} + \frac{1}{2}m\omega_0^2\frac{\hbar}{m\omega_0}\xi^2\right]\psi(\xi) = \hbar\omega_0\varepsilon\,\psi(\xi) \quad \Rightarrow \quad \left[\frac{d^2}{d\xi^2} - \xi^2\right]\psi(\xi) = -2\varepsilon\,\psi(\xi)$$

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$$(-2\varepsilon_0+1)\psi_0(\xi) - \left(\frac{d}{d\xi}+\xi\right)\left(\frac{d}{d\xi}-\xi\right)\psi_0(\xi) = 2\psi_0(\xi)$$

$$\begin{bmatrix} -\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + \frac{1}{2}m\omega_0^2 z^2 \end{bmatrix} \psi(z) = E\psi(z) \qquad \varepsilon = \frac{E}{\hbar\omega_0} \qquad \xi = \sqrt{\frac{m\omega_0}{\hbar}} z$$
$$(-2\varepsilon_0 + 1)\psi_0(\xi) - \left(\frac{d}{d\xi} + \xi\right) \left(\frac{d}{d\xi} - \xi\right) \psi_0(\xi) = 2\psi_0(\xi)$$
$$\left(\frac{d}{d\xi} + \xi\right) \left(\frac{d}{d\xi} - \xi\right) \psi_0(\xi) = (-2\varepsilon_0 - 1)\psi_0(\xi) \qquad \left(\frac{d}{d\xi} - \xi\right) / \dots$$
$$\left(\frac{d}{d\xi} - \xi\right) \left(\frac{d}{d\xi} - \xi\right) \left(\frac{d}{d\xi} - \xi\right) \psi_0(\xi) = (-2\varepsilon_0 - 1) \left(\frac{d}{d\xi} - \xi\right) \psi_0(\xi)$$

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$$(-2\varepsilon_0 + 1)\psi_0(\xi) - \left(\frac{d}{d\xi} + \xi\right) \left(\frac{d}{d\xi} - \xi\right) \psi_0(\xi) = 2\psi_0(\xi) \qquad \left(\frac{d}{d\xi} - \xi\right) \left(\frac{d}{d\xi} - \xi\right) \psi_0(\xi) = (-2\varepsilon_0 - 1)\psi_0(\xi) \qquad \left(\frac{d}{d\xi} - \xi\right) / \dots$$

$$\left(\frac{d}{d\xi} - \xi\right) \left(\frac{d}{d\xi} + \xi\right) \left(\frac{d}{d\xi} - \xi\right) \psi_0(\xi) = (-2\varepsilon_0 - 1) \left(\frac{d}{d\xi} - \xi\right) \psi_0(\xi) = \psi_1(\xi) \qquad \left(\frac{d}{d\xi} - \xi\right) \psi_0(\xi) = \psi_1(\xi) \qquad \left(\frac{d}{d\xi} - \xi\right) \psi_0(\xi) = (-2\varepsilon_0 - 1)\psi_1(\xi) = (-2\varepsilon_1 + 1)\psi_1(\xi) \qquad \varepsilon_1 = \varepsilon_0 + 1$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + \frac{1}{2}m\omega_0^2 z^2\right]\psi(z) = E\psi(z) \qquad \qquad \varepsilon = \frac{E}{\hbar\omega_0} \qquad \xi = \sqrt{\frac{m\omega_0}{\hbar}}z$$

$$\left(\frac{d}{d\xi} - \xi\right)^n \psi_0(\xi) = \psi_n(\xi) \qquad \varepsilon_n = \varepsilon_0 + n$$

$$\left(\frac{d}{d\xi}+\xi\right)^n\psi_0(\xi)=\psi_{-n}(\xi)\qquad \varepsilon_{-n}=\varepsilon_0-n$$

$$\left(\frac{d}{d\xi} - \xi\right)\psi_0(\xi) = \psi_1(\xi)$$
$$\left(\frac{d}{d\xi} - \xi\right)\left(\frac{d}{d\xi} + \xi\right)\psi_1(\xi) = (-2\varepsilon_0 - 1)\psi_1(\xi) = (-2\varepsilon_1 + 1)\psi_1(\xi)$$
$$\varepsilon_1 = \varepsilon_0 + 1$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + \frac{1}{2}m\omega_0^2 z^2\right]\psi(z) = E\psi(z) \qquad \qquad \varepsilon = \frac{E}{\hbar\omega_0} \qquad \xi = \sqrt{\frac{m\omega_0}{\hbar}}z$$

