Modeling the energy spectra of some nanosytems under different conditions

(Quantum dots: periodicity, spatial confinement and external fields)

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A quantum dot is a small crystal of nanometric size. It is built of a huge amount of electrons and nuclei. As in macroscopic crystals, atoms inside quantum dots are arranged according to an ordered pattern, displaying microscopic periodicity. However, nanocrystals and macroscopic crystals display quite different behaviour and properties. In a macroscopic crystal, despite its finite size, most of the properties are bulk-like. At the electronic scale, macroscopic crystal is so huge that electrons see the crystal border as if located at infinity. This allows to fully exploiting translational symmetry, drastically simplifying its quantum mechanical description. If we now introduce a heterojunction (or consider a nanocrystal) we still have local periodicity. However, the border is no longer felt at infinity. Instead, we may consider the border effect as a potential superimposed to the crystalline periodic potential. This extra potential is extremely smooth at the scale of a lattice constant. Physically, it behaves as a *confining potential* which renders a *discrete* character to the electron energy structure. The possibility to precisely control the size of a quantum dot enables to determine the wavelength of the absorption and emission, which in turn determines the colour of light the human eye perceives. Quantum dots can therefore be tuned during production to emit any desired colour light. The smaller the dot, the closer it is to the blue end of the spectrum, and the larger the dot, the closer to the red end. Quantum dots can even be tuned beyond visible light, into the infra-red or into the ultra-violet. In addition to this potential, hereafter referred to as *spatial confining potential*, externally applied fields or just the presence of interfaces may bring about additional sources of confinement, as the magnetic confinement. We can therefore understand why quantum dots are called *artificial atoms*, as the manufacturer can tune its properties in the fabrication process or/and by means of appropriate external sources of confinement. Along two lectures, we will provide a bird's eye view on periodicity and spatial and magnetic confinements on quantum dots. The aim of these talks, more than introducing the world of nanosystems is to revisit some basic knowledge viewed from and used for solid state and nanoscience oriented to the hands on session where some toy-models will be studied.

1. QUANTUM DOTS

1.1. Crystal structure: Translation symmetry

The periodicity of a crystal, i.e., the existence of a lattice, is related to the translation symmetry and has profound consequences in the physical behaviour end the electronic structure of solids. For example, the observable electronic density $\rho(\mathbf{r})$ is periodic ($\rho(\mathbf{r}) = \rho(\mathbf{r+t})$, with $\boldsymbol{t}$ a translation vector). The square of the modulus of the wave function then is periodic, and therefore the wave function is periodic up to a phase. This phases are precisely the characters of the irreducible representations (irreps) of the translation group (since translations commute, the translation group is commutative, so all its irreps are one-dimensional). The linear momentum is the generator of translations ($\hat{T}_n = e^{i\,a\,n\,\hat{p}}$). Then, its eigenfunctions $\{e^{ikx}\}$ can be used as basis of the irreps, the calculation of their characters and the associated quantum number k as label for these irreps. However, while k can assume the value of all possible finite real numbers, the number of non-equivalent irreducible representations of the translation group is much smaller because $e^{ika} = 1$, where a is a point of the Lattice, that means $e^{ikx} = e^{ik(x+a)}$, i.e., k and $(k+a)$ are the same irrep as they have the same set of characters. We see then that for each point of the direct Lattice (a) there is a point k in the so-called *reciprocal* space (units 1/length). The full set of k points form a lattice whose unit cell is known as the *first Brillouin zone*. The reciprocal lattice is extremely useful in the study of crystals.

1.2. Translations in 3D: Bloch functions

The extension to three dimensions implies replacing x by $\boldsymbol{r}$ and k by $\boldsymbol{k}$. Now the label of the three-dimensional translation group is not a number k but a vector $\boldsymbol{k}$. The most general basis of the irreps are the so-called Bloch functions: $\boldsymbol{\Psi_k}(\boldsymbol{r}) = e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}}u(\boldsymbol{r});\ \ u(\boldsymbol{r}+\boldsymbol{a}) = u(\boldsymbol{r})$. We also can define in 3D the reciprocal lattice and identify the labels of all non-equivalent irreps within the 3D first Brillouin zone.

