Chair of Condensed Matter Physics
Institute of Theoretical Physics
Faculty of Physics, Universityof Warsaw

Semester Zimowy 2011/2012

Wykład

Modelowanie Nanostruktur

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Electronic structure of a bulk (3D) in the magnetic field

$$\frac{1}{2m^*}\left(i\hbar\nabla - \frac{e}{c}\vec{A}\right)^2 \Psi(x,y,z) = E\Psi(x,y,z)$$

$$\vec{A} = \nabla \times \vec{B}$$

$$\vec{A} \to \vec{A}' = \vec{A} + \nabla\Lambda, \quad \textit{where} \quad \Lambda(\vec{x},t) \text{ -- scalar function}$$

$$\vec{B} = const = (0,0,B)$$

$$\vec{A}(\vec{r}) = (-By,0,0)$$

$$\vec{A}(\vec{r}) = \frac{1}{2}(-By,Bx,0), \quad [\vec{A}(\vec{r}) = \frac{1}{2}\vec{B}\times\vec{r}]$$

$$\vec{A}(\vec{r}) = (0,Bx,0)$$

Modelowanie Nanostruktur, 2011/2012
Jacek A. Majewski

Wykład 7 – *22 XI 2011*

Pole magnetyczne w nanostrukturach

- Poziomy Landaua w 3D
- Poziomy Landaua w dwu-wymiarowym gazie elektronowym
- Pole magnetyczne w drutach kwantowych
- Pole magnetyczne w kropkach kwantowych
  Stany Focka-Darwina

Electronic structure of a bulk (3D) in the magnetic field (cnt.)

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

$$\Psi(x,y,z) = \exp[i(k_x x + k_z z)]g(y)$$

$$\frac{d^2 g}{dy^2} + \frac{2m^*}{\hbar^2}\left[E - \frac{\hbar^2}{2m^*}k_z^2 - \frac{1}{2m^*}(\hbar k_x - eBy)^2\right]g(y) = 0$$

$$y_0 := \frac{\hbar k_x}{eB} \quad \omega_c := \frac{eB}{m^*} \quad \left(\omega_c := \frac{eB}{cm^*}\right) \quad \varepsilon = E - \frac{\hbar^2}{2m^*}k_z^2$$

$$\frac{d^2 g}{dy^2} + \frac{2m^*}{\hbar^2}\left[\varepsilon - \frac{m^*}{2}\omega_c^2(y-y_0)^2\right]g(y) = 0$$

Electronic structure of a bulk (3D) in the magnetic field (cnt.)

$$\frac{d^2 g}{dy^2}+\frac{2m^*}{\hbar^2}\left[\varepsilon-\frac{m^*}{2}\omega_c^2(y-y_0)^2\right]g(y)=0$$

$$\varepsilon_n=(n+1/2)\hbar\omega_c$$

$$g_n(y)=\left(\frac{2\sqrt{\pi}\alpha}{\Omega 2^n n!}\right)^{1/2}H_n[\alpha(y-y_0)]\exp[-\frac{1}{2}\alpha^2(y-y_0)^2]$$

$$\alpha=\frac{m^*\omega_c}{\hbar}=\frac{eB}{\hbar}=1/l_m$$

Electronic structure of a bulk (3D) in the magnetic field (cnt.)

Degeneracy of the levels

The number of possible k_α $(\alpha = x,y,z)$ in the range Δk_α is equal to $\frac{L_\alpha}{2\pi}\Delta k_\alpha$

The *orbit center* y_0 must lie within the box

$$-L_y/2\le y_0\le L_y/2$$

$$-L_y/2\le\frac{\hbar k_x}{eB}\le L_y/2$$

It determines the range of allowed wavevectors

$$\frac{-L_y eB}{2\hbar}\le k_x\le\frac{L_y eB}{2\hbar}\qquad \Delta k_x=\frac{L_y eB}{\hbar}$$

