

Slides from FYS4411 Lectures

Morten Hjorth-Jensen & Gustav R. Jansen

¹Department of Physics and Center of Mathematics for Applications
University of Oslo, N-0316 Oslo, Norway

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Quantum dots

What are they?

- ▶ **Electrons confined in an external potential.**
- ▶ What happens in semiconductors?
- ▶ Coloumb effects and the Pauli principle keeps an excited electron-hole pair bound.
- ▶ Modelled by a *free* particle with an effective mass in an external potential. Can disregard the crystal lattice.
- ▶ Have the same properties as atoms, only larger size. Are discussed as artificial atoms.
 - ▶ Discrete energy levels.
 - ▶ Selfbound.
 - ▶ Relatively long lifetimes.

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Quantum dots

Properties

- ▶ Energy levels depends on the size of the crystal. (Typically nanometer scale)
- ▶ Smaller crystals have larger energy gaps.
- ▶ Effective mass depends on type of semiconductor and size.
 - ▶ Effective mass much smaller than m_e .
 - ▶ Large de Broglie wavelength - $\lambda = \frac{h}{\gamma m_0 v}$
 - ▶ Quantum effects visible at larger scales.
- ▶ Emits light when electron recombines with hole. Frequency depends on energy gap.
- ▶ There are indications that the shape of the crystal also affect energy gap.
- ▶ Can be modelled as particles in a well.

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Quantum dots

Usage

- ▶ **Quantum laboratory.**
- ▶ Improved transistors.
- ▶ Quantum computers
- ▶ QLED (light emitting diode) and lasers.
 - ▶ Smaller sizes
- ▶ Medical imaging techniques and realtime tracking of molecules/cells.
- ▶ Improved solar panel efficiency.

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Quantum dots, the case of our project

We consider a system of electrons confined in a pure isotropic harmonic oscillator potential $V(\mathbf{r}) = m^* \omega_0^2 r^2 / 2$, where m^* is the effective mass of the electrons in the host semiconductor, ω_0 is the oscillator frequency of the confining potential, and $\mathbf{r} = (x, y, z)$ denotes the position of the particle.

The Hamiltonian of a single particle trapped in this harmonic oscillator potential simply reads

$$\hat{H} = \frac{\mathbf{p}^2}{2m^*} + \frac{1}{2} m^* \omega_0^2 \mathbf{r}^2$$

where \mathbf{p} is the canonical momentum of the particle.

Quantum dots

When considering several particles trapped in the same quantum dot, the Coulomb repulsion between those electrons has to be added to the single particle Hamiltonian which gives

$$\hat{H} = \sum_{i=1}^{N_e} \left(\frac{\mathbf{p}_i^2}{2m^*} + \frac{1}{2} m^* \omega_0^2 \mathbf{r}_i^2 \right) + \frac{e^2}{4\pi\epsilon_0\epsilon_r} \sum_{i < j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|},$$

where N_e is the number of electrons, $-e$ ($e > 0$) is the charge of the electron, ϵ_0 and ϵ_r are respectively the free space permittivity and the relative permittivity of the host material (also called dielectric constant), and the index i labels the electrons.

Quantum dots

We assume that the magnetic field \vec{B} is static and along the z axis. At first we ignore the spin-dependent terms. The Hamiltonian of these electrons in a magnetic field now reads

$$\hat{H} = \sum_{i=1}^{N_e} \left(\frac{(\mathbf{p}_i + e\mathbf{A})^2}{2m^*} + \frac{1}{2} m^* \omega_0^2 \mathbf{r}_i^2 \right) + \frac{e^2}{4\pi\epsilon_0\epsilon_r} \sum_{i<j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}, \quad (1)$$

$$= \sum_{i=1}^{N_e} \left(\frac{\mathbf{p}_i^2}{2m^*} + \frac{e}{2m^*} (\mathbf{A} \cdot \mathbf{p}_i + \mathbf{p}_i \cdot \mathbf{A}) + \frac{e^2}{2m^*} \mathbf{A}^2 + \frac{1}{2} m^* \omega_0^2 \mathbf{r}_i^2 \right) \quad (2)$$

$$+ \frac{e^2}{4\pi\epsilon_0\epsilon_r} \sum_{i<j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}, \quad (3)$$

where \mathbf{A} is the vector potential defined by $\mathbf{B} = \nabla \times \mathbf{A}$.