1.3. Solving the Schrödinger equation

In order to solve the Schrödinger equation of a crystal we use translational symmetry and the characters of the irreducible representation to set the required boundary conditions: since $\hat{\boldsymbol{T}}_{\boldsymbol{a}}\, \boldsymbol{\Psi}(\boldsymbol{r}) = \boldsymbol{e}^{\boldsymbol{i}\,\boldsymbol{ka}}\, \boldsymbol{\Psi}(\boldsymbol{r})$ then, $\boldsymbol{\Psi}_{\boldsymbol{k}}(\text{-}\boldsymbol{a}/2) = \boldsymbol{e}^{\boldsymbol{i}\,\boldsymbol{\phi}}\, \boldsymbol{\Psi}_{\boldsymbol{k}}(\boldsymbol{a}/2), \quad \boldsymbol{\phi} \in [-\boldsymbol{\pi}, \boldsymbol{\pi}]$. We solve the Schrödinger equation for each k value and find a set of low-lying eigenvalues. The plot vs. k of the n-th eigenvalue, $E_n(k)$, represents an energy band.

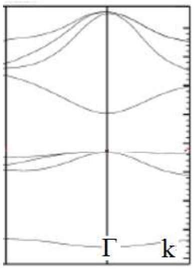


Figure 1.1: energy bands

1.4 Energy band structures

As a starting point to study the energetics of crystal solids, we consider an electron travelling along the crystal. The *quasi-free electron* feels the Coulomb potential exerted by the lattice ions as a perturbation. This kind of carriers is responsible for most of the solid's collective properties.

Let us first assume that the kinetic energy of the electron greatly exceeds the potential, $\varepsilon >> V$ (empty lattice). The Hamiltonian describing the system and its solutions are given by:

$$\frac{p^2}{2m}\Psi(\vec{r}) = \varepsilon_k \Psi(\vec{r}), \qquad \Psi(\vec{r}) = N e^{i\vec{k}\vec{r}}, \qquad \varepsilon_k = \frac{\hbar^2 k^2}{2m}.$$

With $p=\hbar k$ the linear momentum and N the normalization constant. Such a wave function is known as *plane wave*, and its energy structure vs k is shown in figure 1.3a. At zero temperature, the electrons in a solid will occupy the lowest orbitals allowed by the Pauli's exclusion principle, from $k=0$ till $k=k_F$. We then define the *Fermi energy* as $\varepsilon_F=\hbar^2 k_F^2/2m$.

Let us next include the lattice as a weak perturbation. It can be shown that electrons will not feel the lattice unless $k \sim \pi/a$, where a is the lattice constant. If , $k \sim \pi/a$, the plane wave experiences Bragg reflection. This leads to forbidden values of k, where energy gaps appear (figure 1.2b). Depending on the magnitude of the gap and the position of the Fermi energy, we classify solids as insulators, semiconductors and conductors (metals) –figure 1.2c-.

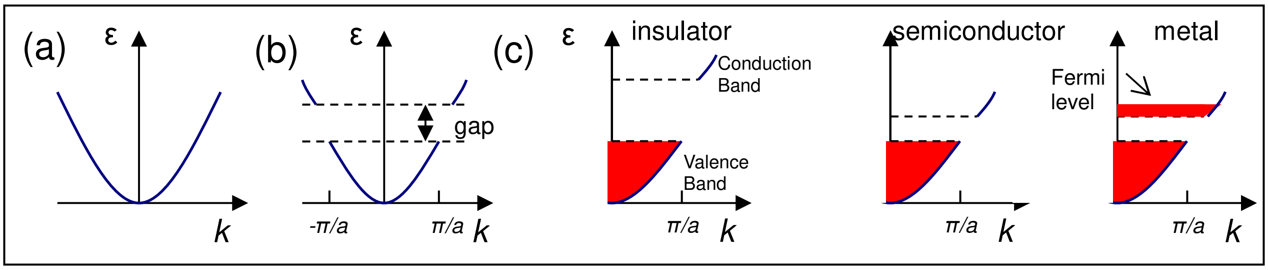


Figure 1.2.

1.5 The k·p model. Effective mass.

A computationally affordable yet reliable description of many semiconductor crystal is obtained using the k·p method. The idea is to project the crystal Hamiltonian, $H=p^2/2m+V_{cr}(\mathbf{r})$, onto a general Bloch function $\psi(r) = N\, e^{ikr}\, u_k(r)$. After operating and left-multiplying by e^{-ikr}, one gets the *k·p Hamiltonian*:

$$\left(\frac{p^2}{2m}+V_{cr}(\vec{r})+\frac{\hbar^2 k^2}{2m}+\hbar k\cdot p\right)u_{nk}=\varepsilon_{nk}\,u_{nk}\,.$$

If we have some information about u_{nk} at a given point $k=0$ (Γ point, at the centre of the Brillouin zone), we can solve the Hamiltonian perturbationally for k near $k=0$. To this end, we expand the Hamiltonian in terms of a basis of functions $u_{nk}(\mathbf{r})=\Sigma_n\, c_{nk}\, u_{n0}(\mathbf{r})$. A general matrix element is of the form:

$$\langle u_{n0}|\hat{H}_{kp}|u_{l0}\rangle=\left(\varepsilon_{n0}+\frac{k^2}{2m}\right)\delta_{nl}+\frac{1}{m}\vec{k}\,\vec{P}_{nl}\,,$$