Number of states with certain k_z

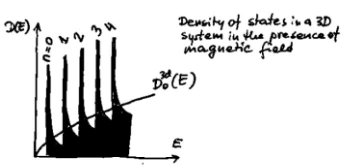
$$p:=\frac{L_x}{2\pi}\Delta k_x=\frac{L_x L_y eB}{2\pi\hbar}=\frac{m^*\omega_c L_x L_y}{2\pi\hbar}$$

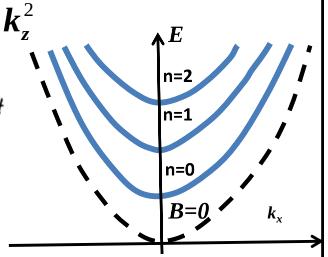
Number of states in Landau level

$$p\Delta k_z=p\frac{L_z}{2\pi}\Delta k_z=\frac{L_x L_y L_z eB}{4\pi^2\hbar}$$

Electronic structure of a bulk (3D) in the magnetic field (cnt.)

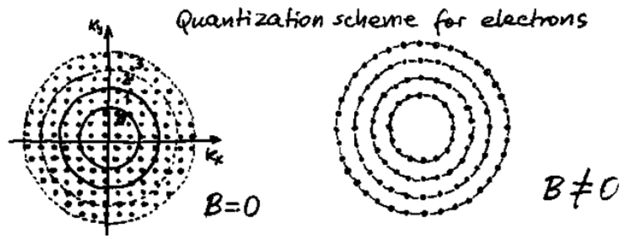
$$E=(n+1/2)\hbar\omega_c+\frac{\hbar^2}{2m^*}k_z^2$$





$$D(E)=\frac{1}{4\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\hbar\omega_c\sum_n[E-(n+1/2)\hbar\omega_c]^{-\frac{1}{2}}$$

Electronic structure of a bulk (3D) in the magnetic field (cnt.)



In the presence of the magnetic field, various k_x, k_y points condense into points on circles which represent constant energy surfaces with energies $\frac{\hbar\omega_c}{2}$, $\frac{3\hbar\omega_c}{2}$, etc.

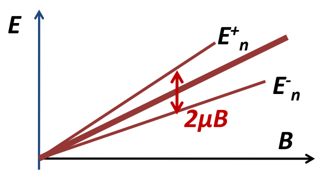
Electronic structure of a bulk (3D) in the magnetic field (cnt.)

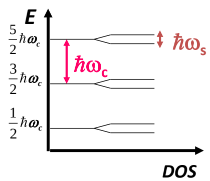
Effect of electron spin on Landau levels

$$\left[\frac{1}{2m*}\left(i\hbar\nabla-\frac{e}{c}\vec{A}\right)^2+\mu\vec{\sigma}\bullet\vec{B}\right]\Psi(x,y,z)=E\Psi(x,y,z)$$

Zeeman term

$$E_n^{\pm}(k_z)=(n+1/2)\hbar\omega_c+\frac{\hbar^2}{2m*}k_z^2\pm\mu B$$





2D structures in the magnetic field

$$\left[\frac{-\hbar^2}{2m_z}\frac{\partial^2}{\partial z^2}+\frac{1}{2m*}\left(i\hbar\nabla_r-\frac{e}{c}\vec{A}_r\right)^2+V_{eff}(z)\right]\Psi(x,y,z)=E\Psi(x,y,z)$$

$$\vec{A}_r=(0,Bx,0)$$

$$\Psi(x,y,z)=\varphi(z)\chi(x,y)$$

$$\left[\frac{-\hbar^2}{2m_z}\frac{\partial^2}{\partial z^2}+V_{eff}(z)\right]\varphi(z)=E_i\varphi(z)$$ Describes confinement

$$\left[\frac{-\hbar^2}{2m*}\frac{\partial^2}{\partial x^2}+\frac{m*\omega_c^2}{2}(x-x_0)^2\right]\chi(x,y)=E_n\chi(x,y)$$

$$x_0:=\frac{1}{eB}\frac{\hbar}{i}\frac{\partial}{\partial y}$$

Electronic states in 2D Electron Gas (2DEG)