$$\left(\frac{d}{d\xi} - \xi\right)^n \psi_0(\xi) = \psi_n(\xi) \qquad \varepsilon_n = \varepsilon_0 + n$$

$$\left(\frac{d}{d\xi}+\xi\right)^n\psi_0(\xi)=\psi_{-n}(\xi)\qquad \varepsilon_{-n}=\varepsilon_0-\varepsilon_0$$

We now choose  $\psi_0(\xi)$ :

$$\psi_{-1}(\xi) = 0$$

$$\left(\frac{d}{d\xi} + \xi\right)\psi_0(\xi) = \psi_{-1}(\xi) = 0$$
$$\psi_0(\xi) = A e^{-\frac{\xi^2}{2}}$$



**FIGURE 4.4.** Potential well V(z), energy levels, and wave functions of a harmonic oscillator. The potential is generated by a magnetic field of 1 T acting on electrons in GaAs.

$$\begin{bmatrix} -\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + \frac{1}{2}m\omega_0^2 z^2 \end{bmatrix} \psi(z) = E\psi(z) \qquad \qquad \varepsilon = \frac{E}{\hbar\omega_0} \qquad \xi = \sqrt{\frac{m\omega_0}{\hbar}} z$$
$$\begin{pmatrix} \frac{d}{d\xi} - \xi \end{pmatrix} \left( \frac{d}{d\xi} + \xi \right) A e^{-\frac{\xi^2}{2}} = (-2\varepsilon_0 + 1) A e^{-\frac{\xi^2}{2}} = 0 \quad \Rightarrow -2\varepsilon_0 + 1 = 0 \Rightarrow \varepsilon_0 = \frac{1}{2}$$
$$= 0 \qquad \qquad \varepsilon_n = n + \frac{1}{2}$$

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$$\psi_{-1}(\xi) = 0$$

$$\left(\frac{d}{d\xi} + \xi\right)\psi_0(\xi) = \psi_{-1}(\xi) = 0$$
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$$\left(\frac{d}{d\xi} - \xi\right) \left(\frac{d}{d\xi} + \xi\right) A e^{-\frac{\xi^2}{2}} = (-2\varepsilon_0 + 1) A e^{-\frac{\xi^2}{2}} = 0 \qquad \Rightarrow -2\varepsilon_0 + 1 = 0 \Rightarrow \varepsilon_0 = \frac{1}{2}$$

$$\varepsilon_n = n + \frac{1}{2}$$

$$E_n = \hbar\omega_0 \left(n + \frac{1}{2}\right)$$

$$\left(\sqrt{m\omega_0}\right) = (-m\omega_0 - \omega_0)^2$$

$$\psi_n(z) = A_n H_n\left(\sqrt{\frac{m\omega_0}{\hbar}}z\right) \exp\left(-\frac{m\omega_0}{2\hbar}z^2\right)$$

 $H_n$  - Hermite's polynomials

$$A_n = \left(2^n n! \sqrt{\frac{\pi\hbar}{m\omega}}\right)^{-1/2}$$





LETTERS

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# Sculpting oscillators with light within a nonlinear quantum fluid

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**Figure 1** | **Spatially mapped polariton-condensate wavefunctions. a**, Experimental scheme with two 1 µm-diameter pump spots separated by 20 µm focused on the planar microcavity. The effective potential V (red) produces multiple condensates (grey image shows  $n_{SHO} = 3$  mode). **b**, Real-space spectra along line between pump spots. **c**, Tomographic images of polariton emission (repulsive potential seen as dark circles around pump spots). Labelled according to  $n_{SHO}$  assigned from **d**. **d**, Extracted mode energies versus quantum number. **e**, Hermite-Gaussian fit of  $\psi_{SHO}^{n=5}(x)$  to image cross-section, dashed in **c**.

