XIIth-IIC-EMTCCM

European Master in Theoretical Chemistry and Computational Modelling

Lecture 2

Magnetic Field:

Classical Mechanics
Aharonov-Bohm effect

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The Hamiltonian of a particle in a magnetic field

charged particle in a magnetic field. The Hamiltonian of such system is:

$$H = \frac{1}{2m}(p - eA)^2 + V(r), \qquad (1)$$

where A is the vector potential of the magnetic field B and $V(r)$ is a confining potential.

The Hamiltonian of a charged particle in a magnetic field reads,

$$\hat{\mathcal{H}} = \frac{(\hat{p} - eA)^2}{2m_e} + V\,, \qquad (1)$$

where $\hat{p}$ is the

Where does this Hamiltonian come from?

and V the spatial confining potential. If the magnetic field is axial and constant, $\vec{B} = B_0\vec{k}$, we may choose the potential vector $\vec{A} = (-\frac{1}{2}y\,B_0, \frac{1}{2}x\,B_0, 0)$ so that the

The Hamiltonian for an electron in the two-dimensional (x,y) plane, in the presence of a magnetic field, reads (in a.u.),

$$\mathcal{H} = \frac{1}{2m^*}(\mathbf{p} + \mathbf{A})^2 + V(x,y), \qquad (1)$$

where m^* stands for the effective mass, $\mathbf{A}$ is the vector po-

Within the effective mass and envelope function approximations, this Hamiltonian for a system in the (x, y) plane is, in atomic units,

$$H = \frac{1}{2m^*}(\mathbf{p} + \mathbf{A})^2 + V(x, y), \qquad (1)$$

where m^* stands for the electron effective mass, $\mathbf{A}$ is the vector potential and $V(x, y)$ represents a finite scalar potential which

motion of the electron in the ring. In atomic units, the Hamiltonian may be written as:

$$H = \frac{1}{2m^*}(\mathbf{p} + \mathbf{A})^2 + V(x, y), \qquad (1)$$

where m^* stands for the electron effective mass, $\mathbf{p}$ is the canonical moment, and $V(x, y)$ is a square-well potential

coordinates of the QR and write the Hamiltonian in atomic units as

$$H = \frac{1}{2m^*}(\mathbf{p} + \mathbf{A})^2 + V(x, y), \qquad (1)$$

where m^* stands for the electron effective mass, $\mathbf{A}$ is the vector potential and $V(x, y)$ represents a finite scalar

Classical Mechanics:

Conservative systems $V = V(q)$ $\quad F = -\frac{\partial V}{\partial q}$

$q = x, y, z$ $\quad F(x, y, z)$

Newton's Law $\frac{d}{dt}p - F = 0$ $\quad p = p_x, p_y, p_z$

Lagrange equation $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q} = 0$ $\quad L = T - V$

$p = \frac{\partial L}{\partial \dot{q}}$ $\quad F = \frac{\partial L}{\partial q} = -\frac{\partial V}{\partial q}$

Hamiltonian $H = p\dot{q} - L = 2T - (T - V) = T + V$

Velocity-dependent potentials

Time-independent field $\vec{B}(x, y, z)$ $\quad \vec{F} = e\,(\vec{v} \wedge \vec{B})$

$\vec{F}(\vec{r}, \vec{v})$

No magnetic monopoles $\vec{\nabla}\vec{B} = 0$ $\quad \vec{B} = \vec{\nabla} \wedge \vec{A}$ $\quad \vec{A}(x, y, z)$

Lagrange function in this case?

Guess: $L = \frac{1}{2}mv^2 + e(\vec{v} \cdot \vec{A})$

Is $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q} = 0$ *equivalent to* $\vec{F} = e\,(\vec{v} \wedge \vec{B})$?