2D structures in the magnetic field (2)

$$\left[\frac{-\hbar^2}{2m*}\frac{\partial^2}{\partial x^2}+\frac{m*\omega_c^2}{2}(x-x_0)^2\right]\chi(x,y)=E_n\chi(x,y)$$

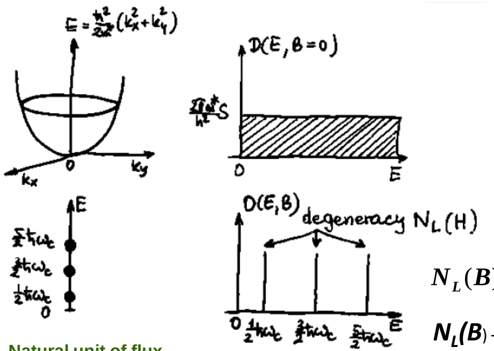
$$\chi(x,y)=\chi(x)e^{ik_y y} \quad \Rightarrow \quad x_0=\frac{\hbar k_y}{eB}$$

$$\chi_n(x)=\left(\frac{2\sqrt{\pi}\alpha}{\Omega 2^n n!}\right)^{1/2}H_n[\alpha(x-x_0)]\exp[-\frac{1}{2}\alpha^2(x-x_0)^2]$$

$$E_n=E_i+\varepsilon_n=E_i+(n+1/2)\hbar\omega_c$$ Discrete levels!!!

$$D(E)\sim\sum_n\delta(E-E_n)$$

2D structures in the magnetic field (3)



$$N_L(B) = BS\frac{e}{hc} = \frac{\Phi}{\Phi_0}$$

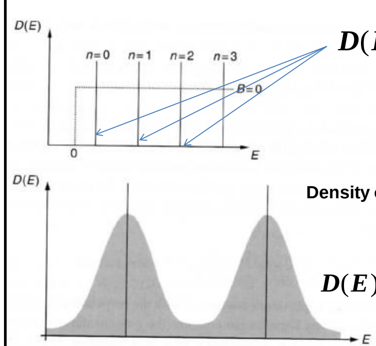
$N_L(B)$ – degeneracy of a level

Natural unit of flux

$$\Phi_0 = \frac{hc}{e} = 4.136\times10^{-7}\ gauss\cdot cm^2$$

Electronic states in 1D systems Quantum Wires

2D structures in the magnetic field (4)

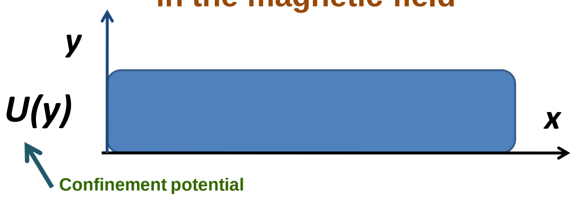


$$D(E) \sim \sum_n \delta(E - E_n)$$

Density of states with **disorder**

$$D(E) = \frac{1}{2\pi l_m^2}\sum_n\left[1 - \left(\frac{E-E_n}{\Gamma_n}\right)^2\right]^{1/2}$$

Confined 2D structures (effectively 1D) in the magnetic field



Landau gauge $A_x = -By \quad A_y = 0$

$$[E_s + \frac{(\hat{p}_x + eBy)^2}{2m*} + \frac{\hat{p}_y^2}{2m*} + U(y)]\Psi(x,y) = E\Psi(x,y)$$

$$\hat{p}_x = -i\hbar\frac{\partial}{\partial x} \qquad \hat{p}_y = -i\hbar\frac{\partial}{\partial y}$$

No analytic solutions for arbitrary confinement potential

Confined 2D structures (effectively 1D) in the magnetic field (3)

$$\Psi(x,y)=\frac{1}{\sqrt{L}}e^{ikx}\chi(y)$$

$$[E_s+\frac{(\hbar k+eBy)^2}{2m*}+\frac{\hat{p}_y^2}{2m*}+U(y)]\chi(y)=E\chi(y)$$

