7th IIC-EMTCCM
European Master in Theoretical Chemistry and Computational Modelling
7th International Intensive Course

DIPARTIMENTO DI MATEMATICA E INFORMATICA

Lecture 2

Magnetic Field:

Classical Mechanics
Magnetism: Landau levels
Aharonov-Bohm effect
Magneto-translations

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Classical Mechanics: an overview

Newton's Law

$$\frac{d}{dt}p - F = 0$$

Conservative systems

$$V = V(q) \qquad F = -\frac{\partial V}{\partial q}$$

Lagrange equation

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

$$L = T - V$$

$$p = \frac{\partial L}{\partial \dot{q}}$$

Velocity-dependent potentials

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

No magnetic monopoles $\int_S \vec{B} d\vec{S} = 0$ ⟺ $\vec{\nabla}\vec{B} = 0$

$\vec{B} = \vec{\nabla} \wedge \vec{A}$ $\vec{A}(x, y, z)$

$$\vec{F} = e\,(\vec{v} \wedge \vec{B}) = e\,(\vec{v} \wedge \vec{\nabla} \wedge \vec{A})$$

$$(\vec{\nabla} \wedge \vec{A})_x = (\partial_y A_z - \partial_z A_y)$$

$$(\vec{v} \wedge \vec{\nabla} \wedge \vec{A})_x = \frac{\partial(\vec{v} \cdot \vec{A})}{\partial x} - \sum_{x,y,z} v_i \left(\frac{\partial A_x}{\partial q_i}\right) = \frac{\partial(\vec{v} \cdot \vec{A})}{\partial x} - \frac{d\,A_x}{d\,t}$$

Velocity-dependent potentials: cont.

$$F_x = e\,(\vec{v} \wedge \vec{\nabla} \wedge \vec{A})_x = e\left[\frac{\partial(\vec{v}\cdot\vec{A})}{\partial x} - \frac{d\,A_x}{d\,t}\right]$$

Define: $U = -e\,(\vec{v}\cdot\vec{A}) \Longrightarrow \dfrac{\partial U}{\partial \dot{x}} = -e\,A_x$

$$F_x = -\frac{\partial U}{\partial x} + \frac{d}{dt}\frac{\partial U}{\partial \dot{x}}$$

$$F_x = \dot{\pi}_x = \frac{d}{dt}\left(\frac{\partial T}{\partial \dot{x}}\right)$$

$$L = T - U$$

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

Velocity-dependent potentials: cont.

kinematic momentum:

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

canonical momentum:

$$p_x = \frac{\partial L}{\partial \dot{x}} = \frac{\partial T}{\partial \dot{x}} - \frac{\partial U}{\partial \dot{x}} = \pi_x + e\,A_x$$

Hamiltonian:

$$H = \sum_{i=x,y,z} p_i\,\dot{x}_i - L = \sum_{i=x,y,z} (\pi_i\,\dot{x}_i + e\,\dot{x}_i\,A_i) - (T - U)$$

$$\Rightarrow \quad H = (2T - U) - (T - U) = T = \frac{\pi^2}{2m}$$

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

Conservative systems: V(x,y,z) & L = T - V

canonical momentum: $p_x = \frac{\partial L}{\partial \dot{x}} = \frac{\partial T}{\partial \dot{x}} - \frac{\partial V}{\partial \dot{x}} = \frac{\partial T}{\partial \dot{x}} = \pi_x$ ***kinematic momentum:***

Hamiltonian:

$$H = \sum_{i=x,y,z} p_i \dot{x}_i - L = \sum_{i=x,y,z} \pi_i \dot{x}_i - (T - V) = 2T - (T - V)$$

$$\Rightarrow \quad H = T + V = \frac{\pi^2}{2m} + V \equiv \frac{p^2}{2m} + V$$

$$\Rightarrow \quad \boxed{H = \frac{p^2}{2m} + V}$$

Gauge

$$B = \nabla \wedge A_1 \quad ; \quad A = A_1 + \nabla\chi \implies B = \nabla \wedge A$$

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

We may select χ :

$$\nabla(A_1 + \nabla\chi) = \nabla A = 0$$

Gauge Coulomb:

$$\boxed{\nabla A = 0}$$

Hamiltonian (coulomb gauge)

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

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

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

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

Axial magnetic field B & coulomb gauge

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

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

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

$$A = (-1/2\, y\, B_0, 1/2\, x\, B_0, 0)$$
$$p = -i\hbar\nabla$$

$\Rightarrow$

$$A^2 = \frac{1}{4} B_0^2 (x^2 + y^2) = \frac{1}{4} B_0^2 \rho^2$$

$\Rightarrow$

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

Hamiltonian: axial magnetic field B & coulomb gauge

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

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

$$A^2 = \frac{1}{4} B_0^2 (x^2 + y^2) = \frac{1}{4} B_0^2 \rho^2$$

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \frac{e^2\, B_0^2}{8m}\rho^2 - \frac{e\, B_0}{2m}\hat{L}_z \quad ; \quad \omega = -\frac{e B}{2m}$$

$$\Rightarrow \quad \hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2} m\omega^2\rho^2 + \omega \hat{L}_z$$

$\omega_c = 2\,\omega$ ***Cyclotron frequency***

Electron in a magnetic field

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

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

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

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

$$= \frac{\hat{p}_z^2}{2m_e} + \hat{\mathcal{H}}_{HO}^{2D} - \frac{eB}{2m_e}\hat{L}_z + V$$

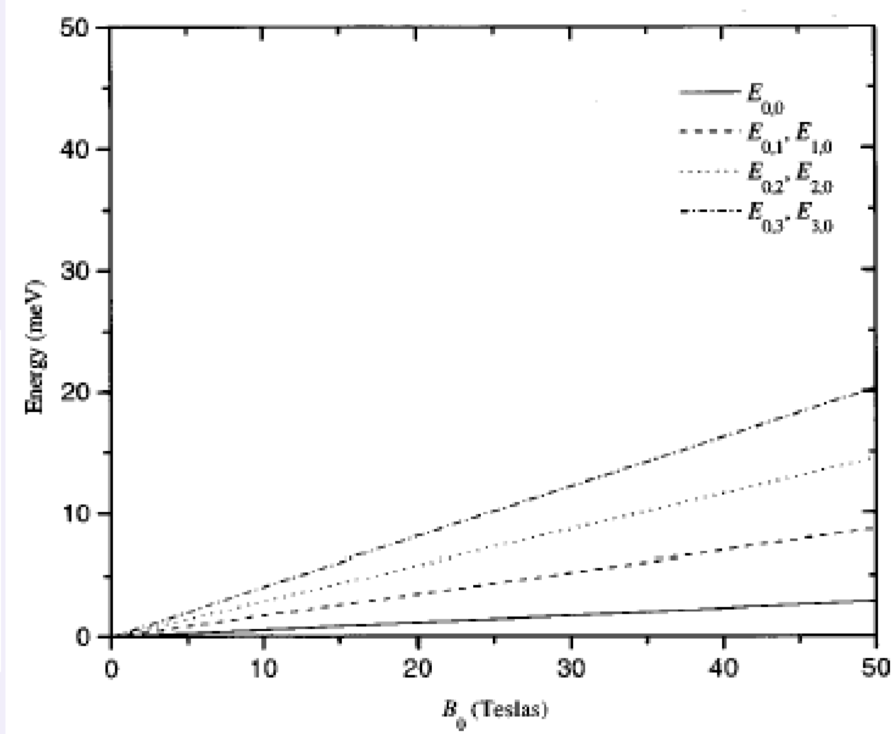
$$E_{HO}^{2D} = (2n + |M| + 1)\,\omega$$