$$L = \frac{1}{2}mv^2 + e(\vec{v}\cdot\vec{A})$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q} = 0$$

$$\frac{d}{dt}\frac{\partial L}{\partial v_x} = \frac{d}{dt}(mv_x + eA_x) = m\frac{dv_x}{dt} + \sum_i \frac{\partial A_x}{\partial q_i}\frac{dq_i}{dt}$$

$$\frac{d}{dt}\frac{\partial L}{\partial v_x} = m\frac{dv_x}{dt} + \sum_i \frac{\partial A_x}{\partial q_i}v_i$$

$$\frac{\partial L}{\partial x} = e\sum_i \frac{\partial A_i}{\partial x}v_i$$

$$m\frac{dv_x}{dt} = e\left(v_y(\partial_x A_y - \partial_y A_x) + v_z(\partial_x A_z - \partial_z A_x)\right)$$

$$= e\left(v_y B_z - v_z B_y\right) = e(v \times B)_x$$

$$\vec{F} = e\left(\vec{v} \wedge \vec{B}\right)$$

$$\vec{B} = \begin{vmatrix} \vec{\imath} & \vec{\jmath} & \vec{k} \\ \partial_x & \partial_y & \partial_z \\ A_x & A_y & A_z \end{vmatrix}$$

$$\vec{v} \times \vec{B} = \begin{vmatrix} \vec{\imath} & \vec{\jmath} & \vec{k} \\ v_x & v_y & v_z \\ B_x & B_y & B_z \end{vmatrix}$$

Lagrangian

$$L = \frac{1}{2}mv^2 + e(\vec{v}\cdot\vec{A})$$

kinematic momentum:

$$\pi_x = \frac{\partial T}{\partial \dot{x}} = m\,\dot{x}$$

canonical momentum:

$$p_x = \frac{\partial L}{\partial \dot{x}} = \pi_x + eA_x$$

Hamiltonian

$$H = \sum_{i=x,y,z} p_i\,\dot{x}_i - L = \sum_{i=x,y,z} (\pi_i\,\dot{x}_i + e\,\dot{x}_i\,A_i) - \sum_{i=x,y,z} (\frac{1}{2}\pi_i\,\dot{x}_i + e\,\dot{x}_i\,A_i) = \frac{1}{2}\sum_{i=x,y,z} \pi_i\,\dot{x}_i = \frac{\pi^2}{2m}$$

$$\Rightarrow \quad H = \frac{1}{2m}(p - e\,A)^2$$

Gauge

$B = \nabla \wedge A_1$; $A = A_1 + \nabla\chi$ $\Longrightarrow$ $B = \nabla \wedge A$

$$\nabla \wedge (\nabla\chi) = \begin{vmatrix} \vec{\imath} & \vec{\jmath} & \vec{k} \\ \partial_x & \partial_y & \partial_z \\ \partial_x\chi & \partial_y\chi & \partial_z\chi \end{vmatrix} = 0$$

We may select χ : $\nabla(A_1 + \nabla\chi) = \nabla A = 0$

Coulomb Gauge : $\boxed{\nabla A = 0}$

Hamiltonian (coulomb gauge)

$H = \frac{1}{2m}(p - e\,A)^2$; $\hat{p} \longrightarrow -i\hbar\nabla$

$$H = \frac{1}{2m}(-i\hbar\nabla - e\,A)^2 = \frac{\hbar^2}{2m}\nabla^2 + \frac{i\hbar}{2m}e\,(\nabla\,A + A\,\nabla) + \frac{e^2}{2m}A^2$$

$$H = \frac{\hbar^2}{2m}\nabla^2 + \frac{i\hbar}{m}e\,A\,\nabla + \frac{e^2}{2m}A^2$$

$$\Longrightarrow \boxed{H = \frac{\hat{p}^2}{2m} - \frac{e}{m}A\cdot\hat{p} + \frac{e^2}{2m}A^2}$$

Axial magnetic field B & coulomb gauge

$$A = (-1/2\, y\, B_0, 1/2\, x\, B_0, 0)$$

$$\nabla \wedge A = \begin{vmatrix} \vec{\imath} & \vec{\jmath} & \vec{k} \\ \partial_x & \partial_y & \partial_z \\ -1/2\, y\, B_0 & 1/2\, x\, B_0 & 0 \end{vmatrix} = B_0\, \vec{k} \quad ;$$

$$\nabla A = \partial_x(-1/2\, y\, B_0) + \partial_y(1/2\, x\, B_0) + \partial_z(0) = 0$$ *gauge*

$$A = (-1/2\, y\, B_0, 1/2\, x\, B_0, 0) \quad p = -i\hbar\nabla \Rightarrow A^2 = \frac{1}{4}B_0^2(x^2 + y^2) = \frac{1}{4}B_0^2\rho^2$$

$$\Rightarrow A \cdot \hat{p} = -\frac{1}{2} i\hbar B_0 (x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}) = \frac{1}{2} B_0 \hat{L}_z$$