#### FIRST:

Coulomb potential in 3D in the semiconductor of dielectric constant  $\varepsilon_r$ , effective mass  $m^*$ :

 $V(r) = -\frac{e^2}{4\pi\varepsilon_r\varepsilon_0}\frac{1}{r}$   $Ry = \left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 \frac{m}{2\hbar^2} = \frac{\hbar^2}{2ma_B^2} = \frac{1}{2}\frac{e^2}{4\pi\varepsilon_0a_B} = 13.6 \text{ eV}$   $a_B = \frac{4\pi\varepsilon_0\hbar^2}{m_0e^2} = 0.5 \text{ Å}$   $E_n = -Ry\frac{1}{n^2}$   $E_n = -\left(\frac{m^*}{m_0}\right)\frac{1}{\varepsilon_r^2}Ry\frac{1}{n^2}$ 

$$E_n = -\left(\frac{m^*}{m_0}\right) \frac{1}{\varepsilon_r^2} Ry \frac{1}{n^2}$$
$$a_B^* = \frac{4\pi\varepsilon_r\varepsilon_0\hbar^2}{m_0e^2} \left(\frac{m_0}{m^*}\right) = a_B\varepsilon_r \left(\frac{m_0}{m^*}\right)$$

Electric charge moving in a plane in Coulomb potential. NOTE: this is not Gauss law in 2D (for which the relationship is like  $(\ln r)$  but the "hydrogen atom" trapped in 2D.

$$V(r) = -\frac{1}{r}$$

$$r = \sqrt{x^2 + y^2}, r \in [0, \infty)$$

$$\phi = \tan^{-1}\frac{x}{y}, \phi \in [0, 2\pi].$$

$$\frac{\partial}{\partial x} = \sin\phi\frac{\partial}{\partial r} + \frac{\cos\phi}{r}\frac{\partial}{\partial\phi}$$

$$\frac{\partial}{\partial y} = \cos\phi\frac{\partial}{\partial r} - \frac{\sin\phi}{r}\frac{\partial}{\partial\phi}.$$

$$\nabla^2 = \frac{\partial}{\partial x^2} + \frac{\partial}{\partial y^2} = \frac{\partial}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial}{\partial \phi^2}$$

Problem Hamiltonian in 2D:

.

V(r)

V

$$\left(-\frac{1}{2}\nabla^2 + V\right)\psi(\mathbf{r}) = -\frac{1}{2}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}\right)\psi(\mathbf{r}) + V(r)\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

Electric charge moving in a plane in Coulomb potential

$$\left(-\frac{1}{2}\nabla^2 + V\right)\psi(\mathbf{r}) = -\frac{1}{2}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}\right)\psi(\mathbf{r}) + V(r)\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

$$-\frac{1}{2}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2} + \frac{2}{r}\right)\psi(\mathbf{r}) = E\psi(\mathbf{r}) \qquad \Psi(\mathbf{r}) = R(r)\Phi(\phi)$$

Angular momentum magnitude:  $\hat{L}_{2D}^2 = -\frac{\partial^2}{\partial \phi^2}$ 

Angular momentum projection  $\hat{L}_z = -i \frac{\partial}{\partial \phi}$ 

$$\frac{r^2}{R(r)} \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{2}{r} + 2E \right) R(r) = -\frac{1}{\Phi(\phi)} \frac{\partial^2}{\partial \phi^2} \Phi(\phi) = m^2 \quad \text{(a number)}$$
$$\Phi(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

From physical reasons  $e^{im\phi} = e^{im(\phi+2\pi)}$  thus  $m = 0, \pm 1, \pm 2, \pm 3 \dots$ 

$$\Psi(\mathbf{r}) = R(r)\Phi(\phi)$$

Radial therm:

$$-\frac{1}{2}\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \frac{m^2}{r^2} + \frac{2}{r}\right)R(r) = ER(r)$$

O! joj-joj-joj! (some substitutions, derivations nad equations):

$$R_{n,m}(\rho) = e^{-\frac{\rho}{2}} \sum_{j=0}^{N(n)} a_0 \frac{|m| + j - n}{j(2|m| + j)} \rho^{|m| + j}$$