$$\hat{H}' = \frac{B\hat{L}_z}{2m}$$

$$E' = \frac{B}{2m} M = \omega M$$

$$[\hat{H}_{HO}^{2D}, \hat{H}'] = 0$$

$$E(n, M) = (2n + |M| + M + 1)\,\omega$$



Rosas et al. AJP 68 (2000) 835

- **Landau levels**
- **No crossings**

Confined electron pierced by a magnetic field

Spherical confinement, axial symmetry

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

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

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

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

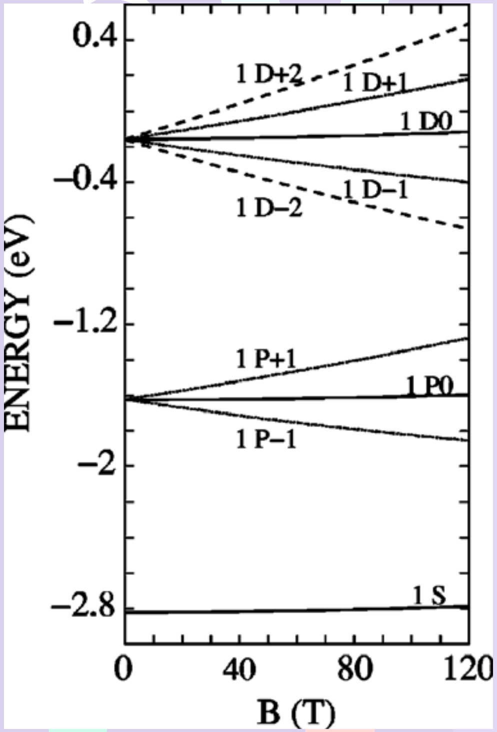
$$\Psi(\rho, z, \phi) = \Phi_{n,M}\; e^{iM\phi}$$

$$|e| = \hbar = 1$$

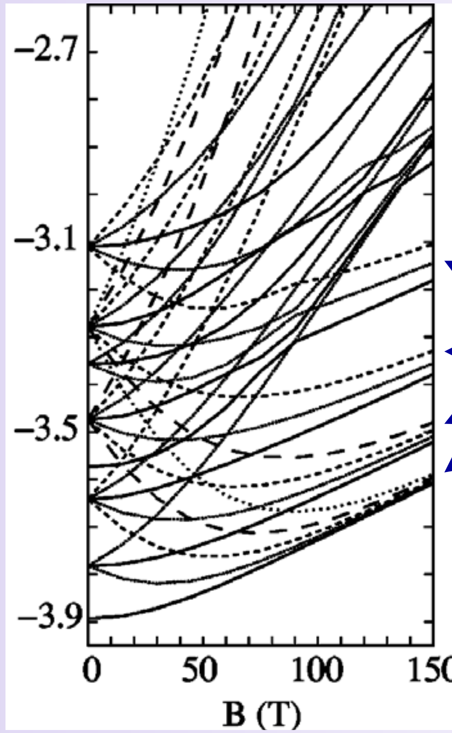
$$\left(-\frac{1}{2m_e}\nabla^2 + \frac{B^2}{8m_e}\rho^2 + \frac{BM}{2m_e} + V_e(\rho, z)\right)\Phi_{n,M} = E_{n,M}\Phi_{n,M}$$

Competition: quadratic vs. linear term

Electron in a spherical QD pierced by a magnetic field



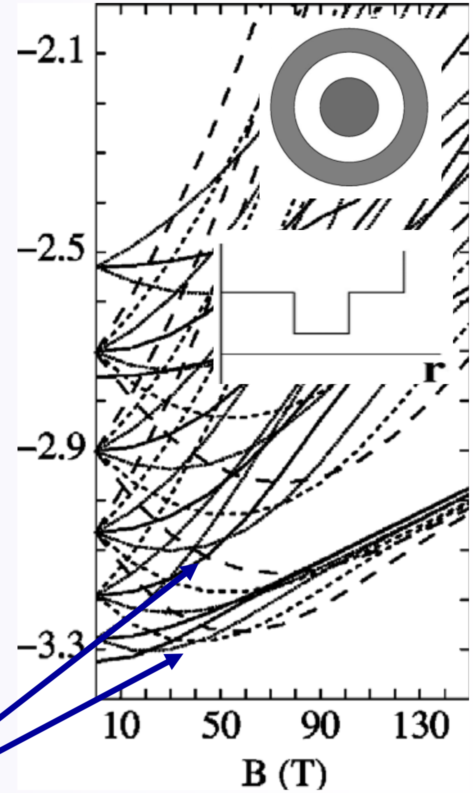
Electron energy levels, *nLM*, R = 3 nm InAs NC



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

Landau levels

AB crossings



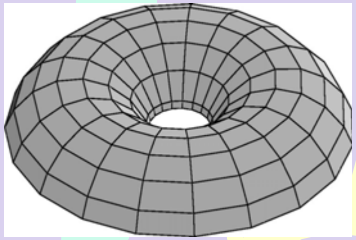
Electron energy levels, *nLM*,

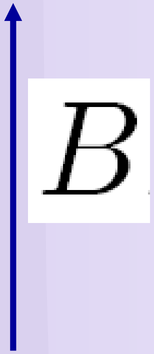
GaAs/InAs/GaAs QDQW

J. Planelles, J. Díaz, J. Climente and W. Jaskólski, PRB 65 (2002) 245302

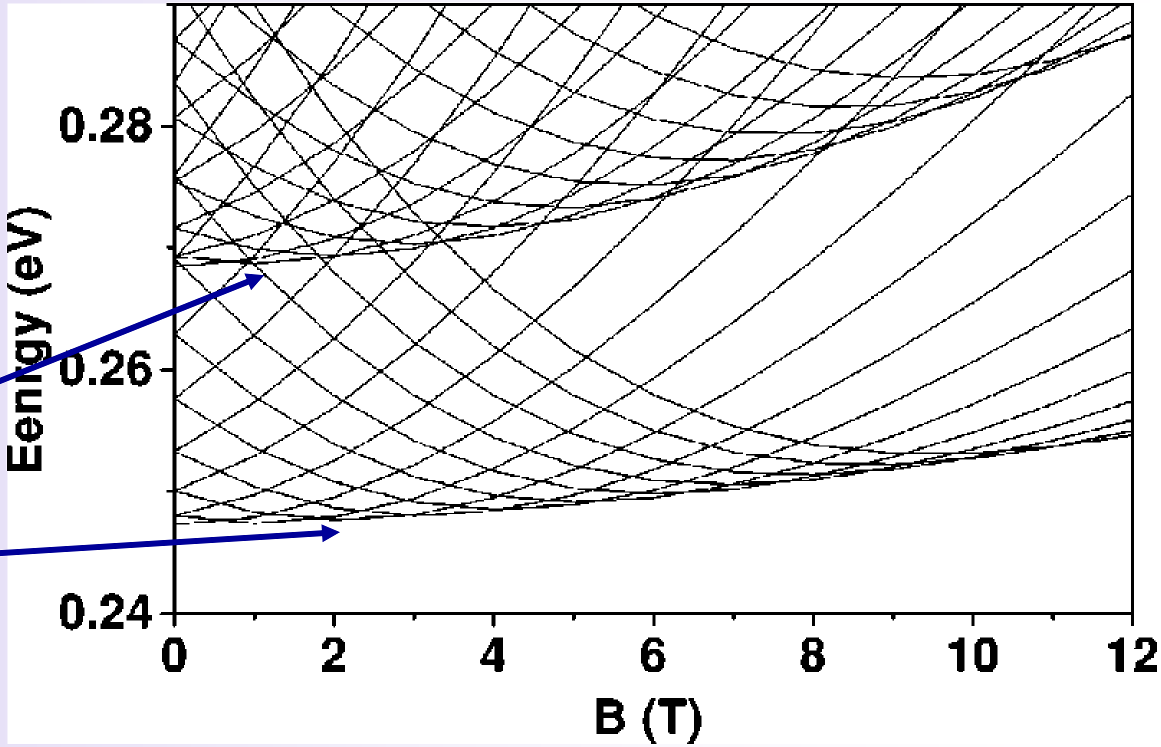
Electron in a QR pierced by a magnetic field

