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1 The quantum dot

During the last century many new designs came to life. Quite a few of those have made our everyday life simpler, more convenient and to some extent more dangerous. Automobiles, electricity, light bulbs, television sets, computers, tumble dryers, etc. The list can go on forever. If we where to discuss which of those invention that have formed our life the most everyone agrees. It's the computer and the bits and pieces that make it tick. Identifying the date of the invention of the first computer is not possible, nor useful. The term computer have evolved during the last 50 years and we don't really have a general description of it. Some would say that a computer is a machine, analog or digital that assist us in calculations and have the possibility to store. To some extent one could say that the old abacus could indeed store and calculate data. The abacus remained until the middle of the 1500s. It's even used by some cultures today. After the 1500s many tried to develop mechanical machines to do some specific calculation. Charles Babbage, Joseph Marie Jacquard and Blaise Pascal was pioneers. Babbage designed a machine he called the "analytical engine" and during the development of programming code for this machine modern concepts of loops and branches was used. This is thought to be one of the very first computer, though it was never finished due to fund problems.

The modern computer, by that we mean a computer controlled by electronics, started in the late 1930s. The Mark I was build by Howard H. Aiken using funds from IBM. It was electromechanical since it used electric relays as binary

switches. Babbage original concepts was finally build. The first complete electronic computer was build in 1939 by John V. Atanasoff using vacuum tubes as switches. However the all-electronic computer who is generally considered to be the first is the ENIAC (Electronic Numerical Integrator and Computer). It was finished in 1946 by John W. Mauchly and J. Presper Eckert, using much of the same concepts as seen in Atanasoff's computer. ENIAC was of course not small, a mere 15000 square feet and a weight of 30 tons. And it's computer power was not even close to a modern calculator.

Inventions that made those computers smaller and more complex was at first the transistor and then the integrated circuits, often consisting of several transistors. However the basics of operation remain the same today as was developed in the 1940s. In 1947, William Shockley, John Bardeen and Walter Brattain build the first functional point-contact transistor. Today the transistor is constructed a bit different but the principle of operation is the same as the point-contact transistor. The integrated circuit was born in late 1950s by Jack Kilby and Robert Noyce at about he same time, but different places.

During the years after the first integrated circuits was born they have been refined many times. Developing from a basic circuit consisting of a few transistors to special devices consisting of millions of transistors. Today it's bot uncommon to have several hundred million transistors in sophisticated integrated circuits. Smaller and smaller sized components are needed and transistors with a size smaller than 50nm are more or less usual today. Processing power of modern computers are more or less dependent of the number of transistors you can pack into the integrated circuits. The search for more and more processing power continues. As the transistors and the spacing between them become smaller, tighter tolerances are needed to keep the circuit working without errors due to electrical leaks. Because of the nature of electricity and the working of to-days transistors we will get serious problems keeping electricity isolated in each transistor. Soon enough we start to encounter small groups of electrons and their interaction with each other and the surroundings. If we want to continue to use the same operation principle as of today we are forced to start looking at the quantum regime. The early 1970s opened a new era of research known as quantum wells. These where flat and thin semiconductor layers placed between two layers with greater conductor-band energy. The potential difference trapped the electrons in the thin layer. Due to the low effective mass the system is quasi-two dimensional. Where the excitation in the perpendicular direction are quantized. Then the 1980s gave birth to the quantum wire, where we have quantized in two dimension. By the middle of the 1980s the quantum dots was realized experimentally, where all three dimensions of motion was quantized.

1.1 Artificial atom and how are they related to quantum dots

The quantum dot is a vague name, but it's often characterized as a conducting "island" with a size comparable to the Fermi wavelength. Usually this "island" is a residence for a number of electrons. The similarities between quantum dots and atoms are present, but there are significant differences. First of all the length scales in a quantum dots is different from any atom. A typical quantum dot have a length scale in the 100nm range, while atoms are smaller, ranging from about 0.05nm to 0.4nm. The confining forces are also different. In atoms,

the attractive force is set up by the nucleus. But in quantum dots we typically have some external field which generates a background charge, thereby confining the particles. Since the length scale is different, the energy scale is also different. Typical values for a atom and a quantum dot is listed in Table 1.1.1 Despite the

	Quantum dot	Atom
Size	100nm	0.1nm
Energy spacing	0.1meV	1eV
Excitation energy	0,1meV	10eV
Magnetic field	10T	10000T

Table 1.1.1: Difference between a typical atom and quantum dot

difference, quantum dots are often called “artificial atoms”. The difference lies in the scaling, but not the working. The quantum dots experience energy bands and excitation just like the atoms. They even show “magic numbers” seen in atoms, although with different values. By controlling the external potential we can determine the number of electrons in the quantum dot showing the analogy with the periodic table and shell filling.