Finally:

$$Ry^* = \left(\frac{e^2}{4\pi\varepsilon_r\varepsilon_0}\right)^2 \frac{m^*}{2\hbar^2} = \frac{1}{2} \frac{e^2}{4\pi\varepsilon_0\varepsilon_r a_B^*} = \left(\frac{m^*}{m_0}\right) \frac{Ry}{\varepsilon_r^2} \qquad a_B^* = \varepsilon_r \left(\frac{m_0}{m^*}\right)$$



$$\Psi(\mathbf{r}) = R(r)\Phi(\phi)$$

Radial therm:

$$-\frac{1}{2}\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \frac{m^2}{r^2} + \frac{2}{r}\right)R(r) = ER(r)$$

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$$E_n = -\frac{Ry^*}{\left(n - \frac{1}{2}\right)^2}$$

For Hydrogen Ry = 13.6 eV and  $a_B = 0.053$  nm For GaAs semiconductor  $Ry^* \approx 5$  meV and  $a_B^* \approx 10$  nm



Finally:

$$Ry^* = \left(\frac{e^2}{4\pi\varepsilon_r\varepsilon_0}\right)^2 \frac{m^*}{2\hbar^2} = \frac{1}{2} \frac{e^2}{4\pi\varepsilon_0\varepsilon_r a_B^*} = \left(\frac{m^*}{m_0}\right) \frac{Ry}{\varepsilon_r^2} \qquad a_B^* = \varepsilon_r \left(\frac{m_0}{m^*}\right)$$

 $E_n = -\frac{Ry^*}{\left(n - \frac{1}{2}\right)^2}$ 

For Hydrogen Ry = 13.6 eV and  $a_B = 0.053$  nm For GaAs semiconductor  $Ry^* \approx 5$  meV and  $a_B^* \approx 10$  nm

#### Polaritons



http://www.stanford.edu/group/yamamotogroup/research/EP/EP\_main.html

## Quantum wells – 2D, 1D, 0D

2017-06-05



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The direct bandgap is required for optoelectronics

 $E_g^{InGaAs} = 0.4105 + 0.6337x + 0.475x^2 \text{ eV} @ 2.0 \text{K}$ 

$$\begin{split} \hbar\omega_n &= \varepsilon_{e,n_e} - \varepsilon_{h,n_h} = \\ &= E_g^{InGaAs} + \frac{\hbar^2 \pi^2 n^2}{2m_0 a^2} \left( \frac{1}{m_e} + \frac{1}{m_h} \right) = \\ &= E_g^{InGaAs} + \frac{\hbar^2 \pi^2 n^2}{2m_0 m_{eh} a^2} \\ \\ m_e &= (0.023 - 0.037x + 0.003x^2) m_0 \\ m_h &= (0.41 - 0.1x) m_0 \end{split}$$



TENSION! - You can not choose only the thickness, an important factor for quantum wells and dots is the stress!



Fig. 12.6. Bandgap energy and lattice constant of various III-V semiconductors at room temperature (adopted from Tien, 1988).

www.LightEmittingDiodes.org

 $(0.4105+0.6337x+0.475x^2)$ 

Full Hamiltonian in our universe has three spatial dimensions  $(x, y, z, t) = (\vec{R}, t)$ 

$$\left[-\frac{\hbar^2}{2m}\,\nabla^2 + V(\vec{R})\right]\psi(\vec{R}) = E\psi(\vec{R})$$

For  $V(\vec{R}) = V(z)$  we obtain:

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(z)\right]\psi(x, y, z) = E\psi(x, y, z)$$

Along directions x and y we have uniform motion (*ruch swobodny*):

$$\psi(x, y, z) = \exp(ik_x x) \exp(ik_y y) u(z)$$

We can show (on the blackboard!), that final eigenenergies of the potential V(z) are:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + V(z)\right]u(z) = \varepsilon u(z) \qquad \qquad \varepsilon = E - \frac{\hbar^2 k_x^2}{2m} - \frac{\hbar^2 k_y^2}{2m}$$







 $\psi_{k_x,k_y,n}(x,y,z) = \exp(ik_x x) \exp(ik_y y) u_n(z) = \psi_{k,n}(r,z) = \exp(i\mathbf{k} \cdot r) u_n(z)$ 



**FIGURE 4.9.** Quasi-two-dimensional system in a potential well of finite depth. Electrons with the same total energy can be bound in the well (A) or free (B).

