Applications of Quantum Physics
winter semester 2017/18

Amanda Matthes

January 1, 2018

Contents

1 Revision about Quantum Mechanics

The state of a quantum system is described by a wave function $\Psi(x,t)$. It is continuous, integrable and single valued. It contains all you can know about a system. The probability of finding a particle between x and $x+dx$ is given by

$$P = |\Psi(x,t)|^2 dx \tag{1}$$

Ψ has to be normalized:

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1 \tag{2}$$

Quantum Mechanics is non-deterministic. It can only predict the probability of outcomes. After a measurement the system is in a new state that is consistent with the outcome of the measurement (collapse of the wave function). The wave function obeys the time dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\Psi = \hat{H}\Psi \tag{3}$$

with

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}) \quad \text{in 3D} \tag{4}$$

To solve this partial differential equation, try

$$\Psi(\vec{r},t) = \psi(\vec{r})T(t) \tag{5}$$

Substitute in the Schrödinger Equation and divide both sides by ψT:

$$\frac{i\hbar}{T}\frac{dT}{dt} = \frac{1}{\psi}\hat{H}\psi \tag{6}$$

Now the left side is a function of t only and the right is a function of $\vec{r}$ only. ($\rightarrow$ separation of variables).
If $\hat{H}$ is time independent this can be made equal to a constant E. This gives two equations:

$$\frac{dT}{dt} = -\frac{iE}{\hbar}T \tag{7}$$

which is solved by

$$T = e^{-iEt/\hbar} \tag{8}$$

and

$$\hat{H}\psi = E\psi \tag{9}$$

which is also called the time independent Schrödinger Equation. It is an **eigenvalue equation**.

In Quantum Mechanics physical quantities are described by Hermitian operators ($\hat{A} = \hat{A}^\dagger$). This guaranties that the eigenvalues are real numbers.

The TDSE is a linear pde so superpositions of solutions are also solutions. The general solution is

$$\Psi(\vec{r}, t) = \sum_n c_n \psi_n(\vec{r}) T_n(t) \tag{10}$$

with ψ_n being the eigenfunctions. So a wave function is not necessarily an eigenfunction itself.

Solutions of the TISE are eigenfunctions of $\hat{H}$

2 Tunnelling Simple Barriers

Simple Solutions of the Time Independent Schrödinger equation

The TISE for a constant potential $V(x) = V_0$ in 1D is

$$\frac{d\psi}{dx^2} = \frac{2m}{\hbar^2}(V_0 - E)\psi \tag{11}$$

For $E > V_0$ this can also be written as

$$\frac{d\psi}{dx^2} = -k^2\psi \tag{12}$$

where $k^2 = \frac{2m}{\hbar^2}(E - V_0)$ and is solved by waves

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \tag{13}$$

In classically forbidden regions ($E < V_0$) we can write

$$\frac{d\psi}{dx^2} = \beta^2\psi \tag{14}$$

with $\beta^2 = \frac{2m}{\hbar^2}(V_0 - E)$ and it is solved by exponentials tunnelling into the region

$$\psi(x) = Ce^{\beta x} + De^{-\beta x} \tag{15}$$

Simple Square Barrier

Consider particles of energy E hitting a square barrier of width b of height V_0 with $E < V_0$ at $x = 0$.

For $x < 0$:

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \tag{16}$$

with $k^2 = \frac{2mE}{\hbar^2}$.

For $0 < x < b$:

$$\psi(x) = Ce^{\beta x} + De^{\beta x} \tag{17}$$

with $\beta^2 = \frac{2m}{\hbar^2}(V_0 - E)$.

And for $x > b$:

$$\psi(x) = Fe^{ikx} \tag{18}$$

Our boundary conditions are given by ψ and $\frac{\psi}{dx}$ being continuous. This gives four boundary conditions. A is determined by the incoming intensity. So we have four unknowns (B, C, D, F) and four linear equations. This is solvable but tedious.

For a high wide barrier $\beta b \gg 1$ we can find a tunnelling factor

$$T = e^{-2\beta b} = \exp\left\{-2b\sqrt{\frac{2m}{\hbar^2}(V_0 - E)}\right\} \tag{19}$$

It can be used to estimate probabilities.