Confined electron pierced by a magnetic field

Spherical confinement, axial symmetry

$$\vec{B} = B_0\vec{k}$$

$$\hat{\mathcal{H}} = \frac{(\hat{p} - eA)^2}{2m_e} + V$$

$$\vec{A} = (-\tfrac{1}{2}y\, B_0, \tfrac{1}{2}x\, B_0, 0)$$

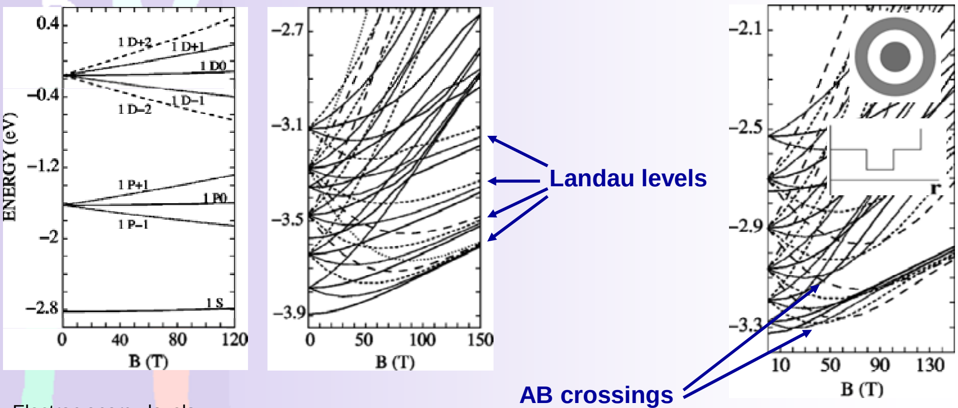
$$\hat{\mathcal{H}} = -\frac{\hbar^2}{2m_e}\nabla^2 - \frac{eB}{2m_e}\hat{L}_z + \frac{e^2B^2}{8m_e}\rho^2 + V(\rho, z)$$

$$\Psi(\rho, z, \phi) = \Phi_{n,M}\, e^{iM\phi} \qquad |e| = \hbar = 1$$

$$\left(-\frac{1}{2m_e}\nabla^2 + \frac{B^2}{8m_e}\rho^2 + \frac{BM}{2m_e} + V_e(\rho, z)\right)\Phi_{n,M} = E_{n,M}\Phi_{n,M}$$

Competition: quadratic vs. linear term

Electron in a spherical QD pierced by a magnetic field



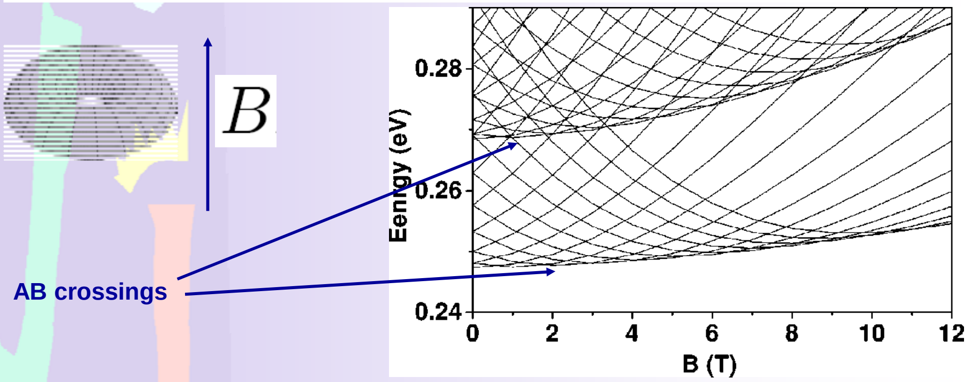
Electron energy levels, *nLM*, R = 3 nm InAs NC