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





AB crossings



Electron energy levels (*n=1, M*) (*n=2,M*), of a InAs QR

Dimensions: r = 10, R=60, h=2

J. Planelles ,W. Jaskólski, and I. Aliaga, PRB 65 (2001) 033306

Peierls/Berry phase

R. Peierls, Z. Phys. ***80*** *(1933) 763;*
M. Graf & P. Volg, PRB ***51*** *(1995) 4940*
M.V. Berry, Proc. R. Soc. A ***392*** *(1984) 45.*
R.Resta, JPCM ***12*** *(2000) R107;*

$\mathcal{H}_0 = \frac{p^2}{2m}$ $\quad \mathcal{H} = \frac{(p+A)^2}{2m}$

$\{E_n^0, \Phi_n^0\}$ $\quad \{E_n, \Psi_n\}$

A phase in is introduced in the wf by the magnetic field: $F(\mathbf{r}) = \int_0^{\mathbf{r}} \mathbf{A}(r')d\mathbf{r}' \leftrightarrow \nabla F = \mathbf{A}$

Choose: $\Psi(\mathbf{r}) = \exp\left[-iF(\mathbf{r})\right]\chi(\mathbf{r})$

$$(-i\nabla + A)\exp\left[-iF(\mathbf{r})\right]\chi(\mathbf{r}) = \exp\left[-iF(\mathbf{r})\right](-i\nabla\chi(\mathbf{r})) \rightarrow$$

$$(-i\nabla + A)^2\exp\left[-iF(\mathbf{r})\right]\chi(\mathbf{r}) = \exp\left[-iF(\mathbf{r})\right](-\nabla^2\chi(\mathbf{r}))$$

$$\frac{1}{2m}(-i\nabla + A)^2\exp\left[-iF(\mathbf{r})\right]\chi(\mathbf{r}) = E\exp\left[-iF(\mathbf{r})\right]\chi(\mathbf{r})$$

$$\longrightarrow \quad -\frac{1}{2m}\nabla^2\chi = E\chi,$$

BCs

Peierls/Berry phase cont

Peierls subtitution: $\Phi(\mathbf{r}) \longrightarrow \exp\left[-i\int_0^{\mathbf{r}} \mathbf{A}(r')d\mathbf{r}'\right]\Phi(\mathbf{r})$

Hamiltonian substitution: $\mathcal{H} = \exp\left[-iF\right]\mathcal{H}_0\exp\left[iF\right]$

$$\nabla(\exp[iF]\Phi) = \exp[iF]\nabla\Phi + \Phi\exp[iF]\nabla F = \exp[iF]\nabla\Phi + i\,A\exp[iF]\Phi$$

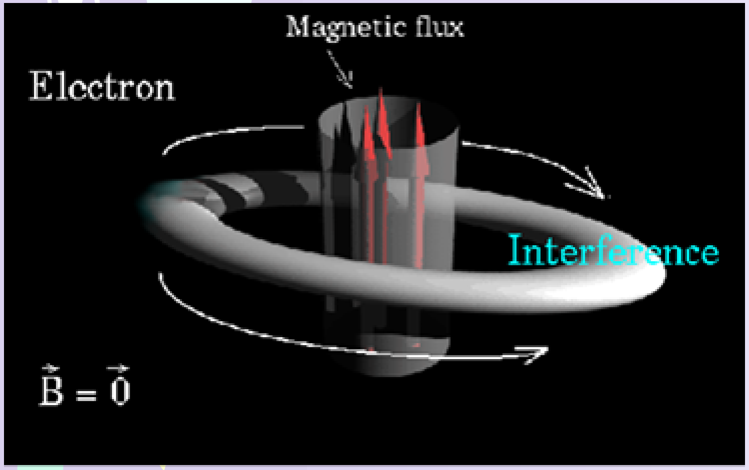
$$-\nabla^2(\exp[iF]\Phi) = \exp[iF](-\nabla^2\Phi + 2\,i\,A\nabla\Phi + A^2\Phi) = \exp[iF](-i\nabla + A)^2\Phi$$

$$\exp[-iF]\left[-\frac{1}{2m}\nabla^2 + V\right]\exp[iF]\Phi = \exp[-iF]\exp[iF]\left[\frac{1}{2m}(-i\nabla + A)^2 + V\right]\Phi$$

$$= \left[\frac{1}{2m}(-i\nabla + A)^2 + V\right]\Phi$$

Aharonov-Bohm Effect

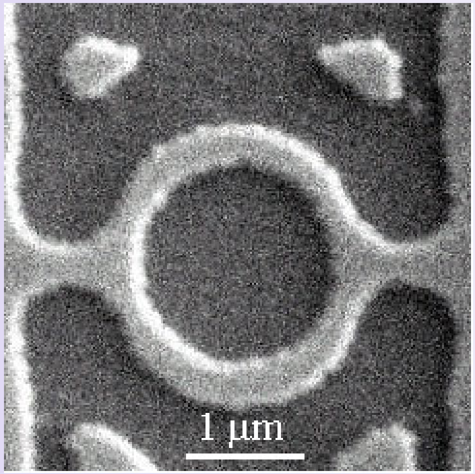
Y. Aharonov, D. Bohm, Phys. Rev. ***115*** *(1959) 485*

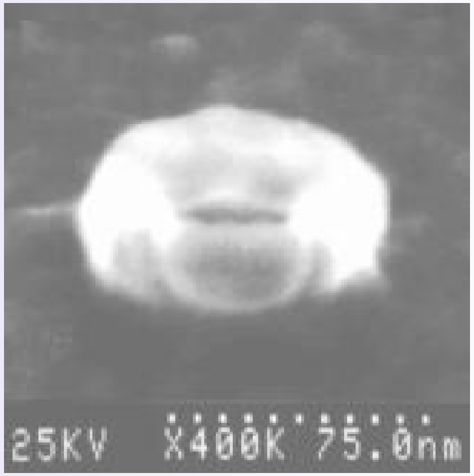


- Classical mechanics: equations of motion can always be expressed in term of field alone.
- Quantum mechanics: canonical formalism. Potentials cannot be eliminated.
- An electron can be influenced by the potentials even if no fields acts upon it.
- Berry's phase (gauge dependent)
- $\oint A dl$ Gauge independent