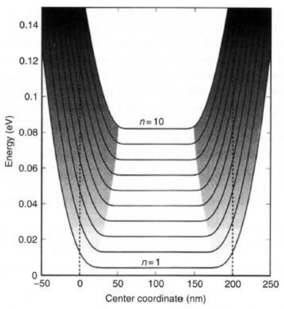
A parabolic potential: $U(y)=\frac{1}{2}m*\omega_0^2y^2$

$$E(n,k)=E_s+(n+\frac{1}{2})\hbar\omega_{co}+\frac{\hbar^2k^2}{2m*}\frac{\omega_o^2}{\omega_{co}^2}$$

$$\omega_{co}=\omega_o+\omega_c \qquad \omega_c=\frac{|e|B}{cm*}$$

Confined 2D structures (effectively 1D) in the magnetic field (3)

An infinite barrier type confining potential *U(y)*:



Calculated energy versus center coordinate y_0 for a **200nm-wide wire** and magnetic field 5T.

The shaded regions correspond to edge states

Confined 2D structures (effectively 1D) in the magnetic field (3)

$$E(n,k)=E_s+(n+\frac{1}{2})\hbar\omega_{co}+\frac{\hbar^2k^2}{2m*}\frac{\omega_o^2}{\omega_{co}^2}$$

Group velocity: $v(n,k)=\frac{1}{\hbar}\frac{\partial E(n,k)}{\partial k}=\frac{\hbar k}{m*}\frac{\omega_o^2}{\omega_{co}^2}$

The wave function of the state *(n,k)* is centered at $y = -- y_k$

$$y_k=\frac{\hbar k}{eB}$$

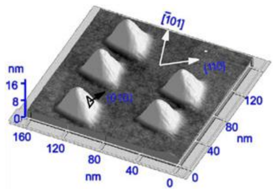
The spatial location of the wave function is proportional to k or group velocity

Electronic states in quantum dots Fock-Darwin theory

Entirely confined systems

$L \approx \lambda = \hbar/(2Em^*)^{1/2}$

0D systems
quantum dots
quantum boxes
artificial atoms
....



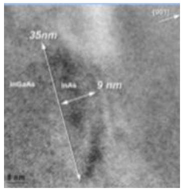
Where physics of solids, atoms, nucleus, quantum chaos meet ➔

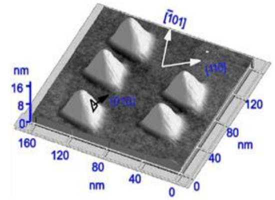
Few body problem

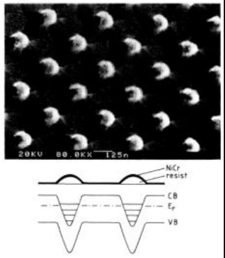
Fock-Darwin theory

Two-dimensional harmonic oscillator in the magnetic field

$L_z << L_x, L_y$ + 2D parabolic potential well
one-electron approximation

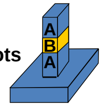




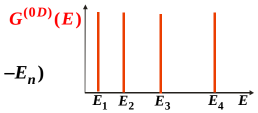


Energy spectrum of 0D systems

0D
Quantum Dots



$$G^{(0D)}(E) = \sum_n \delta(E - E_n)$$



always discreet levels (dimensional quantisation):

- ε_n ψ_n **whose degeneracies, positions, and distribution depend on QD shape and disorder**
- **independently of disorder, spin and time reversal degeneracy if *B* = 0 and no spin interactions**

Analogy to:

- *nucleus*
- *finite elastic bodies (vibration modes)*
- *electromagnetic cavities*

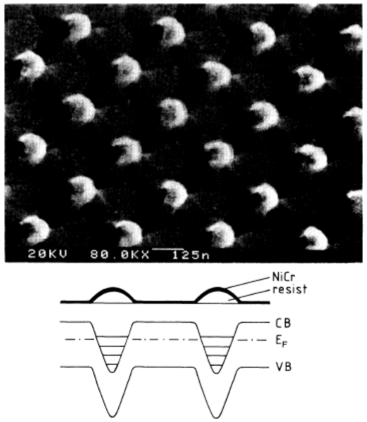


FIG. 1. Scanning electron micrograph of resist dots, with a 125 nm marker, together with a schematical sketch of the band structure across the dots right at the InSb surface. The bright disks give an idea of the geometrical dot size. This monitor sample is shadowed with gold for contrast enhancement.