Example:
Consider two pieces of metal separated by an insulator. This can be thought of as a square barrier.
To remove an electron from metal one needs energy equal to the work function $W = V_0 - E$. So

$$\beta = \sqrt{\frac{2m}{\hbar^2}W} \approx 10.3\frac{1}{nm} \tag{20}$$

Now, if the gap is $b = 5nm$ (That's roughly 25 atoms; The atomic **radius** is $\approx 0.1nm$):

$$T = e^{-2\beta b} \approx 10^{-44} \tag{21}$$

If the gap is just $b = 1nm$ thick (5 atoms), then it quickly goes down to

$$T \approx 10^{-9} \tag{22}$$

A few important notes:

- At nm scales electrons will leak through insulators. This limits circuit miniaturisation.
- The tunnelling microscope makes use of this. Tiny distances from the probe to surface - even at the fraction of an atomic radius - give measurable current changes.
- Quantum mechanics will be important in nanoscale physics.
- Flash memory is made possible thanks to quantum tunnelling.

Note on numerical calculations:
Stick to sensible units (eV and nm for atomic physics, or MeV and fm for nuclear physics). Write masses as rest energies mc^2. Remember

$$\hbar c = 197.33MeV \cdot fm \text{ or } eV \cdot nm \tag{23}$$

If charges are involved, $\frac{e^2}{4\pi\epsilon_0}$ can be deduced from the fine structure constant

$$\alpha = \frac{1}{\hbar c}\frac{e^2}{4\pi\epsilon_0} \approx \frac{1}{137} \tag{24}$$

3 Tunnelling and WKB

More complex barriers can be approximated using a series of square barriers with a width of Δx. The tunnelling probability through one barrier is $T(x_n) \approx exp[-2\Delta x\sqrt{\frac{2m}{\hbar^2}(V(x_n)-E)}]$. The total tunnelling probability is

$$T = \prod T(x_i) = exp[-2\sum\sqrt{\frac{2m}{\hbar^2}(V(x_n)-E)}\Delta x] \tag{25}$$

As $\Delta x \to 0$

$$T = exp[-2\int_a^b \sqrt{\frac{2m}{\hbar^2}(V(x)-E)}dx] \tag{26}$$

This is the WKB approximation. It is only useful for smoothly varying barriers. Also the original term for $T(x_n)$ only works for tall wide barriers, so it's only a good approximation for energies well below the maximum of $V(x)$.

Example: Nuclear fusion in the sun
At a temperature of roughly $10^7 K$ the protons in the sun have a kinetic energy of $\approx 1keV$. At the classical point of closest approach:

$$1keV \approx T = V = \frac{e^2}{4\pi\epsilon_0}\frac{1}{r} \tag{27}$$

$\hbar c = 197 MeV fm$
$\alpha = \frac{1}{137}$

$$r \approx 1400 fm \tag{28}$$

But nuclear forces have a range of about $1fm$. So the only way that fusion can happen is via the tunnelling effect.

$$T_{WKB} = exp[-2\int_{r_N}^{r_C}\sqrt{\frac{2\mu}{\hbar^2}(V(r)-V(r_c)}dr] \tag{29}$$

$$= exp[-2(\frac{2\mu e^2}{4\pi\epsilon_0\hbar^2})^{1/2}\int_{r_N}^{r_C}(\frac{1}{r}-\frac{1}{r_C})^{1/2}dr] \tag{30}$$

We can use

$$\int(\frac{1}{x}-1)^{1/2} = \sqrt{x(1-x)} - cos^{-1}\sqrt{x} + C \tag{31}$$

Substituting $x = \frac{r}{r_C}$ we arrive at

$$T = exp[-(\frac{r}{R_G})^{1/2}] \tag{32}$$

where $R_G = \frac{4\pi\epsilon_0\hbar^2}{e^2 2\pi^2\mu}$. So there is a 1 in 3 billion chance of tunnelling.
It turns out that the diproton is not stable so $p + p \rightarrow^2 He$ doesn't actually happen. What really happens is $p + p \rightarrow^2 H + e^+ + \nu_e$. The diproton β^+ decays. Deuterons go on to fuse with protons to ${}^3He$. And ${}^3He$ fuses to α-particles.
Overall 6 protons and make an α-particle and 2 protons (and energy).