Quantum dots

In coordinate space, \mathbf{p}_i is the operator $-i\hbar\nabla_i$ and by applying the Hamiltonian on the total wave function $\Psi(\mathbf{r})$ in the Schrödinger equation, we obtain the following operator acting on $\Psi(\mathbf{r})$

$$\mathbf{A} \cdot \mathbf{p}_i + \mathbf{p}_i \cdot \mathbf{A} = -i\hbar(\mathbf{A} \cdot \nabla_i + \nabla_i \cdot \mathbf{A}) \Psi \quad (4)$$

$$= -i\hbar(\mathbf{A} \cdot (\nabla_i \Psi) + \nabla_i \cdot (\mathbf{A} \Psi)) \quad (5)$$

Quantum dots

We note that if we use the product rule and the Coulomb gauge $\nabla \cdot \mathbf{A} = 0$ (by choosing the vector potential as $\mathbf{A} = \frac{1}{2} \mathbf{B} \times \mathbf{r}$), \mathbf{p}_i and ∇_i commute and we obtain

$$\nabla_i \cdot (\mathbf{A}\Psi) = \mathbf{A} \cdot (\nabla_i \Psi) + \underbrace{(\nabla_i \cdot \mathbf{A})}_{0} \Psi = \mathbf{A} \cdot (\nabla_i \Psi)$$

Quantum dots

This leads us to the following Hamiltonian:

$$\hat{H} = \sum_{i=1}^{N_e} \left(-\frac{\hbar^2}{2m^*} \nabla_i^2 - i\hbar \frac{e}{m^*} \mathbf{A} \cdot \nabla_i + \frac{e^2}{2m^*} \mathbf{A}^2 + \frac{1}{2} m^* \omega_0^2 \mathbf{r}_i^2 \right) + \frac{e^2}{4\pi\epsilon_0\epsilon_r} \sum_{i<j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|},$$

Quantum dots

The linear term in \mathbf{A} becomes, in terms of \mathbf{B} :

$$\frac{-i\hbar e}{m^*} \mathbf{A} \cdot \nabla_i = -\frac{i\hbar e}{2m^*} (\mathbf{B} \times \mathbf{r}_i) \cdot \nabla_i \quad (6)$$

$$= \frac{-i\hbar e}{2m^*} \mathbf{B} \cdot (\mathbf{r}_i \times \nabla_i) \quad (7)$$

$$= \frac{e}{2m^*} \mathbf{B} \cdot \mathbf{L} \quad (8)$$

where $\mathbf{L} = -i\hbar(\mathbf{r}_i \times \nabla_i)$ is the orbital angular momentum operator of the electron i .

Quantum dots

If we assume that the electrons are confined in the xy -plane, the quadratic term in \mathbf{A} can be written as

$$\frac{e^2}{2m^*} \mathbf{A}^2 = \frac{e^2}{8m^*} (\mathbf{B} \times \mathbf{r})^2 = \frac{e^2}{8m^*} B^2 r_i^2$$

Quantum dots

Until this point we have neglected the intrinsic magnetic moment of the electrons which is due to the electron spin in the host material. We will now add its effect to the Hamiltonian. This intrinsic magnetic moment is given by $\mathcal{M}_s = -g_s^* (e\mathbf{S})/(2m^*)$, where \mathbf{S} is the spin operator of the electron and g_s^* its effective spin gyromagnetic ratio (or effective *g-factor* in the host material). We see that the spin magnetic moment \mathcal{M}_s gives rise to an additional interaction energy linear in the magnetic field,

$$\hat{H}_s = -\mathcal{M}_s \cdot \mathbf{B} = g_s^* \frac{e}{2m^*} B \hat{S}_z = g_s^* \frac{\omega_c}{2} \hat{S}_z$$

where $\omega_c = eB/m^*$ is known as the cyclotron frequency.