Why is quantum dots so important to explore? The reason is two-folded. The first has to do with our need to manufacture smaller and smaller devices. As was mentioned at the very first of this section, the integrated circuits are reaching their maximum operation points due to size. For 15 years ago, quantum dots was not of any particular interest to people doing circuit layout and manufacturing. Today, this situation is far from the truth and research in this field is intense, judging by the number of published articles. Typical transistor operation is a switch that is turned on and of when a voltage is added. Transistors today are building bricks of all integrated electronics. The ultimate transistor would be one that turns on and of when one electron is added or removed, what we call SET (Single Electron Transistor) today. This is also a perfect quantum dot. Knowing its inner workings are essential in a manufacture process.

But in addition to the need of smaller transistors, the quantum dot as a artificial atom have opened a whole new area of research. One thing that makes quantum dots very special are the possibility to control their size, shape, dimension, energy bands and number of electrons. This is something we cannot do with regular atoms. So quantum dots turn out to be a very handy platform for investigating many-body physics. One could also make several interacting quantum dots and form a lattice with shapes not found in nature. Even “artificial molecules” can also be made. This opens up a new world for basic research.

1.2 Structure, manufacture and operational principle

The manufacture process involved making quantum dots is complicated. You need high precision, material purity and a sophisticated controlling device. One of the first method for making quantum dots was developed by Reed et al. [6] during the mid 1980s. The common etching method today is more or less the same, just that the quality in the production is far better. The shape and operation principle is different from design to design, but all need to be produced on

a small scale, typically 10-100nm to yield size quantization. Common semiconductor material is normally used. *GaAs* (Gallium Arsenide) is preferred over *Si* (Silicon) due to its electrical properties. *GaAs* have higher electron mobility, lower breakdown voltages and less noise. *GaAs* can then be made smaller. However Silicon is easy available from quartz sand and are cheap. Silicon also bonds with oxides without problems and *SiO₂* makes an excellent isolator. In addition, hole mobility is greater than *GaAs*. This gives Silicon the advantage when logical gates need to be produces, due to the potential higher speed of a Silicon p-channel transistor over *GaAs*. When you want to manufacture quantum dots mainly for measurements and research, size and error is more important than cost and speed. *GaAs* can be combined with Aluminum to make a isolator. *AlAs* (Aluminum Arsenide) is also a good insulator and both of these combine well with *GaAs*.

To make quantum dots, several methods and designs are available. Manufacturing is not the main topic in this thesis and we will just outline some of the techniques. The outline is the same for all methods. You start with a given dimension and reduce it to create a confinement of some sort, either physical or by some other means, for example electrical fields.

1.2.1 Size restriction using physical boundaries

To make a quantum dot which is physical restricted in one or two dimension we usually use etching. As we have mentioned before, this was the first technique developed and has become the most common since the middle of the 1980s. To prepare the sample for etching one uses lithography. A basic process for making several small transistors and connect them are illustrated in Figure 1.2.1. This process is an analogy to what's going on during the manufacture of quantum dots using lithography and etching. However, since we need far better precision electron or ion beam lithography is used instead of light. First you start with a Silicon or any other material of choice in a wafer form. The making of wafers are dependent on what characteristics you want in the end. Figure 1.2.2(a) show a typical sample of a quantum device. The bottom layer of *GaAs* is doped to work as a reservoir. Then follows a barrier of *AlGaAs* which act as a potential barrier to isolate the next *GaAs* layer by tunneling. The top layer of *Au* works as a electrode. Because of the potential difference between *GaAs* and *AlGaAs* this wafer traps electrons in the middle *GaAs* layer and we have a quantum dot. If we make the two barriers different in such way that electrons can tunnel over one of the barrier, but not the other we can control the electron flow on and of the isolated layer in between. The wafer is layered with a mask on top. By using electron beam lithography, a pattern is made in the mask. We then expose the sample for a etching solution that only etch areas not protected by the mask. Finally we deposit ions to dope the material exposed, or we add a suitable metal. The metal can for example function as an electrode. In the end we're left with a smaller sized confinement as in Figure 1.2.2(b). When we apply potential difference between the electrode and the buffer, we can control the population of electrons inside the middle *GaAs* layer. The form of these quantum dots can vary from design to design, but the principles are the same.