Where ε_{n0} is the *energy gap* and $\mathbf{P}_{nl}=\langle u_{n0}|\mathbf{p}|u_{l0}\rangle$ is the *Kane parameter*. Both magnitudes can be inferred from spectroscopy experiments. Depending on the number *n* of functions in our basis, we speak about *n-band k·p models*. Typical models employed to describe zinc-blende semiconductors are the 1-band model for conduction electrons, 4-band model for valence holes and 8-band model to include coupling between conduction and valence bands.

The 1-band model (all models indeed) is usually solved up to second-order perturbation theory, leading to energies:

$$\varepsilon_{nk}=\varepsilon_{n0}+\sum_{\alpha=x,y,z}\frac{k_\alpha^2}{2}\left(\frac{1}{m}+\frac{2}{m}\sum_{l}\frac{P_{nl}^{(\alpha)2}}{(\varepsilon_{n0}-\varepsilon_{nl})}\right)=\varepsilon_{n0}+\sum_{\alpha=x,y,z}\frac{k_\alpha^2}{2m_\alpha^*}\,.$$

Note that the energy is simply that of a free electron but with an *effective mass m**, which depends on the coupling with other bands. The effective mass can have small and even negative values, which leads to lots of interesting physics in semiconductors.

1.6 Heterostructures. Quantum wells, wires and dots.

So far, we have considered homogeneous crystals. However, current semiconductor research is largely focused on semiconductors made of different materials. How do we model a system with two semiconductor crystals A and B (figure 1.4a)? If both materials have the same crystal structure and similar lattice constant, one usually employs the *envelope function* *approximation*. We replace the usual Bloch function by: $\psi(\mathbf{r}) = N e^{i k_\perp r_\perp} \chi(z)\, u_k(\mathbf{r})$, where $\chi(z)$ is an unknown function in the direction where the translational symmetry has been broken. Noteworthy, $f(\mathbf{r}) = e^{i k_\perp r_\perp} \chi(z)$, varies slowly as compared to the unit cell function $u_k(\mathbf{r})$. Thus, it is often referred to as the envelope function, which is modulated inside each unit cell by u_k. Next, one proceeds as in the homogeneous case, with the additional consideration that the integral $\int_\Omega f(\mathbf{r}) u(\mathbf{r})\, dr^3 \approx 1/\Omega \left(\int_\Omega u(\mathbf{r})\, dr^3 \right) \left(\int_\Omega f(\mathbf{r})\, dr^3 \right)$, with Ω standing for the crystal volume. For a one-band model, eventually this leads to the eigenvalue equation:

$$\left(\frac{p_z^2}{2m} + V(z) + \frac{\hbar^2 k_\perp^2}{2m} + \varepsilon_0^A \right) \chi(z) = \varepsilon\, \chi(z),$$

where $V(z)$ is the spatial confinement potential defined by the alignment between the band gaps of materials A (ε^A) and B (ε^B). As shown in figure 1.4b, for a B/A/B heterostructure the potential can be that of a *quantum well*, and the eigenstates $\chi(z)$ the solutions particle in the box. Thus, semiconductor heterostructures provide the experimental realization of fundamental systems which had hitherto been but theoretical idealizations. It is also possible to fabricate heterostructures where translational symmetry is broken in two and three directions of the space, which gives rise to *quantum wires* and *quantum dots*, respectively. Of particular interest are quantum dots, where a strong spatial confinement in the three directions leads to discrete energy levels, very much as in atoms. Because of this quantum dots are often referred to as artificial atoms or macroatoms. Unlike natural atoms, however, quantum dots can be built with different sizes, shapes and composition, so that the energy spectrum is designed at will. This has opened great prospects for fundamental research and technological developments over the last decades.