Semiconductor Quantum Rings

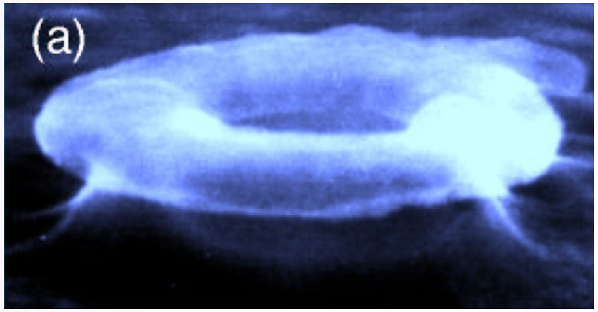
Litographic rings
GaAs/AlGaAs



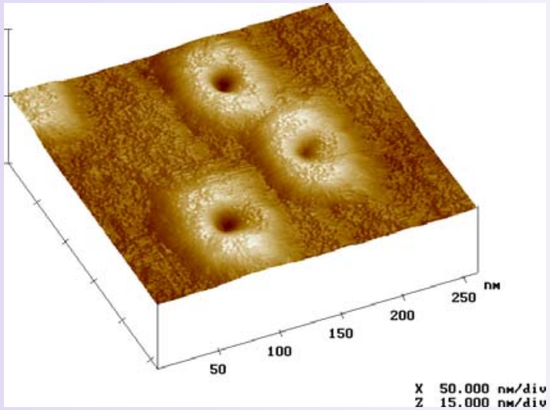


*A.Fuhrer et al., Nature **413** (2001) 822;*

*M. Bayer et al., Phys. Rev. Lett. **90** (2003) 186801.*



self-assembled rings
InAs

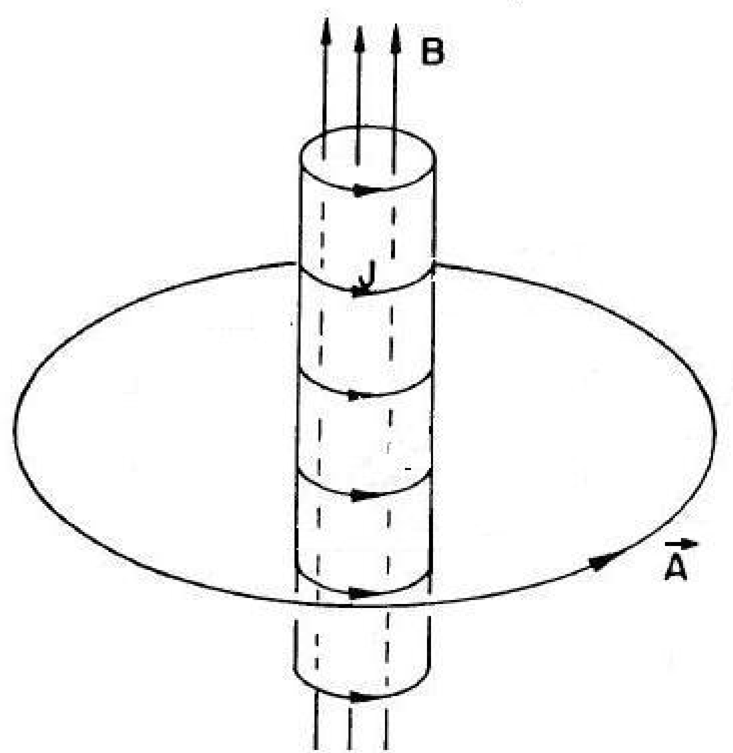


*J.M.García et al., Appl. Phys. Lett. **71** (1997) 2014*

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

*B.C. Lee, C.P. Lee, Nanotech. **15** (2004) 848*

Example 1: Quantum ring 1D



$$\vec{A} = A_\phi \vec{u}_\phi = \begin{cases} \frac{1}{2} B \rho \vec{u}_\phi & 0 < \rho < a \\ \frac{Ba^2}{2\rho} \vec{u}_\phi & a < \rho < \infty \end{cases}$$

$$F(\mathbf{r}) = \int_0^{\mathbf{r}} \mathbf{A}(r')d\mathbf{r}' = \int_0^\theta \frac{Ba^2}{2\rho} \rho d\phi = \frac{B\pi a^2}{2\pi} \theta = F\theta$$

$$\Psi(\theta) = e^{-iF\theta} e^{iM\theta}$$

$$(M - F) = 0 \pm 1 \pm 2 ...$$

BCs: $\Psi(\theta + 2\pi) = \Psi(\theta)$

$$E_M = \frac{M^2}{2I}$$

No magnetic field: $M = 0 \pm 1 \pm 2 ... \in \mathcal{Z}$

With field: $M = F, F \pm 1, F \pm 2 ... \in \mathcal{R}$

Electron in a potential vector but no magnetic field

$B = B_0$ if $0 < \rho < a$ and $B = 0$ otherwise

$$\vec{A} = A_\phi \vec{u}_\phi = \begin{cases} \frac{1}{2} B \rho \vec{u}_\phi & 0 < \rho < a \\ \frac{Ba^2}{2\rho} \vec{u}_\phi & a < \rho < \infty \end{cases}$$

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

$$\hat{\mathcal{H}} = -\frac{\hbar^2}{2m_e}\nabla^2 + \frac{i\hbar e}{m_e}\frac{Ba^2}{2\rho^2}\frac{\partial}{\partial\phi} + \frac{e^2 B^4 a^4}{8 m_e \rho^4} + V$$

$$\frac{\partial}{\partial\phi} \to \frac{\partial}{\partial\phi} - \frac{i\,eB\,a^2}{2\,\hbar} = \frac{\partial}{\partial\phi} + i\frac{\Phi}{\Phi_0}$$

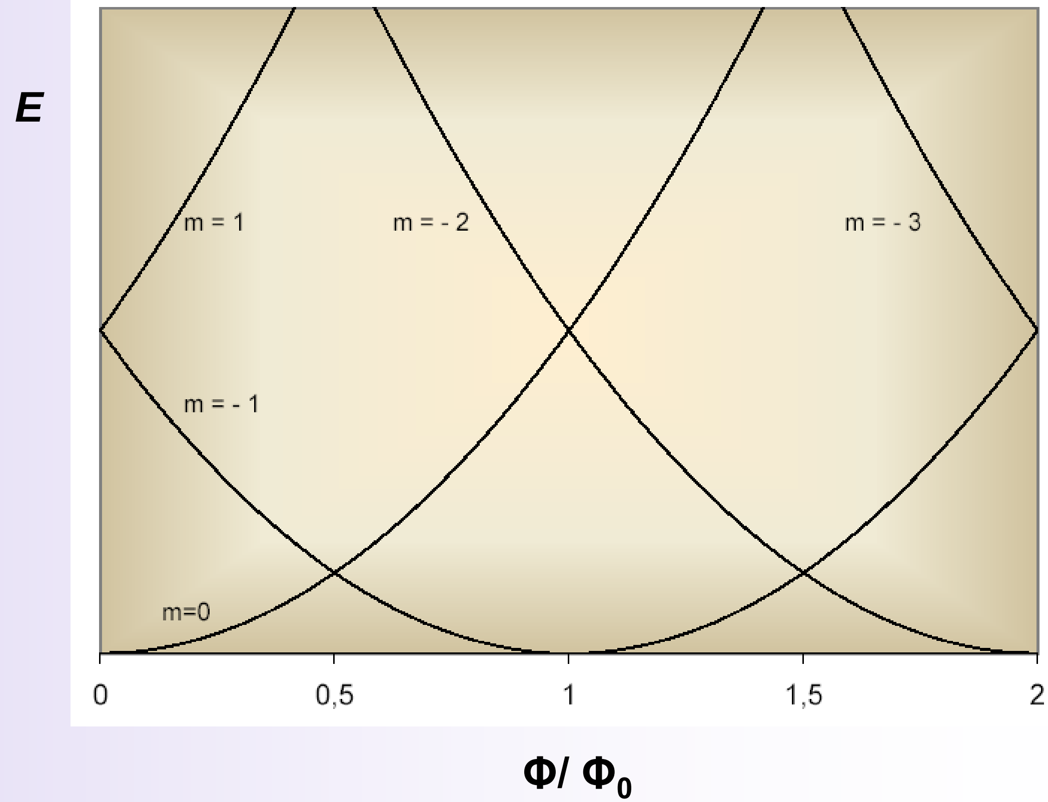
Aharonov-Bohm Effect

1D QR

$$\hat{\mathcal{H}} = -\frac{\hbar^2}{2m_e R^2}\left(\frac{\partial}{\partial\phi} + i\frac{\Phi}{\Phi_0}\right)^2$$