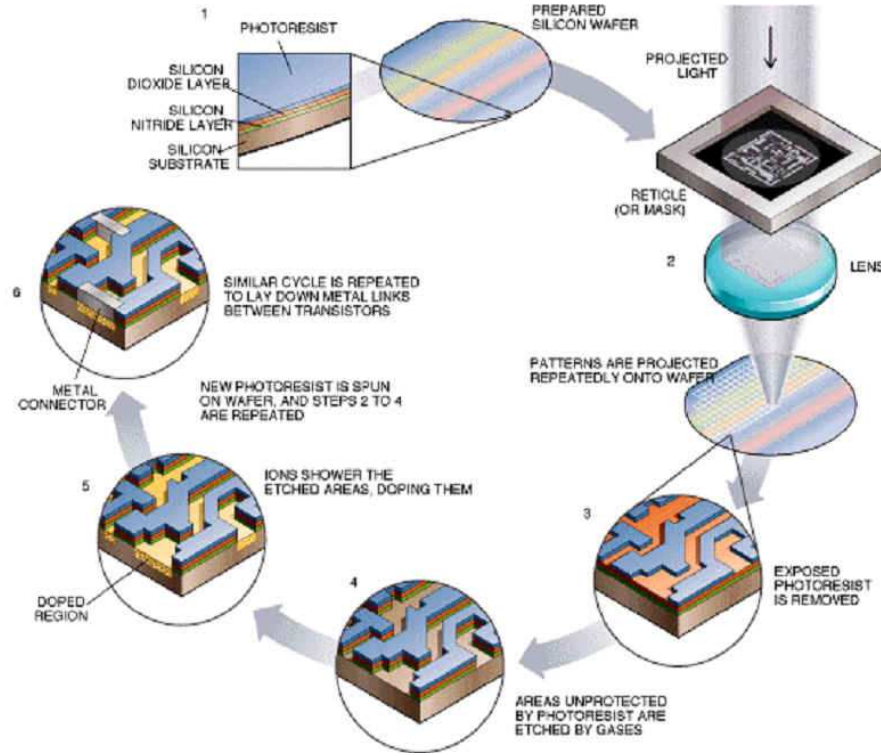


Figure 1.2.1: Light lithography used to create advanced integrated circuits

1.2.2 Size restriction using electrical fields

The etching technique is a physical process and if we need to change some variable in the produced dot, other than the potential difference between the buffer and the electrode, we need to manufacture another sample. This can be time consuming. We also introduce other deviations in data if we were to compare samples from two different production runs. The manufacture process cannot produce the exact same sample twice. Another method using lithography on a substrate to make conductors is more flexible. One example is shown in Figure 1.2.3. Here lithography is used to carve out the conductors on top of a $GaAlAs$ layer covered with a mask. We then deposit metal on top, usually gold. By applying potential difference between the finger gate and Q_1 and Q_2 we form what is called QPC (Quantum Point Contacts) which regulates the population of the isolated dot between the barriers by tunneling. We can then regulate the potential on the center gate to give geometric properties wanted in the dot. On each side of the QPCs we have drain and source. So, by using electrical fields we have greater flexibility. Another important feature is that we have no, or very little edge effects compared to the physical confinement.

There are several other methods developed, but the two explained here are the most useful. For the curious reader, what is called selective growth is outlined by Fukui et al. [2] and Lebens et al. [3]. Microcrystal semiconductors by Ekimov et al. [1]. Self-assembled dots are promising due to their small confinement size down to about 30nm. Experiments have been done by Marzin et al.

	polymer mask
GaAs	cap
AlGaAs	barrier
GaAs	quantum dot/well
AlGaAs	barrier
GaAs	buffer/substrate

(a) Wafer

Au	electrode
GaAs	cap
AlGaAs	barrier
GaAs	quantum dot
AlGaAs	barrier
GaAs	buffer/substrate

(b) End result

Figure 1.2.2: Layers in *GaAs* quantum dot sample

[4] and Raymond et al. [?]

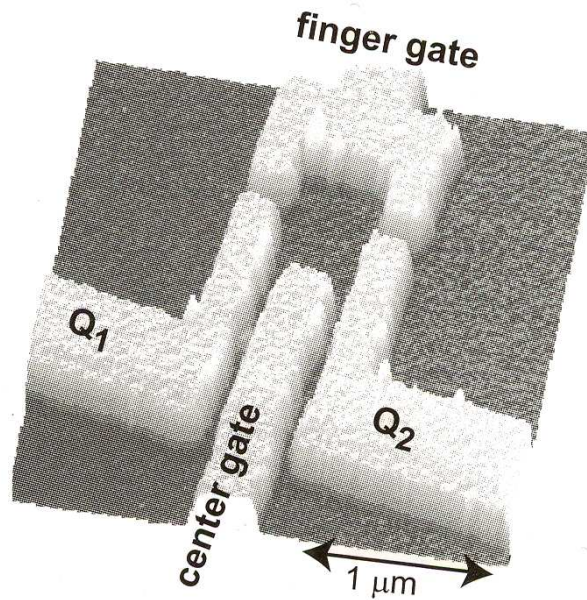


Figure 1.2.3: Typical quantum dot

1.3 Charge quantization

In addition to size quantization we also have what is called charge quantization. In electromagnetism we have a well known device known as the capacitor. Two metal plates are spaced so they are isolated. Then a potential is applied over the plates. This cause a build up of charge at one plate and a reduction of equal charge on the other. In this way the capacitor stores energy. The displaced charge are electron gas and the charge buildup is more or less continuous with applied potential. It's not quantized. One defines Capacitance as the difference between the charges q and the potential V between the plates, $C = q/V$. The energy stored in a capacitor is defined as $E = q^2/2C$.