Quantum Dot in Magnetic Field

$$\mathsf{H}_i = \frac{(\mathsf{p}_i - q_i \mathsf{A}_i)^2}{2m^*} + \tfrac{1}{2} m^* \omega_0^2 \mathsf{r}_i^2 + \frac{g^* \mu_\mathrm{B}}{\hbar} \mathbf{B} \cdot \mathsf{s}_i$$

$$\nabla \times \mathbf{A} = \mathbf{B} \qquad \mu_\mathrm{B} = |q|\hbar/2m_0$$

Single Particle Eigenstates

$$\psi_{n,m} \propto H_n(x) H_m(y) \mathrm{e}^{-\frac{1}{2}(x^2+y^2)}$$

Coulomb Gauge → $\nabla \cdot \mathbf{A} = 0$

$$\mathbf{A} = -\tfrac{1}{2} B \,(y\mathbf{i} - x\mathbf{j})$$

Fock-Darwin Eigenstates

$$\mathsf{H} = -\tfrac{1}{2}\nabla^2 + \tfrac{1}{2} r^2 + \tfrac{1}{2}\omega_c \left(\mathsf{l}_z + \gamma^* \mathsf{s}_z\right)$$

$$\psi_{n_L,l}(r,\theta) = C_{n_L,l}\; r^{|l|}\, \mathrm{e}^{il\theta}\, L_{n_L}^{(|l|)}(r^2)\ \exp\left(-\tfrac{1}{2} r^2\right)$$

$$n_L \geq 0 \text{ and } |l| \leq n_L \qquad C_{n_L,l}^2 = \frac{n_L!}{\pi (n_L + |l|)!}$$

$L_n^{(k)}$ is an associated Laguerre polynomial

$$(n+1) L_{n+1}^{(k)}(x) = (2n + k + 1 - x) L_n^{(k)}(x) - (n+k) L_{n-1}^{(k)}(x)$$

$$L_0^{(k)}(x) = 1\,, \quad \text{and}$$

$$L_1^{(k)}(x) = 1 - x + k$$

$$\mathsf{A} \cdot \mathsf{p} = \tfrac{1}{2} B\, \mathsf{l}_z, \qquad \mathsf{A}^2 = \tfrac{1}{4} B^2 \mathsf{r}^2$$

In the symmetric gauge

$$\mathsf{H} = \frac{\mathsf{p}^2}{2m^*} + \frac{\mu_\mathrm{B}^*}{\hbar} B\, \mathsf{l}_z + \tfrac{1}{2} m^* \left(\frac{qB}{2m^*}\right)^2 \mathsf{r}^2 + \tfrac{1}{2} m^* \omega_0^2 \mathsf{r}^2 + \frac{g^* \mu_\mathrm{B}}{\hbar} B \mathsf{s}_z$$

$$= \frac{\mathsf{p}^2}{2m^*} + \tfrac{1}{2} m^* \left(\omega_0^2 + \tfrac{1}{4}\omega_c^2\right) \mathsf{r}^2 + \frac{\mu_\mathrm{B}^* B}{\hbar} \left(\mathsf{l}_z + \gamma^* \mathsf{s}_z\right)$$

$$\mu_\mathrm{B}^* = \mu_\mathrm{B}/m_\mathrm{r} \quad \gamma^* = g^* m_\mathrm{r} \quad \omega_c = |q| B/m^*$$

$$\hbar = m^* = |q| = \omega = 1$$

$$\mathsf{H} = -\tfrac{1}{2}\nabla^2 + \tfrac{1}{2} r^2 + \tfrac{1}{2}\omega_c \left(\mathsf{l}_z + \gamma^* \mathsf{s}_z\right)$$