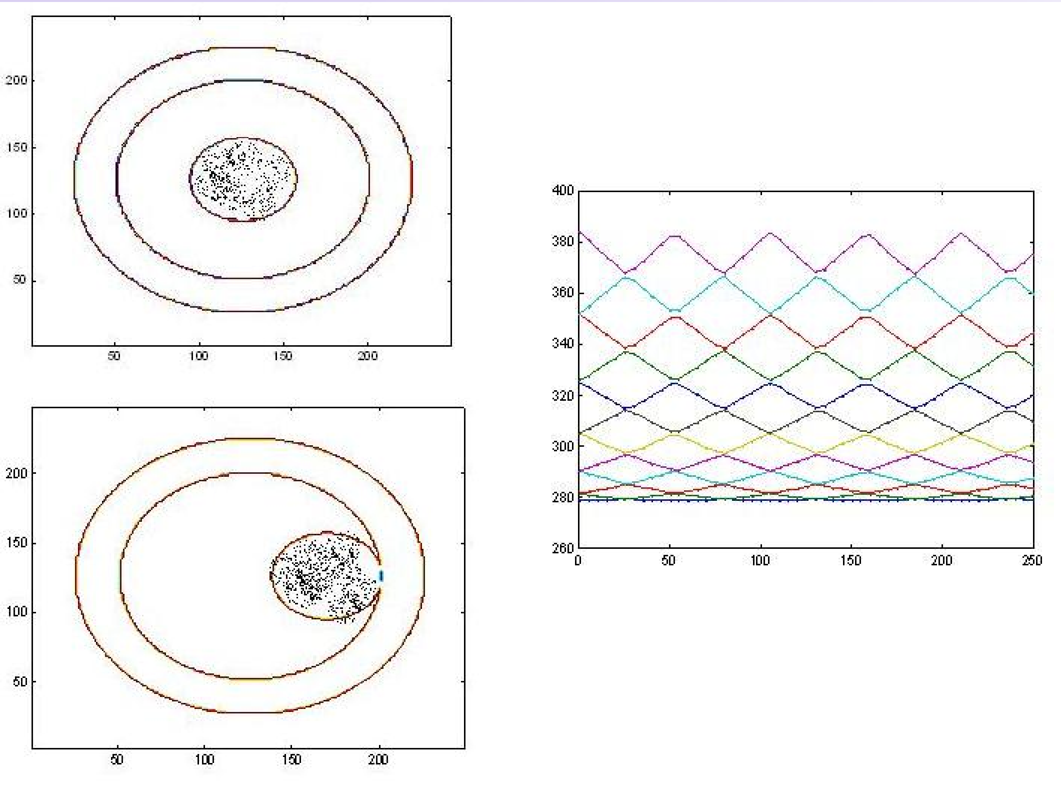
$$E_m = \frac{1}{2}(m+F)^2$$

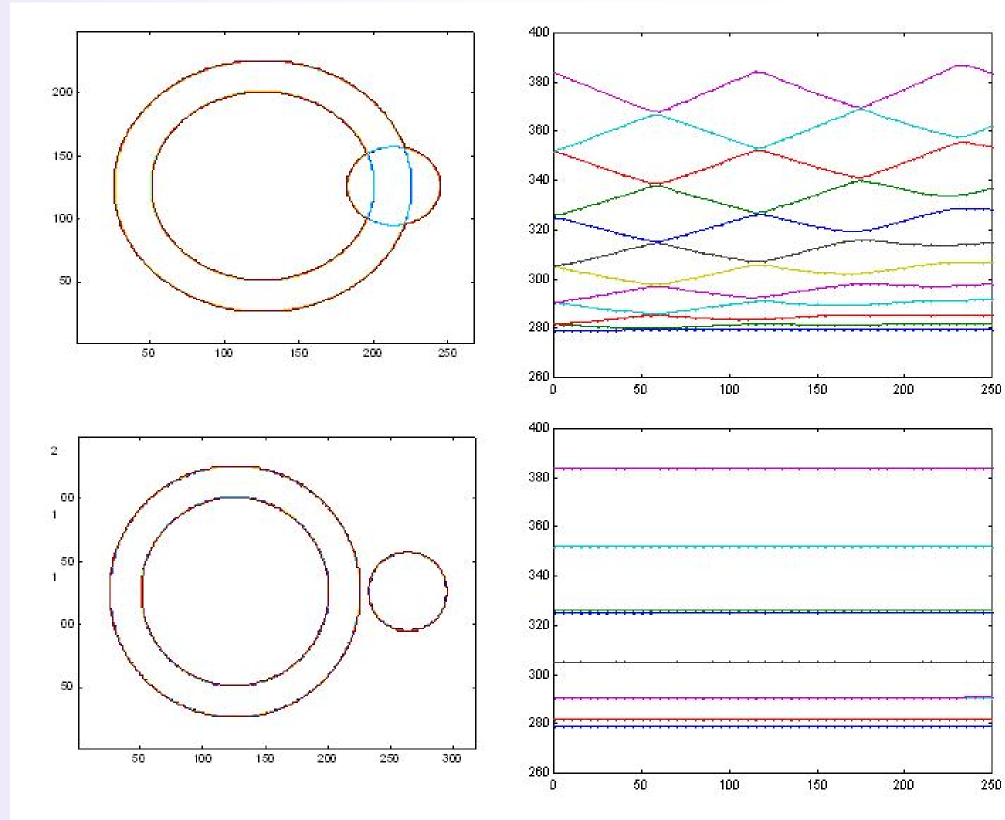
$$m = 0 \pm 1 \pm 2 ... \in Z$$



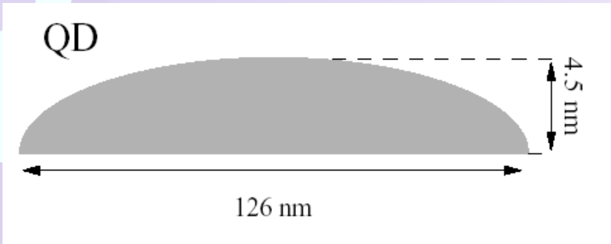
- Periodic symmetry changes of the energy levels
- Energetic oscillations
- Persistent currents