4 Multiple Barriers and Resonant Tunnelling

In this part we want to explore tunnelling trough two barriers. To do this we start with a particle in a box and then look at a particle trapped between two square barriers and then finally at the actual tunnelling.

Particle in a box:
Consider a particle with energy $E < V_0$ in a square well potential of width a with $V = 0$ inside and $V = V_0 = \infty$ outside. For $0 < x < a$:

$$\psi = A\sin(kx) \text{ with } k = \frac{n\pi}{a} \text{ and } n = 1, 2, 3... \tag{33}$$

The particle can only have discrete energy levels

$$E = \frac{\hbar^2 n^2 \pi^2}{2ma^2} \tag{34}$$

A more realistic model for certain physical systems is $V_0 < \infty$. This problem is not analytically solvable. However we can make a few qualitative observations. In the classically forbidden regions the wavefunction will be an exponential. Due to this exponential spillage the wavefunction in the allowed region will be less curved than in the case of the infinite square well. That means that the wavelength is longer so the momentum is lower. This means that the energy levels will be lower in the finite well.

Particle inside double barrier:
Consider a particle with $0 < E < V_0$ between two square barriers. Let the potential be $V = 0$ everywhere but at the barriers, where $V = V_0$.
If you pop a particle in, it isn't bound. It leaks out by tunnelling. So its not strictly a stationary state with definite energy.
A wave packet inside will decay away with a certain lifetime τ related to the tunnelling probability. The uncertainty principle tells us

$$\tau \Delta E \approx \hbar \tag{35}$$

This is a bit like a classical damped oscillator.
But if $E \ll V_0$ the tunnelling probability is low, and τ might be a long time so ΔE might be small. We can then talk about quasi-bound states with energies similar to a square well.

Particle incident on double barrier:

Recall that for one barrier

$$\psi_{before} = e^{ikx} + \frac{B}{A}e^{-ikx} \tag{36}$$

$$\psi_{after} = \frac{F}{A}e^{ikx} \tag{37}$$

That way

$$\text{reflection amplitude } = \frac{B}{A} = re^{i\phi_r} \tag{38}$$

$$\text{transmission amplitude } = \frac{F}{A} = te^{i\phi_t} \tag{39}$$

Note that these can be complex.

Now for the double barrier. There are 5 regions. We are interested in what comes out at the end in region 5. This can happen in several ways. The particle can tunnel through the first barrier and then immediately tunnel through the second one or it can get reflected a few (even number of) times.

$$\psi_5 = te^{i\phi_t}[1 + re^{i\phi_r}e^{i\phi_r}e^{2ika} + (re^{i\phi_r}re^{i\phi_r})^2e^{4ika} + ...]te^{i\phi_t}e^{ikx} \tag{40}$$

$$= t^2e^{2i\phi_t}e^{ikx}\sum_{n=0}^{\infty}(r^2e^{2i\phi_r}e^{2ika})^n \tag{41}$$

This is a geometric series

$$= \frac{t^2e^{2i\phi_t}e^{ikx}}{1 - r^2e^{2i\phi_r}e^{2ika}} \tag{42}$$

That means that the tunnelling probability for a double barrier is

$$\text{Tunnelling prob. for double barrier } = |\frac{t^2e^{2i\phi_t}}{1 - r^2e^{2i(\phi_r+ka)}}|^2 \tag{43}$$

This reaches a maximum for $e^{2i(\phi_r+ka)} = 1$

$$\text{Max double tunnelling prob. } = |\frac{T}{1 - R}|^2 \tag{44}$$

But $T^2 + R^2 = 1$ so the maximum double tunnelling probability is 100%! (for the right energy)

In this resonance condition

$$e^{2ika} = 1 \rightarrow \cos 2ka = 1 \rightarrow k = \frac{n\pi}{a} \tag{45}$$

So half a λ fits in between the barriers.