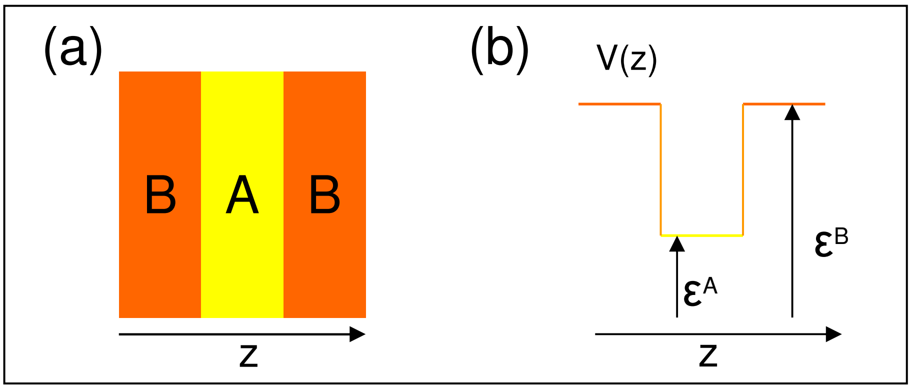


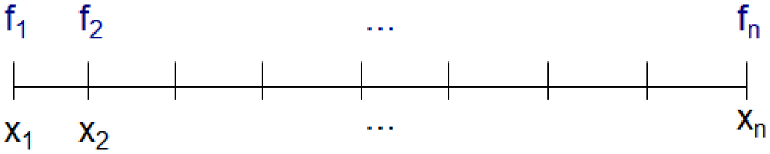
Figure 1.3.

1.7. A toy-case: solving a differential eigenvalue equation with finite differences

We will present here a toy example. We will address cases more sophisticated in the hands on session. Let us consider by now the simple case of stationary states of a particle in a box with finite walls defined by the equation:

$$[-\frac{1}{2m}\frac{d^2}{dx^2}+V(x)]f(x)=Ef(x)\,.$$

Then, we define grid in the coordinate domain:



and approximate the analytical *f(x)* by a numerical list { f_i } defined on the grid. The goal of finding the analytical *f(x)* function solving the differential equation turns into the search of the numerical list { f_i } of *f*-values defined on the grid. The differential equation in a given node of the grid reads:

$$-\frac{f_i^{''}}{2m}+V_i f\ =Ef_i\,.$$

Next, we approximate derivatives by finite differences:

$$f^{'}(x_i)=f_i^{'}=\frac{f_{i+1}-f_{i-1}}{2h}=\frac{f_{i+1/2}-f_{i-1/2}}{h}\,,$$

where h is the grid step. The first definition allows defining the derivative on the grid nodes. The second one will be useful to find second derivatives, as follows:

$$f^{''}(x_i)=f_i^{''}=\frac{f_{i+1/2}^{'}-f_{i-1/2}^{'}}{h}=\frac{f_{i+1}+f_{i-1}-2f_i}{h^2}$$

These expressions replace derivatives on node i by the values of the function on it and the nearest neighbor nodes. We can achieve better accuracy by employing information from further nodes. For example, the coefficients of the five-points second derivative,

$$f_i^{''}=\frac{1}{h^2}(a\ f_{i+2}+b\ f_{i-1}+c\ f_i+d\ f_{i-1}+e\ f_{i-2})$$

can be determined by imposing that this derivative must be exact if *f(x)* is a polynomial of degree four. It is not difficult to find out the coefficient values: $a=e=-1/12$, $b=d=4/3$ and $c=-5/2$. For the sake of easiness, we will employ 3-points finite differences in this example, thus yielding:

$$-\frac{1}{2\,m\,h^2}[f_{i+1}-2f_i+f_{i-1}]+V_i\ f_i=E\,f_i$$

By grouping coefficients we have: $b\,f_{i-1}+a_i\ f_i+b\,f_{i+1}=E\,f_i$, a set of equations with *i=2,n-1* involving the function on the *n* nodes of the grid. The two boundary conditions ($f_1 = f_n = 0$ in this case) close the system of equations:

$$\begin{array}{lcl}
i=2 & \rightarrow & b\,\cancelto{0}{f_1}+a_2\,f_2+b\,f_3 \;=\; E\,f_2 \\
\vdots & & \qquad\qquad\vdots \qquad\qquad\quad \vdots \\
i=n-1 & \rightarrow & b\,f_{n-2}+a_{n-1}\,f_{n-1}+b\,\cancelto{0}{f_n}=E\,f_{n-1}
\end{array}$$

What remains is just solving this homogeneous system of equations that turns into the diagonalization of a tridiagonal matrix:

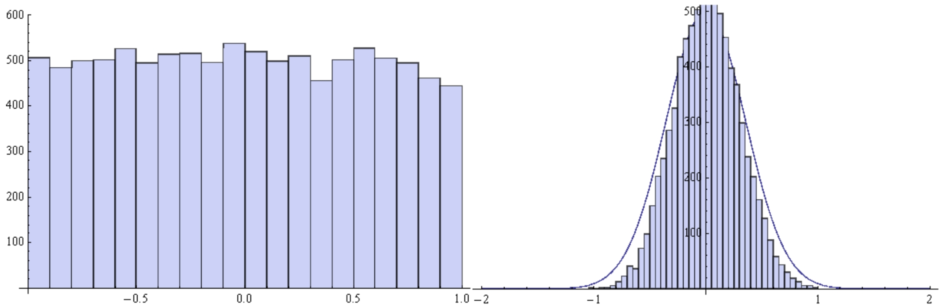
$$\begin{bmatrix}
a_2 & b & & & \\
b & a_3 & b & & \\
 & \ddots & \ddots & \ddots & \\
 & & b & a_{n-2} & b \\
 & & & b & a_{n-1}
\end{bmatrix}
\cdot
\begin{bmatrix} f_2 \\ f_3 \\ \vdots \\ f_{n-2} \\ f_{n-1} \end{bmatrix}
= E
\begin{bmatrix} f_2 \\ f_3 \\ \vdots \\ f_{n-2} \\ f_{n-1} \end{bmatrix}$$

1.8. Stochastic methods to solve eigenvalue equations in a variational manner.

The energy spectrum of multiexcitions in a QD is a many-body problem. Among the several methods employed to address the study de multiexcitions, we can say that, like in atoms and small molecules, the use of rather simple variational functions may provide accurate results. Solving a variational problem with a many-variable many-parameter wave function is a huge task that can be made feasible with the use of stochastic methods. We present an outline of the Variational Quantum Monte Carlo (VQMC) method applied to some toy-models. In VQMC one should carefully choose a trial wave function which depends on a set of variational parameters and then, evaluate the expectation value of the energy < E > (a multi-dimensional integral).

$$\langle E\rangle = \frac{\int \mathrm{d}R\ \Psi^{*}_{\mathrm{T},\alpha} H \Psi_{\mathrm{T},\alpha}}{\int \mathrm{d}R\ |\Psi_{\mathrm{T},\alpha}|^2}$$

The technical problem is that this multi-dimensional integral must be evaluated many times as the program searches the position in the parameter space where the energy < E > has a minimum. Stochastic methods build a sample of random numbers in the R domain of coordinates. Then, averages the integrand on the sample and estimates the energy accuracy by means of the associated variance. It should be said that by using random numbers uniformly distributed across the R domain of coordinates, information is spread all over R so that regions of very high and very low probability are treated on equal foot. A simple transformation allows Monte Carlo to generate far better results: drawing random numbers from non-uniform density $|\psi|^2$. How to do it? By using a Metropolis-like algorithm. This algorithm generates a *random walk* in the R domain modulated by the transition probability $w(r_i \rightarrow r_j)$ whose asymptotic probability approaches $|\psi|^2$ after a large number of steps.

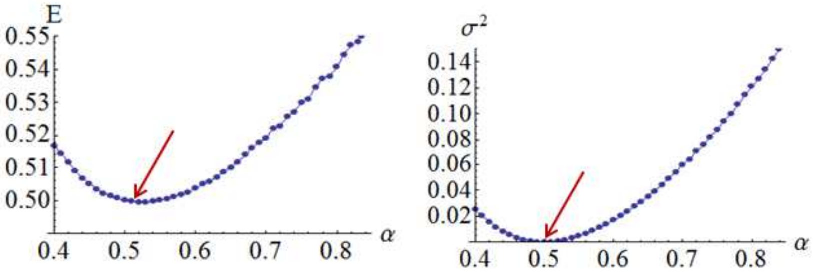


On the left of the above figure we show a histogram of 10.000 calculated random numbers uniformly distributed in the domain (-1,1). The histogram on the right shows 10.000 random numbers distributed according to a non-uniform density $|\psi|^2$ in the domain (-1,1), calculated using the Metropolis algorithm.

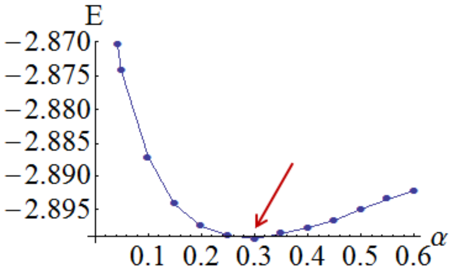
We will introduce VQMC using the toy models of one-dimensional harmonic oscillator and the helium atom. In the former case, the form of the trial function will be a Gaussian with an unknown exponent. In the second, we will employ the following function,

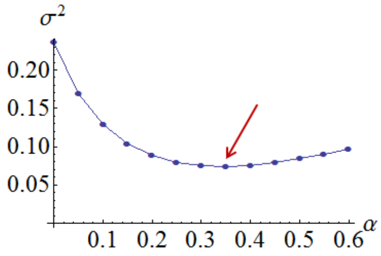
$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = e^{-Zr_1} e^{-Zr_2} e^{\frac{\beta r_{12}}{(1+\alpha r_{12})}}$$

which depends on three variational parameters. To assure a high-quality wave function it is particularly important that the wave function satisfy the cusp conditions (R. T. Pack and W. B. Brown, J. Chem. Phys. 45 (1966) 556), representing the behavior of the exact wave function at the coalescence of two particles. It is achieved in the above function be setting Z=2 and β=1/2.