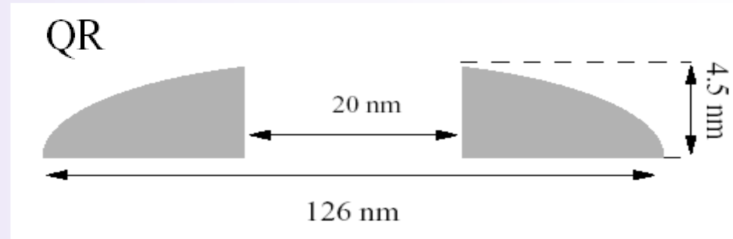
Some 2D calculations: off-centering

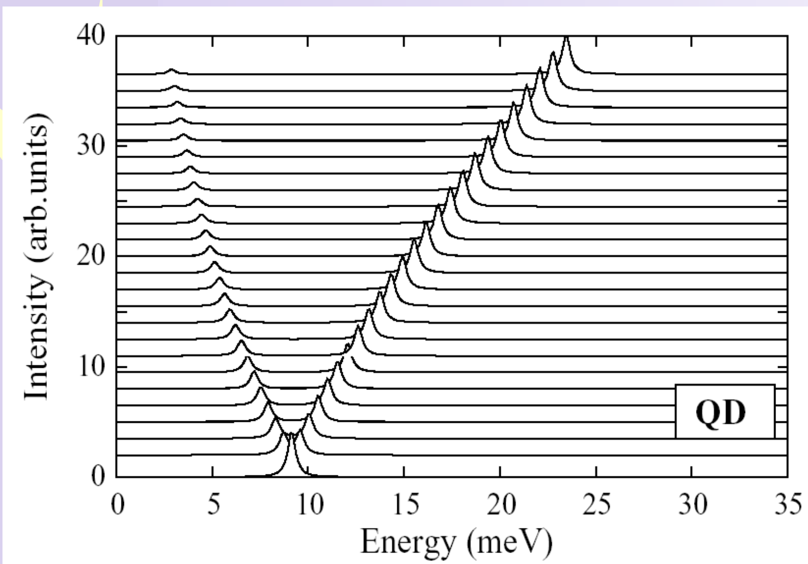


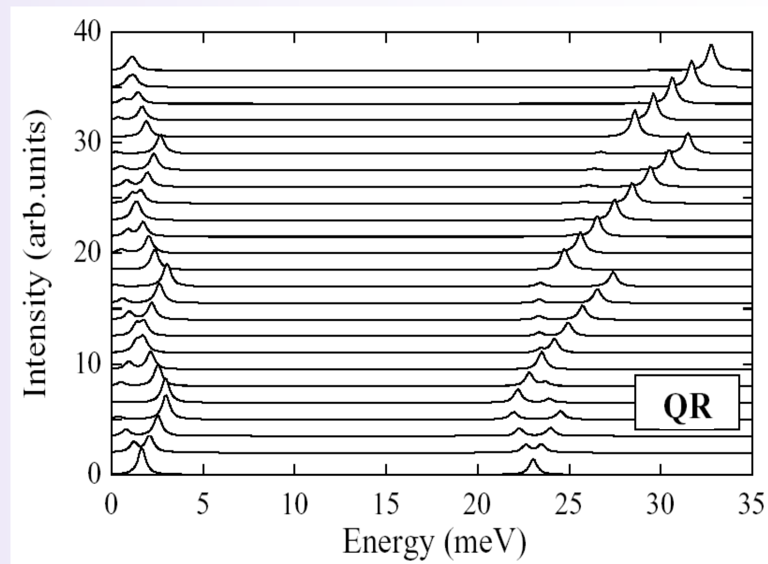


FIR absorption of one electron in QD and QR



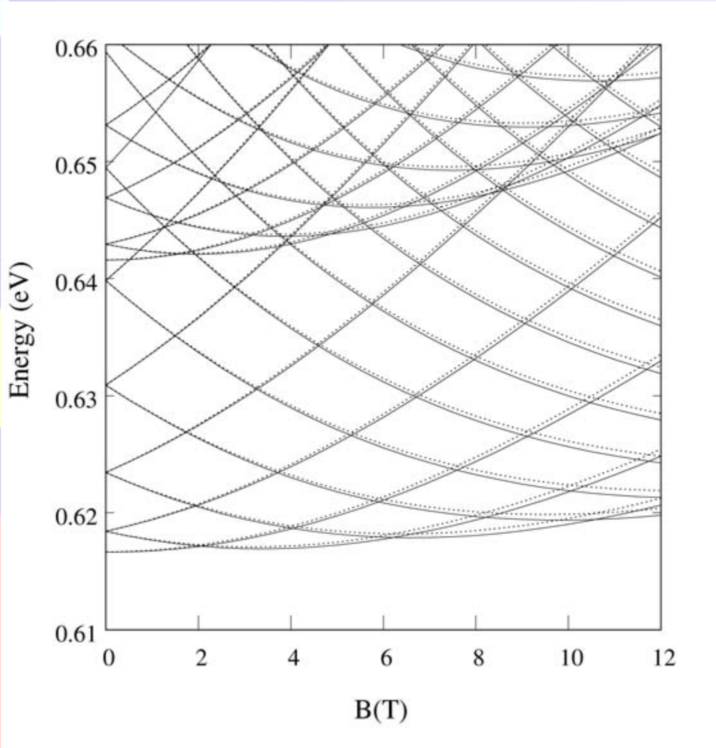


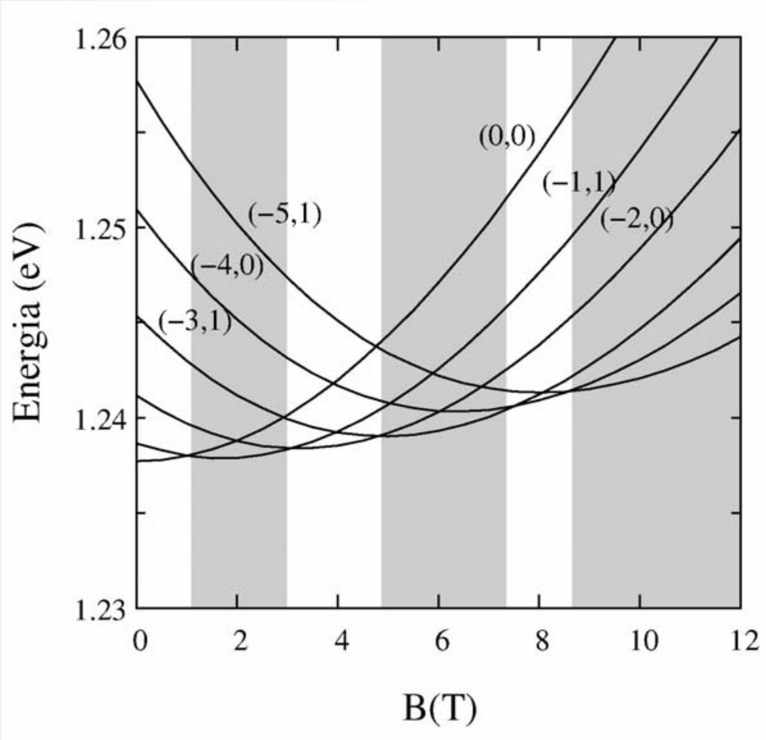




J. Planelles and J. I. Climente, Collect. Czech. Chem. Commun. 70 (2005) 605
arXiv: cond-mat/0412552;

Fractional Aharonov-Bohm Effect





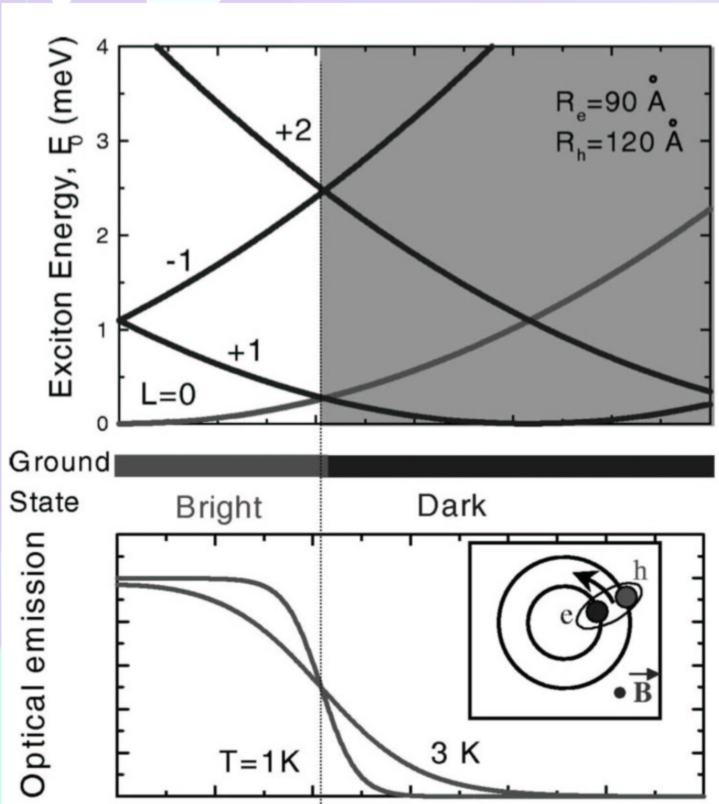
1 electron

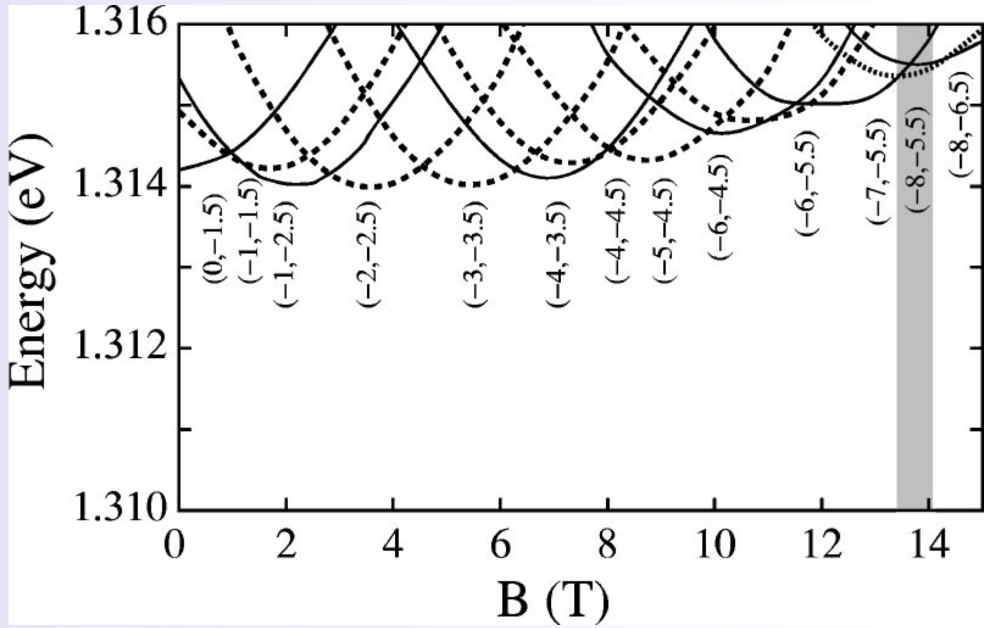
2 electrons coulomb interaction

J.I. Climente , J. Planelles and F. Rajadell,J. Phys. Condens. Matter ***17*** *(2005) 1573*

Optic Aharonov-Bohm effect

The Aharonov-Bohm effect leads to changes in electron and hole symmetry at different B values:

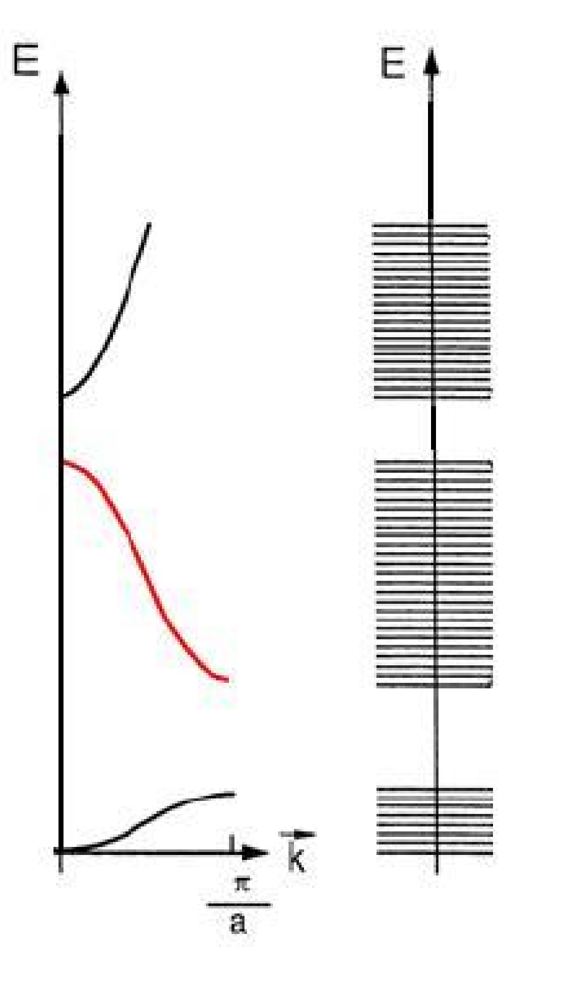




J. Climente, J. Planelles and W. Jaskólski, Phys. Rev. B 68 (2003) 075307