If we now make the distance between the plates small so it acts as a tunnel junction, the charge transfer between the plates is quantized. This mechanism is called Coulomb blockage. To outline the Coulomb blockage model, let us look at Figure 1.2.3. The island is isolated between two QPC, which work as tunneling barriers. We can now think of the island and the two QPCs as a quantized capacitor. This is a approximation since we've completely disregarded the Pauli exclusion principle, which also adds to the energy difference, but it is suppressed in comparison. The potential difference between the two gates is a bit more complex than in a regular capacitor, due to the presence of several gates. But let us call it V_g for simplicity. If we add a charge q to the island, the change in energy would be

$$\Delta E = qV_g + \frac{q^2}{2C} \quad (1)$$

The first term accounts for the work involved moving in the potential field, while the second is the energy of Coulomb repulsion of the island, the capacitor. The electron, either single or multiple is responsible for the charge transfer. For N electrons with charge $-e$ we have that $q = -Ne$. This give the energy difference as a function of the electron number n

$$\Delta E(n) = -NeV_g + N^2 \frac{e^2}{2C} \quad (2)$$

The change in energy from $n + 1$ electron to n electron is given as

$$\Delta E(n+1) - E(n) = -eV_g + \left(\frac{1}{2} + n\right) \frac{e^2}{C} \quad (3)$$

When the energy difference vanish, electrons can be transfered on and off the island. This happens when the gate potential is

$$V_g = \left(\frac{1}{2} + n\right) \frac{e}{C} \quad (4)$$

This give rise to a special property regarding current flow through the islands of quantum dots. A plot of conductance as a function of gate potential is shown in Figure 1.3.4. We see that Coulomb blockage occur between the peaks. However, if we measure the conductance of a typical quantum dot without any kind of filtering device we would observe more noise and imperfection than what is shown in Figure 1.3.4. Typically one would have main peaks which arise due to Coulomb blockage and noise which has to do with the size quantization. Also, when the gate potential increases we often see that we get closer spaced

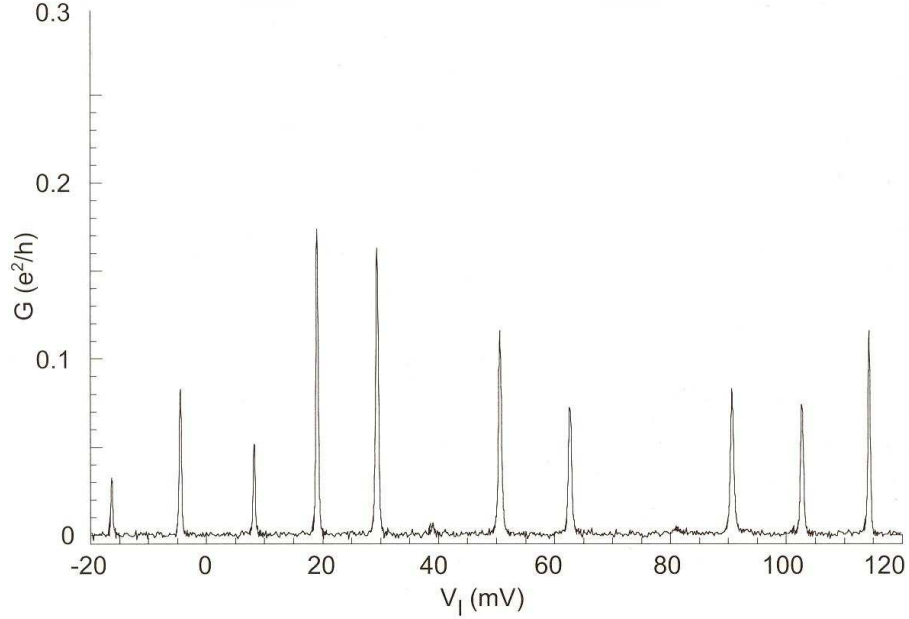


Figure 1.3.4: Conductance through an island as a function of the gate potential. We clearly see that current mostly flows at certain gate potentials

peaks. One explanation for this is that the dot increases in size, approaching the electrodes which increases conductance. The first peak can be the first electron on the dot, but it can also be the tenth. It depends on how we have tuned the tunnel barriers. When the barriers are sufficient close to the confining center for tunneling to happen, we normally see the first electron in the leftmost peak. If the distance is larger, we need to increase the radius of the electron cloud sitting in the center of the confinement. Since electrons repel each other, each time we add an electron, the size of the confined cloud increases and hence the distance to the tunnel barriers decrease. Since a increase in temperature adds more thermal fluctuations, the width of the peaks are directly related to the temperature of the sample.