#### Finite potential well – square well



masses  $m_W = 0.067$  in the well and  $m_B = 0.15$  in the barrier.

Effective mass in the barrier  $m_B$  and in the well  $m_W$ 

$$\left[-\frac{\hbar^2}{2m_0 m_{W,B}} \nabla^2 + V(\vec{R})\right] \psi(\vec{R}) = E\psi(\vec{R})$$

For separated wave functions:  $\psi(\vec{R}) = \psi_{k,n}(r,z) = \exp(i\mathbf{k} \cdot r) u_n(z)$ 

$$\begin{bmatrix} -\frac{\hbar^2}{2m_0 m_W} \nabla^2 + E_W \end{bmatrix} \psi(\vec{R}) = E\psi(\vec{R})$$
$$\begin{bmatrix} -\frac{\hbar^2}{2m_0 m_B} \nabla^2 + E_B \end{bmatrix} \psi(\vec{R}) = E\psi(\vec{R})$$

We got (on the blackboard!):

$$\left[-\frac{\hbar^2}{2m_0 m_W}\frac{d^2}{dz^2} + \frac{\hbar^2 k^2}{2m_0 m_W} + E_W\right]u_n(z) = \varepsilon u_n(z)$$
$$\left[-\frac{\hbar^2}{2m_0 m_B}\frac{d^2}{dz^2} + \frac{\hbar^2 k^2}{2m_0 m_B} + E_B\right]u_n(z) = \varepsilon u_n(z)$$

The particle moves in the well which potential depends on  $\boldsymbol{k}$ , in fact  $k = |\boldsymbol{k}|$ 

$$\begin{bmatrix} -\frac{\hbar^2}{2m_0 m_W} \frac{d^2}{dz^2} + \frac{\hbar^2 k^2}{2m_0 m_W} + E_W \end{bmatrix} u_n(z) = \varepsilon u_n(z)$$
$$\begin{bmatrix} -\frac{\hbar^2}{2m_0 m_B} \frac{d^2}{dz^2} + \frac{\hbar^2 k^2}{2m_0 m_B} + E_B \end{bmatrix} u_n(z) = \varepsilon u_n(z)$$

$$V_0(k) = (E_B - E_W) + \frac{\hbar^2 k^2}{2m_0} \left(\frac{1}{m_B} - \frac{1}{m_W}\right)$$

The particle gains partially the effective mass of the barrier:

E.g. in GaAs-AlGaAs heterostructure  $m_B > m_W$  thus the well gets "shallow"

$$E_n(k) = \varepsilon_n(k) + \frac{\hbar^2 k^2}{2m_0 m_W} \approx \varepsilon_n(k=0) + \frac{\hbar^2 k^2}{2m_0 m_{eff}}$$
  
energy of the bound state depends on  $k$ 

$$m_{eff} \approx m_W P_W + m_B P_B$$
  
the probability of finding a particle

The particle moves in the well which potential depends on  $\boldsymbol{k}$ , in fact  $k = |\boldsymbol{k}|$ 

$$\begin{bmatrix} -\frac{\hbar^2}{2m_0 m_W} \frac{d^2}{dz^2} + \frac{\hbar^2 k^2}{2m_0 m_W} + E_W \end{bmatrix} u_n(z) = \varepsilon u_n(z)$$
$$\begin{bmatrix} -\frac{\hbar^2}{2m_0 m_B} \frac{d^2}{dz^2} + \frac{\hbar^2 k^2}{2m_0 m_B} + E_B \end{bmatrix} u_n(z) = \varepsilon u_n(z)$$

$$V_0(k) = (E_B - E_W) + \frac{\hbar^2 k^2}{2m_0} \left(\frac{1}{m_B} - \frac{1}{m_W}\right)$$

**TABLE 4.2** Dependence on transverse wave vector  $\mathbf{k}_{\perp}$  of the energies of the states bound in a well 5 nm wide and 1 eV deep, with effective mass  $m_{\rm W} = 0.067$  inside the well and  $m_{\rm B} = 0.15$  outside.