We achieve resonance when the reflected waves travel an extra distance which is a

multiple of λ. This gives constructive interference. So there is a large probability of finding a particle in the well and a large tunnelling probability.
This also means that the incoming energy matches that of the quasi-bound levels in the well. Higher quasi bound levels have a larger tunnelling out probability and a larger width because the lifetime is shorter.

This phenomenon is important for

- loading quantum dots
- resonant tunnelling diodes
- graphene-BN-graphene layering
- nuclear fission

Summary: In the case of two wide square barriers, the transmission probability is unity for certain incident energies. This is the same energy of a quasi-bound state in the square well formed by the two barriers.

5 Trapped Particles-Nanocubes

A quantum dot is a small (small enough for quantum behaviour) region of space that traps particles in a 3D-potential. A quantum wire is the same thing in 2D and a quantum well traps particles in 1D. Typical dimensions of such a contraption are $5 - 100nm$, that's roughly $25 - 500$ atoms (atomic radius $\approx 0.1nm$).

Example: metallic nanocubes of silver with dimensions $a \approx 50 - 100nm$
Electrons are free to move until they hit the edge. This can be treated as a 3D infinite square well.

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi \tag{46}$$

Substituting $k^2 = \frac{2Em}{\hbar^2}$ gives

$$\nabla^2\psi = -k^2\psi \tag{47}$$

The boundary conditions are

$$\psi(0, y, z) = 0 \tag{48}$$

$$\psi(a, y, z) = 0 \tag{49}$$

and the same for y and z.
Try:

$$\psi(x, y, z) = X(x)Y(y)Z(z) \tag{50}$$

now

$$\frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\frac{d^2Y}{dy^2} + \frac{1}{Z}\frac{d^2Z}{dz^2} = -k^2 \tag{51}$$

all three terms on the left side are only dependant on one variable each, so they must each be constant:

$$-k_x^2 - k_y^2 - k_z^2 = -k^2 \tag{52}$$

Our boundary conditions imply $X(0) = 0$, $X(a) = 0$ and so on.
The problem can now be solved by solving

$$\frac{d^2}{dx^2}X = -k_x^2 X \tag{53}$$

with boundary conditions $X(0) = 0$ and $X(a) = 0$. This is solved by

$$X(x) = A\cos(k_x x) + B\sin(k_x x) \tag{54}$$

The boundary conditions and normalising yields

$$B = \sqrt{\frac{2}{a}} \tag{55}$$

and

$$k_x = \frac{n_x \pi}{a} \tag{56}$$

with $n_x = 1, 2, ...$ So the full solution is

$$\psi(x, y, z) = (2/a)^{3/2} sin\frac{n_x \pi x}{a} sin\frac{n_y \pi y}{a} sin\frac{n_z \pi z}{a} \tag{57}$$

The Energies are

$$E_{n_x, n_y, n_z} = \frac{\hbar^2 k^2}{2m} = \frac{1}{2m}(\frac{\hbar\pi}{a})^2(n_x^2 + n_y^2 + n_z^2) \tag{58}$$

Notice the degeneracy of all possible Energies.
For $a = 50nm$ the ground state energy is $\approx 0.45eV$. A cube of that size made from silver atoms contains roughly 5×10^6 atoms. With electron repulsion single electron energy levels are irrelevant. The optoelectronic properties are determined by the sea of electrons (plasmon). The oscillations of this electron gas are quantized and dictate the colour of materials.

6 Semiconductor Quantum Dots

Using semiconductors we can control the number of electrons by doping and/or connecting the material to external potentials.

Semiconductor quantum dots come in two varieties. There are things that are called *colloidal systems*. These are suspended in liquid. These are about 10 to 50 atoms in diameter. The size determines the properties. Alternatively quantum dots can be constructed on surfaces of Silicon chips using epitaxy or lithography. They are like miniature transistors but with quantum behaviour. This is the type we want to concentrate on.

They are basically nanoscale lumps of undoped semiconductor with three electrical contacts. That means that the conduction band is initially empty. The **drain** is the source of the electrons if $V_d < V_s$[1] The **source** then drains the electrons.