Observing Coulomb blockage in real life is not easy. First of all, the resistance in the QPC need to be sufficiently large. We need to observe single electrons tunneling through the QPC. This means, that the tunneling event time dt need to be significantly larger than the tunneling time τ . The tunneling time has been estimated as $\tau = \hbar/eV$ [5]. Now, if we estimate the tunneling event time

$$V = RI. \quad (5)$$

The current is known as dq/dt , which gives

$$dt = \frac{Rdq}{V}. \quad (6)$$

As the difference in charge is e , we simply get a crude approximate for the

tunneling event time as

$$dt = Re/V. \quad (7)$$

Now, to observe a single electron transfer we would like to have $dt \gg \tau$, that is

$$R \gg \frac{\hbar}{e^2} \quad (8)$$

The temperature is also an important aspect. If the operational temperature is too high, we can have thermal fluctuations and excitations. Since we need a large tunnel resistor we quickly run into practical problems with cooling. Today, these limitations are seldom a problem and quantum dots made out of silicon are able to operate at room temperature.

1.4 Theoretical description of quantum dots, take one

Quantum dots are complex devices. It is not easy to give a simple, yet complete theoretical explanation. Effects of electron-electron interactions, the Pauli exclusion principle, edge effects and external fields all need to be accounted for. And combinations are also possible. For a two-electron quantum dot, we only need to account for the two body interaction. However, as the electron number increases many body interactions occur and advanced band structures are revealed much due to a balance between the Pauli principle and electron-electron interaction.

Now, to start off, let us look at a quantum dot confined with a harmonic oscillator potential, making restrictions in the x-y directions, while we let the third dimension be locked down by a manufacture technique. We will also apply a constant magnetic field along this third dimension axis. This is often the case of real life quantum dots.

The two dimensional Hamilton operator for free electrons in a harmonic oscillator potential is

$$H = \sum_{i=1}^N \left(\frac{p_i^2}{2m^*} + \frac{1}{2} m^* \omega^2 (x_i^2 + y_i^2) \right), \quad (9)$$

where the electron number is N , the reduced electron mass m^* and the electron momentum p_i . The coordinates are given as x_i and y_i . By introducing an external vector field \vec{A} we get a modified Hamiltonian

$$H = \sum_{i=1}^N \left(\frac{1}{2m^*} (\vec{p}_i + \vec{A}_i)^2 + \frac{1}{2} m^* \omega^2 (x_i^2 + y_i^2) + e\phi + \vec{\rho}_i \cdot \vec{B} \right). \quad (10)$$

In addition to the added vector potential, we get a contribution from the electrical potential ϕ and the magnetic field B . The electron charge is e . The magnetic moment ρ is introduced due to the spin coupling with magnetic fields. The magnetic moment is known as $\vec{\rho} = q\vec{L}/2m$. However, since it is the electron spin that couples, we write $\vec{\rho} = -eg\vec{S}/2m^*$, where g is the Landé g-factor. Since the two last terms in the Hamiltonian in Equation (10) are scalars and not operators, they can be taken outside and disregarded during calculations. We can reintroduce them in the final result if we want. We also see that Equation (10) is separable in single electron Hamiltonians. From now on we only consider

the Hamiltonian for one electron. Let us look closer at Equation (10). Without the scalar terms we have

$$H = \frac{1}{2m^*}(\vec{p} - \frac{e}{c}\vec{A})^2 + \frac{1}{2}m^*\omega_0^2(x^2 + y^2), \quad (11)$$

expanding the first term gives

$$(\vec{p} - \frac{e}{c}\vec{A})^2 = p^2 - \frac{e}{c}(\vec{p} \cdot \vec{A} + \vec{A} \cdot \vec{p}) + \frac{e^2}{c^2}A^2, \quad (12)$$

The momentum and vector field does not commute general. However, by selecting a proper gauge they do. See Appendix ?? for details. Since we want a constant magnetic field along the z-axis we can for example chose

$$\vec{A} = \frac{B}{2}\{-y, x, 0\}, \quad (13)$$

where B now is the amplitude of the applied magnetic field. We can verify the chosen vector field. By Maxwell's equations we have

$$\vec{B} = \nabla \times \vec{A}, \quad (14)$$

which gives

$$\vec{B} = B\vec{e}_z. \quad (15)$$

Putting the vector field from Equation (13) into Equation (12), we get

$$(\vec{p} - \frac{e}{c}\vec{A})^2 = p^2 - \frac{eB}{c}(xp_y - yp_x) + \frac{e^2B^2}{4c^2}(x^2 + y^2). \quad (16)$$

Substitute this back into Equation (11) gives

$$H = \frac{1}{2m^*} \left(p^2 - \frac{eB}{c}(xp_y - yp_x) + \frac{e^2B^2}{4c^2}(x^2 + y^2) \right) + \frac{1}{2}m^*\omega_0^2(x^2 + y^2). \quad (17)$$