Quantum dots

The final Hamiltonian reads

$$\hat{H} = \sum_{i=1}^{N_e} \left(\frac{-\hbar^2}{2m^*} \nabla_i^2 + \overbrace{\frac{1}{2} m^* \omega_0^2 \mathbf{r}_i^2}^{\text{Harmonic oscillator potential}} \right) + \overbrace{\frac{e^2}{4\pi\epsilon_0\epsilon_r} \sum_{i<j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}}^{\text{Coulomb interactions}}$$
$$+ \underbrace{\sum_{i=1}^{N_e} \left(\frac{1}{2} m^* \left(\frac{\omega_c}{2} \right)^2 \mathbf{r}_i^2 + \frac{1}{2} \omega_c \hat{L}_z^{(i)} + \frac{1}{2} g_s^* \omega_c \hat{S}_z^{(i)} \right)}_{\text{single particle interactions with the magnetic field}}, \quad (9)$$

Quantum dots

In order to simplify the computation, the Hamiltonian can be rewritten on dimensionless form. For this purpose, we introduce the following constants:

- ▶ the oscillator frequency $\omega = \omega_0 \sqrt{1 + \omega_c^2 / (4\omega_0^2)}$,
- ▶ a new energy unit $\hbar\omega$,
- ▶ a new length unit, the oscillator length defined by $l = \sqrt{\hbar / (m^* \omega)}$, also called the characteristic length unit.

We rewrite the Hamiltonian in dimensionless units using:

$$\mathbf{r} \longrightarrow \frac{\mathbf{r}}{l}, \quad \nabla \longrightarrow l \nabla \quad \text{and} \quad \hat{L}_z \longrightarrow \hat{L}_z$$

Quantum dots

It leads to the following Hamiltonian:

$$\hat{H} = \sum_{i=1}^{N_e} \left(-\frac{1}{2} \nabla_i^2 + \frac{1}{2} r_i^2 \right) + \overbrace{\frac{e^2}{4\pi\epsilon_0\epsilon_r} \frac{1}{\hbar\omega l}}^{\text{Dimensionless confinement strength } (\lambda)} \sum_{i < j} \frac{1}{r_{ij}} + \sum_{i=1}^{N_e} \left(\frac{1}{2} \frac{\omega_c}{\hbar\omega} \hat{L}_z^{(i)} + \frac{1}{2} g_s^* \frac{\omega_c}{\hbar\omega} \hat{S}_z^{(i)} \right), \quad (10)$$

Lengths are now measured in units of $l = \sqrt{\hbar/(m^*\omega)}$, and energies in units of $\hbar\omega$.

Quantum dots

A new dimensionless parameter $\lambda = l/a_0^*$ (where $a_0^* = 4\pi\epsilon_0\epsilon_r\hbar^2/(e^2 m^*)$ is the effective Bohr radius) describes the strength of the electron-electron interaction. Large λ implies strong interaction and/or large quantum dot.

Since both \hat{L}_z and \hat{S}_z commute with the Hamiltonian we can perform the calculations separately in subspaces of given quantum numbers L_z and S_z .