Electron energy levels, *nLM*, R = 12 nm InAs NC

Electron energy levels, *nLM*, GaAs/InAs/GaAs QDQW

Electron in a QR pierced by a magnetic field

$$\left(-\frac{1}{2m_e}\nabla^2+\frac{B^2}{8m_e}\rho^2+\frac{BM}{2m_e}+V_e(\rho,z)\right)\Phi_{n,M}=E_{n,M}\Phi_{n,M}$$



Aharonov-Bohm Effect

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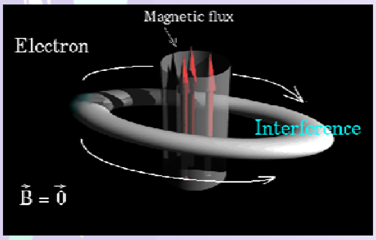
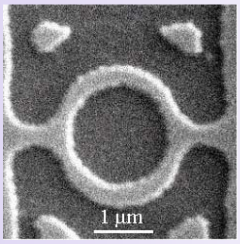
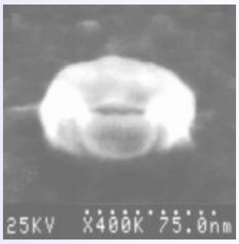


- Classical mechanics: equations of motion can always be expressed in term of field alone.
- Quantum mechanics: canonical formalism. Potentials cannot be eliminated.
- An electron can be influenced by the potentials even if no fields act upon it.

Semiconductor Quantum Rings

Litographic rings
GaAs/AlGaAs





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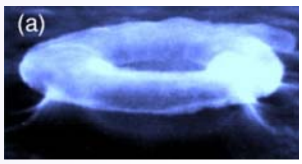
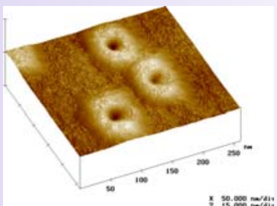


self-assembled rings
InAs



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T. Raz et al., Appl. Phys. Lett ***82*** *(2003) 1706*

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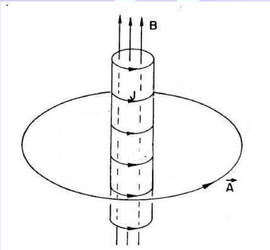
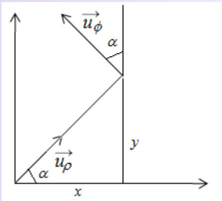
Toy-example : Quantum ring 1D



$$\begin{cases} A_1 = A(0<\rho<a) = \frac{1}{2} B_0\, \rho\, \vec{u}_\phi \\ A_2 = A(a<\rho<\infty) = \frac{1}{2\rho} B_0\, a^2\, \vec{u}_\phi \end{cases}$$



$$\vec{u}_\phi = \vec{\imath}\,(-\sin\alpha) + \vec{\jmath}\,(\cos\alpha) = \frac{1}{\rho}(-y, x, 0)$$

$$\begin{cases} A_1 = \frac{B_0}{2}(-y,x,0) \;\rightarrow\; \vec{B} = \nabla \times A = B_0\ \vec{k} \\ A_2 = \frac{B_0}{2}\frac{a^2}{\rho^2}(-y,x,0) \;\rightarrow\; \vec{B} = \nabla \times A = 0 \end{cases}$$

Quantum ring 1D

$$E = H = L = \frac{1}{2} I \omega^2 = \frac{1}{2} I\, \dot{\phi}^2 \rightarrow p_\phi = \frac{\partial L}{\partial\, \dot{\phi}} = I\, \dot{\phi} = I\omega = L_z$$

$$I = mR^2$$

$$\vec{A} = \frac{B_0 a^2}{2R} \vec{u}_\phi$$

$$H = \frac{p^2}{2m} = \frac{L_z^2}{2mR^2} \xrightarrow{B \neq 0} H = \frac{(p+A)^2}{2m} = \frac{L_z^2}{2mR^2} + \frac{A \cdot L_z}{mR} + \frac{A^2}{2m}$$

$$= \frac{1}{2mR^2}\left(L_z^2 + B_0 a^2 L_z + \frac{B_0^2 a^4}{4}\right)$$

$$= \frac{(L_z + \Phi)^2}{2mR^2}$$

$$\Phi = \frac{B_0 \pi a^2}{2\pi}$$

$$E = \frac{(M + \Phi)^2}{2mR^2}$$