Where the second expression can be associated with the z-component of the angular momentum. See Appendix A.3. Now, if we define

$$\omega_B = \frac{eB}{2m^*c}, \quad (18)$$

and

$$\omega^2 = \omega_0^2 + \omega_B^2, \quad (19)$$

together with the substitution $p \rightarrow -i\hbar\nabla$. We get a more compact notation of the Hamilton. Also note that for example $p_x \rightarrow -i\hbar\partial/\partial x$

$$H = \frac{1}{2m^*} \left(\hbar^2\nabla^2 + i\hbar B(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}) \right) + \frac{1}{2}m^*\omega^2(x^2 + y^2). \quad (20)$$

Changing to polar coordinates r and θ . Details for the transformation are given

in Appendix A.3

$$H = -\frac{\hbar^2}{2m^*} \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} + i \frac{eB}{\hbar c} \frac{\partial}{\partial \theta} \right) + \frac{1}{2} m^* \omega^2 r^2 \quad (21)$$

At first sight changing to polar coordinates r and θ seem more complicated, but it is not. Doing this, we will end up solving a rather simple one dimensional equation. Now is the time to bring in the Schrödinger equation

$$H\Psi = E\Psi \quad (22)$$

With the Hamiltonian in our case we now have the equation

$$-\frac{\hbar^2}{2m^*} \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} + i \frac{eB}{\hbar c} \frac{\partial}{\partial \theta} \right) \Psi(r, \theta) + \frac{1}{2} m^* \omega^2 r^2 \Psi(r, \theta) = E\Psi(r, \theta) \quad (23)$$

This equation is separable in R and θ . We can then assume

$$\Psi(r, \theta) = e^{im\theta} \psi(r), \quad (24)$$

Where m takes certain values, since $\theta + 2\pi = \theta$, at least physically. This gives restrictions such that $m = 0, \pm 1, \pm 2, \dots$. Substitute this into Equation (23) results in the following Schrödinger equation

$$-\frac{1}{2m^*} \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{m^2}{r^2} - \frac{emB}{\hbar c} \right) \psi(r) + \frac{1}{2} m^* \omega^2 r^2 \psi(r) = E\psi(r) \quad (25)$$

See Appendix A.2 for the solutions.

A Appendix

A.1 Gauge transformations

A.2 Solution of the two dimensional radial equation

We want to solve the following Schrödinger equation

$$-\frac{1}{2m^*} \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{m^2}{r^2} - \frac{emB}{\hbar c} \right) \Psi(r, \theta) + \frac{1}{2} m^* \omega^2 r^2 \Psi(r, \theta) = E\Psi(r, \theta). \quad (26)$$

Define

$$\epsilon = 2m^* E - \frac{emB}{\hbar c}, \quad (27)$$

and substitute

$$x = r^2, \quad (28)$$

into Equation (26) to get

$$-\left(4x \frac{\partial^2}{\partial x^2} + 4 \frac{\partial}{\partial x} + \frac{m^2}{x} \right) \psi'(x) + m^* \omega^2 x \psi'(x) = \epsilon \psi'(x). \quad (29)$$

To get rid of the first derivative we can do the substitution $\psi'(x) = x^{-1/2}u(x)$. After a bit of algebra we get the equation

$$-\frac{\partial^2 u}{\partial x^2} + \frac{1}{4} \left(m^{*2} \omega^2 - \frac{\epsilon}{x} - \frac{(m^2 + 1)}{x^2} \right) u = 0 \quad (30)$$

To make the equation dimensionless, substitute $y = m^* \omega x$. This gives

$$-\frac{\partial^2 u}{\partial y^2} + \frac{1}{4} \left(1 - \frac{\epsilon}{m^* \omega y} - \frac{(m^2 + 1)}{y^2} \right) u = 0 \quad (31)$$

We now have a much simpler equation compared to what we started out with. However, we still need to make some general considerations in the limits to get to the wanted solutions. Let us consider what is going on if we let $y \rightarrow \infty$. When this happens we get a very simple equation

$$\frac{\partial^2 u}{\partial y^2} \simeq \frac{1}{4} u, \quad (32)$$

which have a approximate solution which goes as $u(y) \simeq e^{\pm y/2}$. But we need the solution to be finite, even at $y \rightarrow \infty$. Then, only the solution for the negative y is allowed. That is

$$u(y) \simeq e^{-y/2} \quad (33)$$

Now, let us consider $y \rightarrow 0$. In this regime we get a equation

$$\frac{\partial^2 u}{\partial y^2} \simeq \frac{m^2 - 1}{4y^2} \quad (34)$$

This equation has two solution

$$u(y) \simeq y^{(m+1)/2}, \quad (35)$$

$$u(y) \simeq y^{(m-1)/2}. \quad (36)$$

Since this should be finite at $y = 0$ and if $m > 0$ we see that the only valid solution is the first. Combining Equation (33) and Equation (35) we can now substitute

$$u(y) = y^{(m+1)/2} e^{-y/2} \rho(y), \quad (37)$$

into Equation (31) and get, again after tedious algebra

A.3 Polar coordinate transformation

Let us now develop the needed transformations from a Cartesian coordinate system to a Polar one. First, we define what is called general curvilinear coordinates. The orthogonal coordinates will be used here. They cover cartesian, polar, spherical and several others. We assume that the functions used in the derivations are continues and differentiable. Let us say that the vector $\vec{r}(x_1, x_2, x_3, \dots)$ points at a point in space. Then this vector has tangents as the most elementary basis. We can define them as $\vec{e}_i = \partial \vec{r} / \partial x_i$ for $i = 1, 2, 3, \dots$. Each \vec{e}_i will be a tangent to each x_i -curve in a direction of increasing x_i values.