<i>k</i> (nm <sup>-1</sup> )	$\frac{\hbar^2 k^2}{2m_0 m_W}$ (eV)	$\frac{\hbar^2 k^2}{2m_0 m_{\rm B}}$ (eV)	<i>V</i> <sub>0</sub> ( <i>k</i> ) (eV)	ε <sub>1</sub> (eV)	ε <sub>2</sub> (eV)	ε3 (eV)	m <sub>eff</sub>
0.0	0.000	0.000	1.000	0,108	0.446	0.969	0.057
0.5	0.142	0.064	0.921	0.106	0.435	0.919	0.069
1.0	0.570	0.254	0.685	0.096	0.397		0.076

E.g. in GaAs-AlGaAs heterostructure  $m_B > m_W$  thus the well gets "shallow"





 $\psi_{k_x,m,n}(x, y, z) = u_{m,n}(x, y) \exp(ik_z z)$  = albo np. =  $u_{n,l}(r, \theta) \exp(ik_z z)$ 



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$$\psi_{k_x,m,n}(x, y, z) = u_{m,n}(x, y) \exp(ik_z z)$$
 = albo np. =  $u_{n,l}(r, \theta) \exp(ik_z z)$ 

$$E_n(k_x,k_y) = \varepsilon_{m,n} + \frac{\hbar^2 k_z^2}{2m}$$

Square quantum well 2D  $L_{\chi}L_{\gamma}$ , infinite potential:

 $\psi_{k_x,m,n}(x,y,z) = u_{m,n}(x,y) \exp(ik_z z) = \exp(ik_m x) \exp(ik_n y) \exp(ik_z z)$ 

With boundary conditions  $L_x k_m = n_x \pi$  and  $L_y k_n = n_y \pi$  (dicrete spectrum)



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**Fig. 2.13.** The first four modes of the quantum wire. Since in this example,  $L_x > L_y$  the  $n_x = 2$ ,  $n_y = 1$  mode has lower energy than the  $n_x = 1$ ,  $n_y = 2$  mode.

Rectangular wire  $(a \times b)$  – solutions like:

$$\varepsilon_{n_x,n_y} = \frac{\hbar^2 \pi^2}{2m} \left( \frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} \right)$$



http://wn.com/2d\_and\_3d\_standing\_wave

Rectangular wire  $(a \times b)$  – solutions like:

$$\varepsilon_{n_x,n_y} = \frac{\hbar^2 \pi^2}{2m} \left( \frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} \right)$$



http://www.almaden.ibm.com/vis/stm/images/stm14.jpg

Cylindrical well (with infinite walls)

$$-\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} + V_0 \right) \psi(r, \theta) = E\psi(r, \theta)$$

$$\psi(r, \theta) = u(r) \exp(il\theta)$$

$$\frac{\psi(r, \theta) = u(r) \exp(il\theta)}{\left[ -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} \right) + \frac{\hbar^2 l^2}{2mr^2} + V_0 \right] u(r) = Eu(r)$$
hat gives solutions in the form Bessel functions
$$\frac{d^2 u}{dt^2} = \frac{du}{dt}$$

What gives solutions in the form Bessel functions

$$r^{2}\frac{d^{2}u}{dr^{2}} + r\frac{du}{dr} + [(kr)^{2} - l^{2}]u = 0 \qquad J_{l}(kr) \sim \sqrt{\frac{2}{\pi kr}\cos\left(kr - \frac{1}{2}l\pi - \frac{1}{4}\pi\right)}$$
$$k = \sqrt{2m(E - V_{0})}/\hbar$$

$$\phi_{nl}(r) \propto J_l\left(\frac{J_{l,n}r}{a}\right) \exp(il\theta) \qquad \qquad \varepsilon_{nl} = \frac{\hbar^2 j_{l,n}^2}{2ma}$$

Zeros of the Besseel function are  $j_{l,n}$ 

Cylindrical well

low temperature scanning tunneling microscope (STM)



en.ibm.com/vis/stm/corral.htm l#stm16



Cylindrical well

low temperature scanning tunneling microscope (STM)







http://www.almaden.ibm.com/vis/stm/images/stm17.jpg