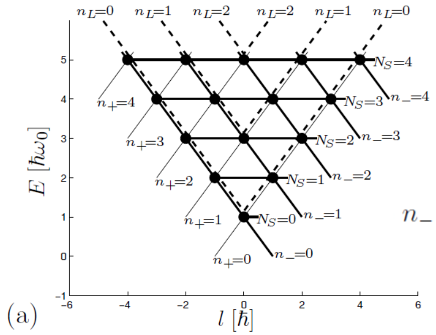
Fock-Darwin Eigenstates

$$\mathsf{H} = -\tfrac{1}{2}\nabla^2 + \tfrac{1}{2} r^2 + \tfrac{1}{2}\omega_c \left(\mathsf{l}_z + \gamma^* \mathsf{s}_z\right)$$

$$\psi_{n_L,l}(r,\theta) = C_{n_L,l}\; r^{|l|}\, \mathrm{e}^{il\theta}\, L_{n_L}^{(|l|)}(r^2)\ \exp\left(-\tfrac{1}{2} r^2\right)$$

$$E_{n_L,l} = 1 + 2n_L + |l| + \tfrac{1}{2}\omega_c \left(l + \gamma^* s\right)$$

Single Particle Energy Levels in Zero Magnetic Field



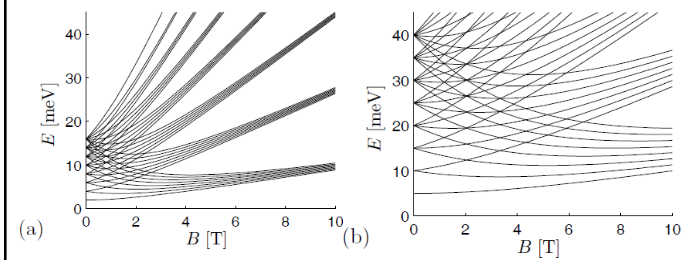
$$N_S = 2n_L + |l|$$

$$n_- = n_L + \frac{1}{2}(|l| + l)$$

$$E_{n_L,l} = 1 + 2n_L + |l| + \frac{1}{2}\omega_c\,(l + \gamma^* s)$$

The single particle energy levels (without Zeeman Energy) as a function of magnetic field

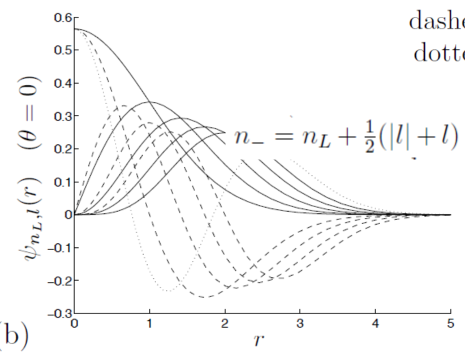
$\hbar\omega_0 = 2\,\mathrm{meV}$ $\hbar\omega_0 = 5\,\mathrm{meV}$



$m_r = 0.067$

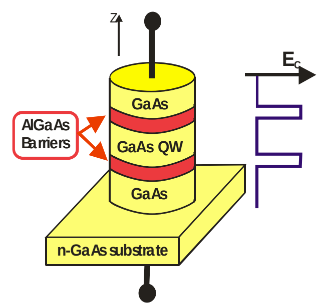
Formation of Landau Levels for B → inf is clearly seen

Radial parts of the Fock-Darwin single particle states



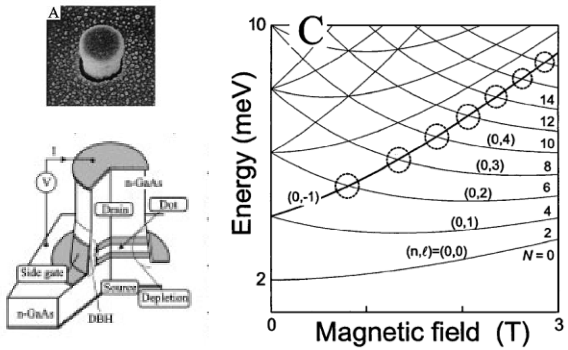
Example of Quantum Transport: Coherent Tunneling

Resonant Tunneling Diode (RTD)



Esaki, Chang, Tsu (IBM, 1974)

Fock-Darwin states



Tarucha et al.., PRL'00