If we now normalize these vectors we get

$$\vec{e}_i = \frac{1}{a_i} \frac{\partial \vec{r}}{\partial x_i}. \quad (38)$$

Where a_i is the length of each vector. The metric tensor is defined as

$$g_{ij} = \frac{\partial \vec{r}}{\partial x_i} \cdot \frac{\partial \vec{r}}{\partial x_j}. \quad (39)$$

In the orthogonal case g_{ij} is a matrix with a_i^2 on the diagonal. Now, a infinitesimal displacement along \vec{r} in three dimensions can be written as

$$d\vec{r} = \frac{\partial \vec{r}}{\partial x_1} dx_1 + \frac{\partial \vec{r}}{\partial x_2} dx_2 + \frac{\partial \vec{r}}{\partial x_3} dx_3, \quad (40)$$

in terms of \vec{e}_i we get

$$d\vec{r} = a_1 dx_1 \vec{e}_1 + a_2 dx_2 \vec{e}_2 + a_3 dx_3 \vec{e}_3. \quad (41)$$

We introduce a vector potential $\psi(x_1, x_2, x_3, \dots)$. A infinitesimal change in three dimensions in x_i gives the change of ψ as follows

$$d\psi = \frac{\partial \psi}{\partial x_1} dx_1 + \frac{\partial \psi}{\partial x_2} dx_2 + \frac{\partial \psi}{\partial x_3} dx_3. \quad (42)$$

Comparing this result with Equation (40), we observe that we can write

$$d\psi = \nabla \psi \cdot d\vec{r}, \quad (43)$$

where

$$\nabla \psi = \frac{\vec{e}_1}{a_1} \frac{\partial \psi}{\partial x_1} + \frac{\vec{e}_2}{a_2} \frac{\partial \psi}{\partial x_2} + \frac{\vec{e}_3}{a_3} \frac{\partial \psi}{\partial x_3}, \quad (44)$$

giving the *nabla* operator

$$\nabla = \frac{\vec{e}_1}{a_1} \frac{\partial}{\partial x_1} + \frac{\vec{e}_2}{a_2} \frac{\partial}{\partial x_2} + \frac{\vec{e}_3}{a_3} \frac{\partial}{\partial x_3}. \quad (45)$$

We have now developed an general expression for the gradient and del operator in three dimension curvilinear coordinates. We also need the divergence to calculate the Laplace operator. Define a vector field

$$\vec{f} = f_1 \vec{e}_1 + f_2 \vec{e}_2 + f_3 \vec{e}_3, \quad (46)$$

calculate the divergence

$$\nabla \cdot \vec{f} = \nabla \cdot (f_1 \vec{e}_1) + \nabla \cdot (f_2 \vec{e}_2) + \nabla \cdot (f_3 \vec{e}_3). \quad (47)$$

Observing what will happen to the first term if we write it out

$$\nabla \cdot (f_1 \vec{e}_1) = \frac{\partial f_1}{\partial x_1} + f_1 \left(\frac{\partial \vec{e}_1}{\partial x_1} \right) \cdot \vec{e}_1. \quad (48)$$

The last term is problematic since we have no direct way of calculating it. Calculate the gradient of x_1 by using the developed term for the del operator in Equation (45)

$$\nabla x_1 = \frac{1}{a_1} \vec{e}_1, \quad (49)$$

and similar for the other two components. We also note that

$$\vec{e}_1 = \vec{e}_2 \times \vec{e}_3, \quad (50)$$

which gives, using Equation (49)

$$\vec{e}_1 = a_2 \nabla x_2 \times a_3 \nabla x_3. \quad (51)$$

Again we write out the first term in Equation (47), but now with the help of Equation (51)

$$\nabla \cdot (f_1 \vec{e}_1) = \nabla(f_1 a_2 a_3) \cdot (\nabla x_2 \times \nabla x_3) + f_1 a_2 a_3 \nabla \cdot (\nabla x_2 \times \nabla x_3), \quad (52)$$

writing out the last term, we see that

$$\nabla \cdot (\nabla x_2 \times \nabla x_3) = \nabla x_3 \cdot (\nabla \times \nabla x_2) - \nabla x_2 \cdot (\nabla \times \nabla x_3), \quad (53)$$

is $\vec{0}$ since $\nabla \times \nabla x_i = \vec{0}$. Using Equation (49) again we get

$$\nabla \cdot (f_1 \vec{e}_1) = \frac{1}{a_2 a_3} (\vec{e}_2 \times \vec{e}_3) \nabla(f_1 a_2 a_3), \quad (54)$$

using Equation (50) and Equation (45) gives

$$\nabla \cdot (f_1 \vec{e}_1) = \frac{\vec{e}_1}{a_2 a_3} \left(\frac{\vec{e}_1}{a_1} \frac{\partial}{\partial x_1} (f_1 a_2 a_3) \right). \quad (55)$$