Observed in stacked type II QDs*: Kuskovsky et al . Phys. Rev. B 76 (2007) 035342; Sellers et al PRL 100, 136405 (2008).*

Translations and magneto-translations I

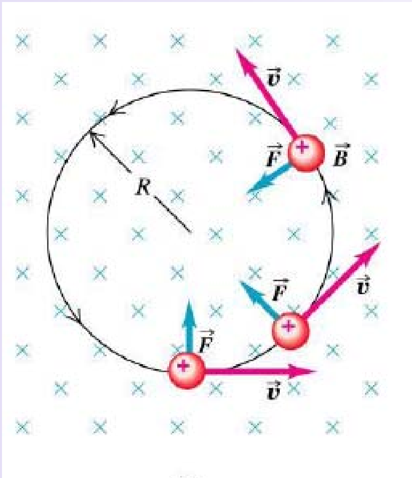


$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2}+V(x)u(x)=Eu(x)$$

$$[\hat{T}_a,\hat{\mathcal{H}}]=0 \quad \hat{T}_a=e^{-ia\hat{p}}$$

$$u(x)=u(x+a).$$

Simultaneous eigenfunctions: Bloch functions



Switching the magnetic field on: No translational symmetry

Though, can we get Bloch functions?

Translations and magneto-translations II

$$\hat{T}_m(\mathbf{r}_0) = \exp\left[-i\mathbf{r}_0 \cdot (\mathbf{p} - \mathbf{A})\right]$$

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

Commute …. but

$$[\hat{T}_m(\mathbf{R}_1), \hat{T}_m(\mathbf{R}_2)] = 2i\sin(\frac{\phi}{2})T_m(\mathbf{R_1} + \mathbf{R_2})$$

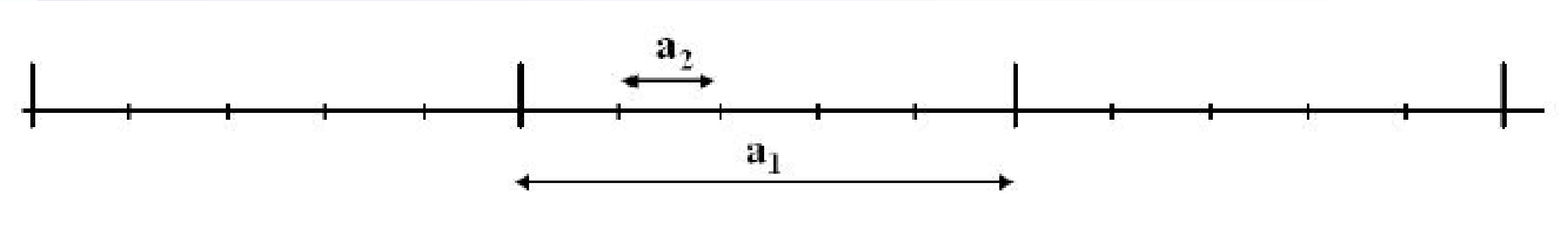
Commute …. if $\frac{\phi}{2} = q\pi,\; q \in Z$ and we can get Bloch functions