Quantum dots

The simplified dimensionless Hamiltonian becomes

$$\hat{H} = \sum_{i=1}^{N_e} \left[-\frac{1}{2} \nabla_i^2 + \frac{1}{2} r_i^2 \right] + \lambda \sum_{i < j} \frac{1}{r_{ij}} + \sum_{i=1}^{N_e} \left(\frac{1}{2} \frac{\omega_c}{\hbar \omega} L_z^{(i)} + \frac{1}{2} g_s^* \frac{\omega_c}{\hbar \omega} S_z^{(i)} \right),$$

Quantum dots

The last sum which is proportional to the magnetic field involves only the quantum numbers L_z and S_z and not the operators themselves. Therefore these terms can be put aside during the resolution, the squeezing effect of the magnetic field being included simply in the parameter λ . The contribution of these terms will be added when the other part has been solved. This brings us to the simple and general form of the Hamiltonian:

$$\hat{H} = \sum_{i=1}^{N_e} \left(-\frac{1}{2} \nabla_i^2 + \frac{1}{2} r_i^2 \right) + \lambda \sum_{i < j} \frac{1}{r_{ij}}.$$

Quantum dots

The form

$$\hat{H} = \sum_{i=1}^{N_e} \left(-\frac{1}{2} \nabla_i^2 + \frac{1}{2} r_i^2 \right) + \lambda \sum_{i < j} \frac{1}{r_{ij}},$$

is however not so practical since the interaction carries a strength λ . Why?

Quantum dots

We rewrite it as a one-body part

$$\hat{H}_0 = \sum_{i=1}^{N_e} \left(-\frac{1}{2} \nabla_i^2 + \frac{\omega^2}{2} r_i^2 \right),$$

and interacting part

$$\hat{V} = \sum_{i < j}^{N_e} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}.$$

Your task till next week is to show this. The unperturbed part of the Hamiltonian yields the single-particle energies

$$\epsilon_j = \omega (2n + |m| + 1), \quad (11)$$

where $n = 0, 1, 2, 3, \dots$ and $m = 0, \pm 1, \pm 2, \dots$. The index i runs from $0, 1, 2, \dots$.

Harmonic oscillator in 2D with cartesian coordinates

Hamilton operator

$$\hat{H}_0 = \sum_{i=1}^N \left(-\frac{1}{2} \nabla_i^2 + \frac{1}{2} \omega^2 r_i^2 \right)$$

Eigenvalues and eigenfunctions

$$\begin{aligned} \phi_{n_x, n_y}(\mathbf{x}, \mathbf{y}) &= A H_{n_x}(\sqrt{\omega}x) H_{n_y}(\sqrt{\omega}y) \exp(-\omega(x^2 + y^2)/2) \\ E &= \omega(n_x + n_y + 1) \end{aligned}$$

Leads to a shell structure, similar to atomic and nuclear systems.

Hermite polynomials

The Hermite polynomials are the solutions of the following differential equation

$$\frac{d^2H(x)}{dx^2} - 2x\frac{dH(x)}{dx} + (\lambda - 1)H(x) = 0. \quad (12)$$

The first few polynomials are

$$H_0(x) = 1,$$

$$H_1(x) = 2x,$$

$$H_2(x) = 4x^2 - 2,$$

$$H_3(x) = 8x^3 - 12x,$$

and

$$H_4(x) = 16x^4 - 48x^2 + 12.$$

They fulfil the orthogonality relation

$$\int_{-\infty}^{\infty} e^{-x^2} H_n(x)^2 dx = 2^n n! \sqrt{\pi},$$

and the recursion relation

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x).$$

Tasks for next week

- ▶ Set up the harmonic oscillator wave function in cartesian coordinates for an electron with $n_x = n_y = 0$ and find the oscillator energy.
- ▶ Use this result to find the unperturbed energy

$$\int \Phi^* \hat{H}_0 \Phi d\tau = \sum_{\mu=1}^N \langle \mu | h | \mu \rangle.$$

for two electrons with the same quantum numbers. Is that possible?

- ▶ Repeat for six electrons (find the relevant harmonic oscillator quantum numbers)
- ▶ Read chapter 5 of Lars Eivind Lervåg's thesis, it deals with quantum dots and gives a good introduction to the physics of quantum dots.
- ▶ For the project, finish parts 1a and 1b, including analytical derivatives and the profile analysis.