This is of course cyclic in the coordinates and we can finally write out the divergence in Equation (47) as

$$\nabla \cdot \vec{f} = \frac{1}{a_1 a_2 a_3} \left(\frac{\partial}{\partial x_1} (f_1 a_2 a_3) + \frac{\partial}{\partial x_2} (f_2 a_1 a_3) + \frac{\partial}{\partial x_3} (f_3 a_1 a_2) \right) \quad (56)$$

The remaining part is to calculate a general expression for the Laplace operator. This is rather simple. We can just put $\vec{f} = \nabla$ and we get

$$\nabla^2 = \frac{1}{a_1 a_2 a_3} \left(\frac{\partial}{\partial x_1} \left(\frac{a_2 a_3}{a_1} \frac{\partial}{\partial x_1} \right) + \frac{\partial}{\partial x_2} \left(\frac{a_1 a_3}{a_2} \frac{\partial}{\partial x_2} \right) + \frac{\partial}{\partial x_3} \left(\frac{a_1 a_2}{a_3} \frac{\partial}{\partial x_3} \right) \right) \quad (57)$$

In our case, we want to use cylindrical polar coordinates. Define

$$x = r \cos(\theta), \quad (58)$$

$$y = r \sin(\theta), \quad (59)$$

$$z = z, \quad (60)$$

where r is the radial distance from the origin to the point P , while θ is the anticlockwise angle from the x-axis up to P . The last coordinate z is the same as in the Cartesian case. Transforming the vector \vec{r} from Cartesian to polar coordinates results in the following \vec{r}

$$\vec{r} = \begin{bmatrix} r \cos(\theta) \\ r \sin(\theta) \\ z \end{bmatrix}. \quad (61)$$

We need to calculate the normalizations variables. Remember that

$$a_i = \left\| \frac{\partial \vec{r}}{\partial x_i} \right\|. \quad (62)$$

This gives

$$a_r = 1, \quad (63)$$

$$a_\theta = r, \quad (64)$$

$$a_z = 1. \quad (65)$$

We put this into Equation (57) and get

$$\nabla^2 = \frac{1}{r} \left(\frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) \right) + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} + \frac{\partial^2}{\partial z^2}. \quad (66)$$

Observe that in we could also write out the first term as a second and first derivate. In the two-dimensional case this would be

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2}. \quad (67)$$

One term remains. This term is associated with what is known as the angular momentum.

$$\vec{L} = \vec{r} \times \vec{p}, \quad (68)$$

written in components

$$L_x = yp_x - zp_y, \quad (69)$$

$$L_y = zp_y - xp_x, \quad (70)$$

$$L_z = xp_y - yp_x. \quad (71)$$

In two dimensions, x and y , the only term that survives is L_z . We now need to transform this into polar coordinates as we did with the Laplace operator. By the substitution $p_x \rightarrow -i\hbar \partial/\partial x$ and the analogy in p_y we can write the z-component angular momentum operator as

$$L_z = i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right). \quad (72)$$

Just like Equation (42) we can write

$$\frac{\partial \psi}{\partial x} = \frac{\partial r}{\partial x} \frac{\partial \psi}{\partial r} + \frac{\partial \theta}{\partial x} \frac{\partial \psi}{\partial \theta}, \quad (73)$$

$$\frac{\partial \psi}{\partial y} = \frac{\partial r}{\partial y} \frac{\partial \psi}{\partial r} + \frac{\partial \theta}{\partial y} \frac{\partial \psi}{\partial \theta}. \quad (74)$$

Using the same \vec{r} as in Equation (61) with any given vector potential ψ gives

$$\frac{\partial \psi}{\partial x} = \cos(\theta) \frac{\partial \psi}{\partial r} - \frac{\sin(\theta)}{r} \frac{\partial \psi}{\partial \theta}, \quad (75)$$

$$\frac{\partial \psi}{\partial y} = \sin(\theta) \frac{\partial \psi}{\partial r} + \frac{\cos(\theta)}{r} \frac{\partial \psi}{\partial \theta}. \quad (76)$$

Now substitute this back into Equation (72) we immediately see that the angular momentum operator in polar coordinates is

$$L_z = -i\hbar \frac{\partial}{\partial \theta} \quad (77)$$

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