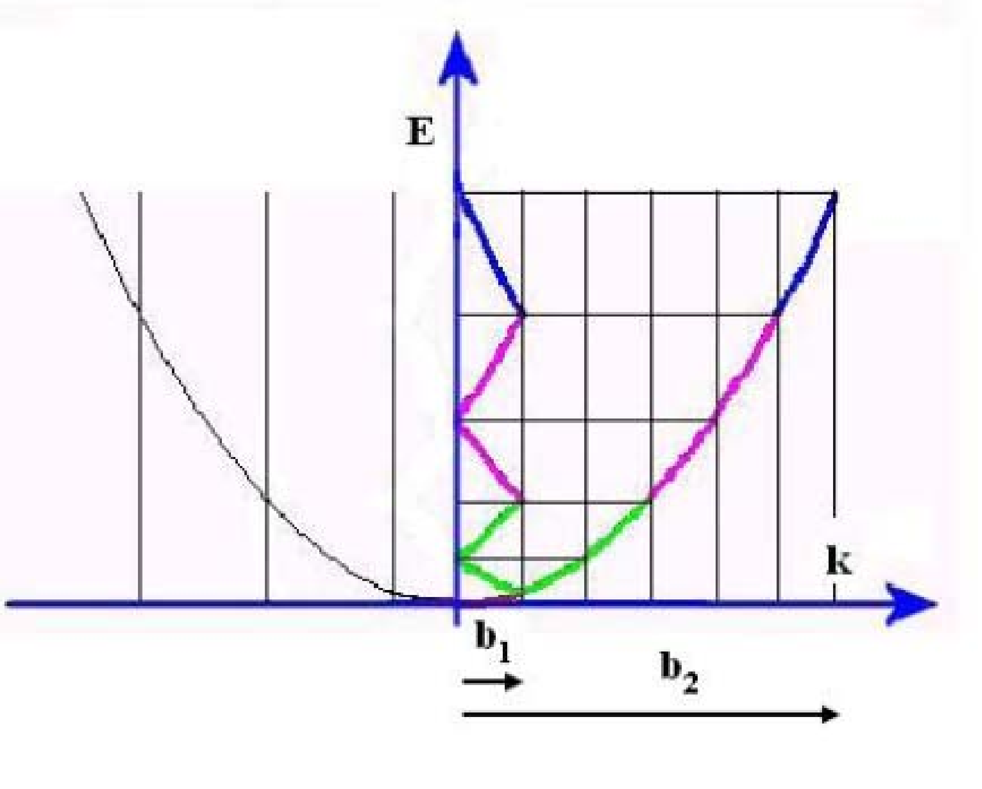
Two-fold periodicity: magnetic and spatial cells

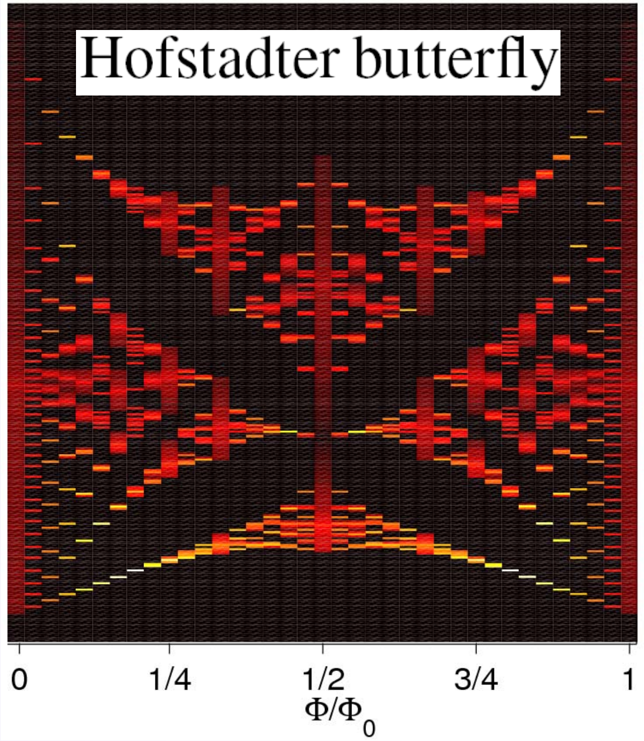
Physical meaning: Translation + Lorentz Strength compensation

Translations and magneto-translations III

Two-fold periodicity: magnetic and spatial cells







J.L. Movilla and J. Planelles, PRB 83 (2011) 014410

SUMMARY

Magnetic field: summary

No magnetic monopoles: $\vec{\nabla}\vec{B} = 0$ → $\vec{B} = \vec{\nabla} \wedge \vec{A}$ ***vector potential***

No conservative field: → ***velocity-dependent potential:*** $U = -e\left(\vec{v} \cdot \vec{A}\right)$

Lagrangian: $L = T - U$

kinematic momentum

Canonical momentum:

$$p_x = \frac{\partial L}{\partial \dot{x}} = \frac{\partial T}{\partial \dot{x}} - \frac{\partial U}{\partial \dot{x}} = \pi_x + e\,A_x$$

Hamiltonian:

$$H = p\,\dot{x} - L = T = \frac{\pi^2}{2m} = \frac{1}{2m}(p - e\,A)^2$$

Coulomb gauge: $\nabla A = 0$

Hamiltonian operator:

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

Magnetic field: summary (cont.)

axial symmetry

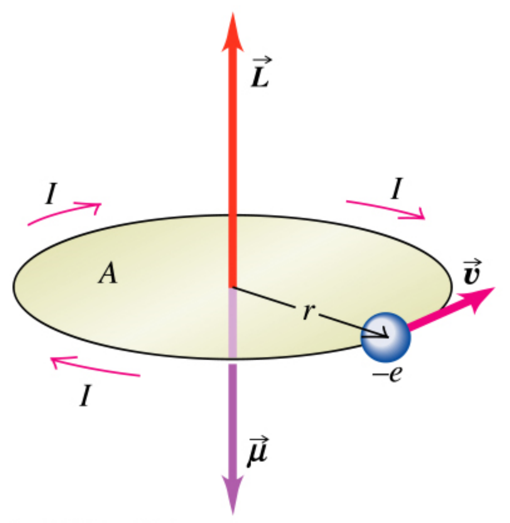
$$\vec{B} = B_0 \vec{k} \rightarrow \hat{\mathcal{H}} = -\frac{1}{2m_e}\nabla^2 + \frac{B^2}{8m_e}\rho^2 + \frac{BM}{2m_e} + V_e(\rho, z)$$

Relevant at soft confinement (nanoscale and bulk)

dominates at strong confinement (atomic scale)

Spatial confinement

Aharonov-Bhom oscillations in non-simple topologies



$$\vec{\mu} = i\vec{S} = \frac{ev}{2\pi r}\pi r^2 \vec{n} = \frac{evr}{2}\vec{n} = \frac{e}{2m_e}\vec{L}$$

$$W = -\vec{\mu}\vec{B} = -\frac{eB_0}{2m_e}M$$

Magnetic field: summary (cont.)

Periodicity and homogeneous magnetic field

↓

Magneto-translations and Super-lattices

↓

B-dependent (super)-lattice constant

↓

Fractal spectrum (Hofstadter butterfly)