On the left/right of the above figure, we show the profile energy/variance vs. the Gaussian exponent of the harmonic oscillator variational wave function calculated by means of 300 random walks with 10.000 steps. The next one corresponds to the He atom taking $Z=2$ and $\beta=1/2$ and varying a. These profiles corresponds to 500 random walks of 300.000 steps.





2. QUANTUM DOTS IN A MAGNETIC FIELD

2.1. Lagrange equations with velocity-dependent potentials

The concept of a Lagrangian L is introduced in order to reformulate classical Newton mechanics. In the case of conservative systems, the Lagrangian is defined as the velocity-dependent kinetic energy T of the system minus its coordinate-dependent potential energy V, $L=T-V$, and the Lagrange equation,

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

can be seen as a rewriting of the Newton law $\frac{d}{dt}(p)-F=0$, as can be easily checked. When the potential does not depend on the velocity, kinetic momentum (velocity-derivative of the kinetic energy) and canonic momentum (velocity-derivative of the Lagrangian) coincide. In this case, the Hamiltonian (Lagrange transformation of the Lagrangian function) is just the total energy $H=T+V$.

When the potentials also dependent on velocity, $U(x,v)$, kinetic π and canonic p momenta are different and the Hamiltonian coincides with the kinetic energy. It can be check in the case of a particle in a magnetic field, described by the potential $U=-e(v\cdot A)$, with A being the potential vector, related to the magnetic field by the equation $B=\nabla\wedge A$. One can easily find that $p=\pi+eA$, and that the Hamiltonian can be written as $H=\dfrac{1}{2m}(p-eA)^2$.

2.2. Coulomb gauge and quantification

We can realize that, as far as $\chi(x)$ is a scalar potential, two vector functions, $A(x)$ and $A(x)+\nabla\chi(x)$, yield the same magnetic field (since $\nabla\wedge\nabla\chi(x)=0$). This means that we have some freedom to select the potential vector. Having in mind the transition to quantum mechanics, where momentum $(-i\hbar\nabla)$ and coordinate do not commute, it is customary to select $\chi(x)$ such that it yields a null the divergence of A ($\nabla\cdot A=0$). This is called the Coulomb gauge. Assuming this gauge, the quantification ($p\rightarrow -i\hbar\nabla$, $x\rightarrow x$) of the Hamilton function yields

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

In the case of a uniform axial magnetic field, $B = B_0\,\vec{k}$, we can select a potential vector $A = [-yB_0/2, xB_0/2, 0]$ and this equation turns into:

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \frac{e^2 B_0^2}{8m}\rho^2 - \frac{e B_0}{2m}\hat{L}_z, \text{ with } \rho = \sqrt{x^2 + y^2}\,.$$

2.3. Magnetic Confinement: Landau levels

By introducing the notation $\omega = -e\,B_0/2m$, the above equation can be rewritten as:

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2\rho^2 + \omega\hat{L}_z = \frac{\hat{p}_z^2}{2m} + H_{HO}^{2D} + \omega\hat{L}_z$$

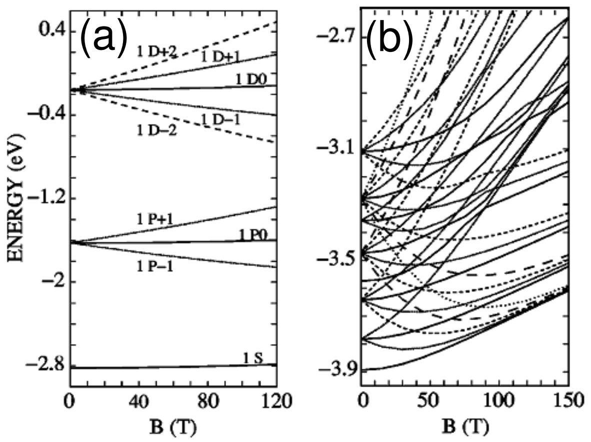
Since the two-dimensional harmonic oscillator Hamiltonian, $\hat{H}_{2D}^{HO}$, commutes with the z-component of the angular momentum, $\hat{L}_z$, in addition to the kinetic energy along *z*, the energy of the system is just $E(m,M) = (2n + |M| + M + 1)\omega$, where ω is proportional to the magnetic field. These are the so-called Landau levels of a free electron in a uniform magnetic field. As we see, the energy levels grow linearly without crossings as the magnetic field increases.

2.4. Spatial and magnetic confinement in quantum dots

When an additional, spatial confining potential co-exists with the magnetic confinement, the above Landau levels mix and we find out a competition between linear and the quadratic terms of the magnetic field. For example, the case of a spherical quantum dot in a homogeneous magnetic field is described by the following eigenvalue equation

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

We find a very different behaviour for short/large radius, owing to the ρ^2 factor appearing in the second term of the above equation. As a result, for small radius the response to the magnetic field is atomic-like (just an energy splitting due to $W = -\mu B$, see figure 2.1a) while for larger systems one may envisage the formation of Landau levels for extremely large magnetic fields, where the magnetic confinement overpasses the spatial one –figure 2.1b-.



R = 3 nm InAs NC R = 12 nm InAs NC

Figure 2.1

2.5. Multiple-connected quantum systems: Aharonov-Bohm effect

The response of a system with a multiply connected topology, as for example a quantum ring, is even more complex, showing level crossings as the magnetic field increases. This is related to the so-called Aharonov-Bhom effect. In figure 3.2 (from J. Planelles ,W. Jaskólski, and I. Aliaga, Phys. Rev. B 65 (2001) 033306) we show the two low-lying bands of a prototypical InAs quantum ring.

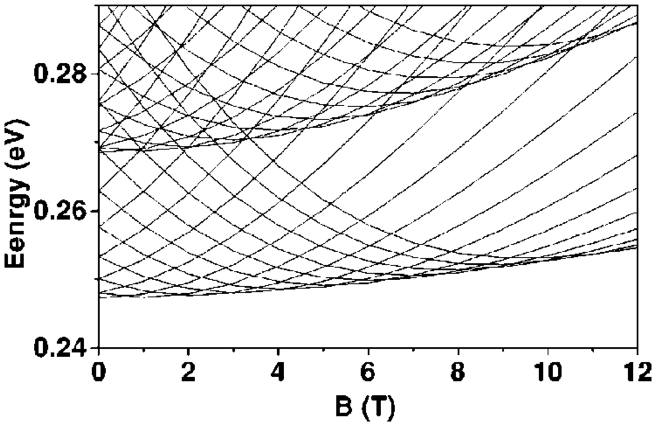
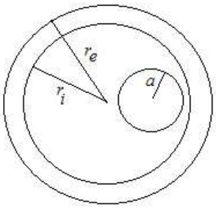
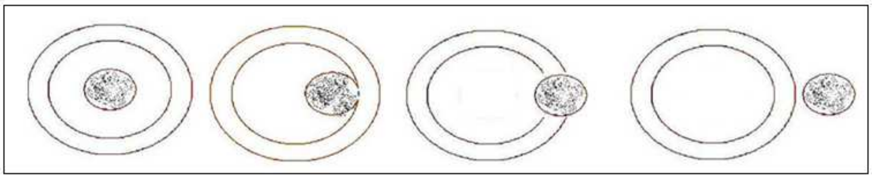


Figure 2.2

The most intriguing aspect of the Aharonov-Bhom effect is that these crossings can be predicted even in the case that the magnetic field pierces the inner hole of the ring only, i.e. no magnetic field acts on the ring section, the region where the electron is located. The mathematical reason comes from the fact that it is the potential vector and not the magnetic field itself that comes into the Hamiltonian, so that an electron can be influenced by the potentials even if no fields act upon it. The physical counterpart is a set of experimental observations that can only be understood as coming from this purely quantum effect without a classical correspondence.

2.6. Case study: effects on the energy spectrum of a beam of magnetic flux restricted to a small area inside, outside and piercing the ring.



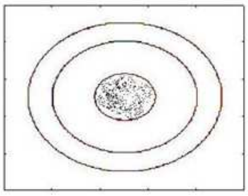


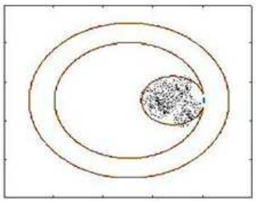
We consider a 2D quantum ring pierced by a magnetic field derived from the potential vector:

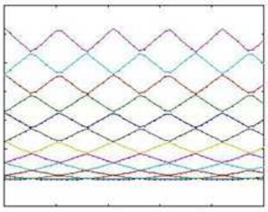
$$A = \begin{Bmatrix} \dfrac{1}{2} B_0 \, \rho \, \vec{u}_\phi & ; & 0 < \rho < a \\ \dfrac{1}{2\rho} B_0 \, a^2 \, \vec{u}_\phi & ; & a < \rho < \infty \end{Bmatrix}$$

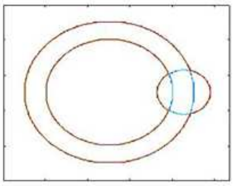
It produces an axial uniform magnetic field crossing a circle of radius *a,* and zero everywhere else. We will consider the disk off-centered by an amount x_0 from the center of a quantum ring. This destroys the axial symmetry we need two coordinates on equal foot to describe the system. For the sake of easiness we chose Cartesian coordinates. The eigenvalue equation of a particle in this ring is a two-coordinate homogenous partial differential equation. We assume that $a < r_i$, where r_i is the internal ring radius. We proceed to numerically integrate the eigenvalues differential equation for different values of x_0, from $x_0 = 0$ up to $x_0 > r_e + a$, where r_e is the external ring radius.

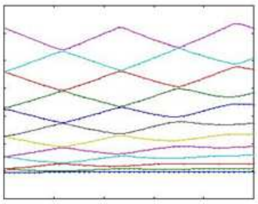
The results will show that the effect of the magnetic field (the Aharonov-Bhom effects) is independent of the off-centering of the magnetic disk if it is confined within the ring hole. The magnetic field does not affect the system if the magnetic disk is external to the ring and has a changing effect depending on how much the field pieces the region where the particle is confined (the ring). We will discuss the origin of this non-classical response of the particle in a ring to the magnetic field.

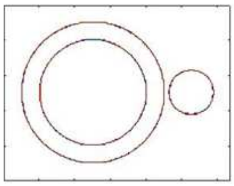


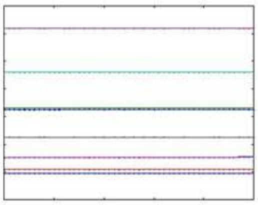












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3. HANDS ON SESSION

The aim of this session is to introduce the students to the task of identifying a system, the Hamiltonian describing its physical behaviour and, then translate it into a differential equation, numerically integrate it and plot the results. To this end we propose a set of elementary examples of increasing difficulty. The first and most simple case of determining the bottom of the bands in a quantum well (or equivalently, the energy spectrum of a 1D QD) is fully developed and used to introduce some key matlab/octave commands that will be used in the later examples. Also, some basic on differences finites to numerically integrate differential equations, choice of appropriate boundary conditions, building up appropriate matrix representation and further diagonalization are outlined. Then the rest of examples are sketched with some hints.

Exercise 1. Write a code to calculate the electron energy spectrum of a 1D GaAs/AlGaAs QD as a function of the size. Consider GaAs effective mass, m*=0.05, all over the structure. Justify the assumed simplification. The GaAs/AlGaAs band off set amounts 0.25 eV. Assume a well width L=25nm. Repeat the calculations for L ranging in [5, 50] nm and plot a few low-lying energies vs. L. Discuss the obtained results.

Exercise 2. Write a code to calculate the electron energy spectrum of two coupled GaAs/AlGaAs QDs as a function of their separation S.

Exercise 3. Write a code to calculate the electron energy spectrum of N=20 coupled GaAs/AlGaAs QDs as a function of their separation S.

Exercise 4. Write a code to calculate the energies of an electron in a 2D GaAs/AlGaAs cylindrical quantum disk/ring with inner radius R_{in} and outer radius R_{out}, subject to an axial magnetic field B. The system (disk/ring) is made of GaAs. The surrounding matrix and inner hole of the ring is made of AlGaAs. Consider a finite width L_b for the surrounding AlGaAs matrix, L_b=10 nm, (i.e., assume that beyond of this distance the wave function is zero). Calculate the energies as a function of B in the range 0-20 T, both, for a structure with (R_{in}, R_{out})=(0, 30) nm –i.e. a quantum disk- and for (3, 30) nm –a quantum ring-. Discuss the role of the linear and quadratic magnetic terms in each case.

Exercise 5. Write a code to calculate the energies of an electron in a 2D GaAs/AlGaAs quantum ring under the influence of a beam of magnetic flux restricted to a small area inside, outside and piercing the ring. Now since the system has no polar symmetry, no analytical partial integrations are possible so that the differential equation will be discretized in a two-dimensional grid.

Exercise 6. In general, the differential equation describing interacting carriers in a QD cannot be integrated numerically. Then a configuration interaction (CI) after the single-particle calculation is called for. Alternatively, for excitons and multiexcitions in a QD, appropriate variational functions may provide accurate results. The goal of this exercise is to write a variational Quantum Monte Carlo VQMC code to solve some toy-problems.

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