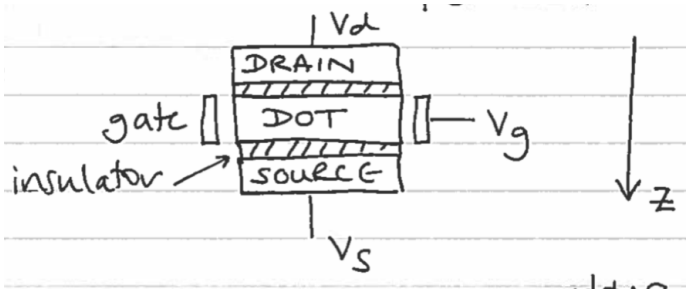


Figure 1: Vertical Section of a cylindrical dot

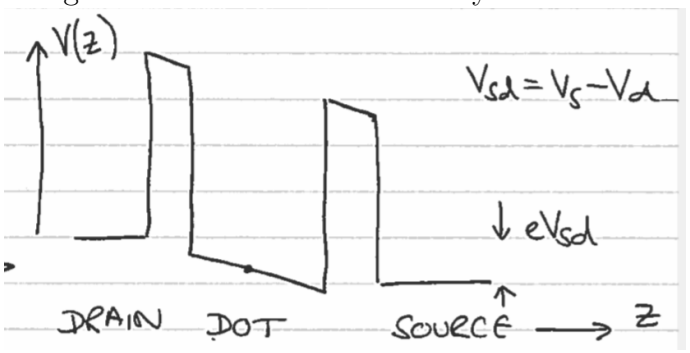


Figure 2: Potential landscape of a quantum dot

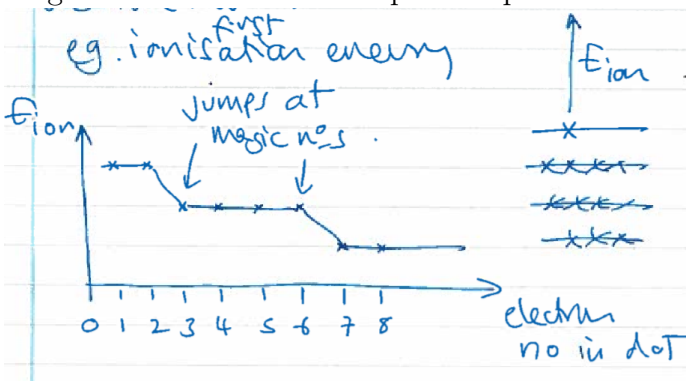


Figure 3: Ionisation energies in a quantum dot

The **gate** is wrapped cylindrically around the dot. It changes the average potential in the dot.

These dots are a lot wider than they are tall. The electrons moving in them have an **effective mass**. This effectively accounts for the results of the many interactions with the surrounding material: $m^\star = 0.06 m_e$.

To a reasonable approximation the potential in x and y can be described by a 2D

[1] remember that negatively charged particles lower their potential energy by being in places of higher potential.

harmonic oscillator:

$$V(x,y) = \frac{1}{2}k(x^2+y^2) \tag{59}$$

We can write $k = m^\star\omega^2$. In practice we find that $\hbar\omega \approx 5meV$.
If the insulating walls are high and the effect of the tilting floor low, the z-direction is described by an infinite square well and looks like in 2. The potential in the centre is controlled by the gate voltage.
The Hamiltonian is therefore

$$\hat{H} = -\frac{\hbar^2}{2m^\star}\nabla^2 + \frac{m^\star\omega^2}{2}(x^2+y^2) \tag{60}$$

Again, we can write

$$\psi(x,y,z) = X(x)Y(y)Z(z) \tag{61}$$

and separate this in three eigenvalue problems:

- two 1D Harmonic oscillators

$$-\frac{\hbar^2}{2m}\frac{d^2X}{dx^2} + \frac{1}{2}kx^2X = E_xX \tag{62}$$

  and for y respectively.

- one infinite square well

$$-\frac{\hbar^2}{2m^\star}\frac{d^Z}{dz^2} = E_zZ \tag{63}$$

So the eigenvalues are

$$E_x = (n_x+\frac{1}{2})\hbar\omega \quad E_y = (n_y+\frac{1}{2})\hbar\omega \quad E_z = \frac{\hbar^2}{2m^\star}(\frac{n_z\pi}{a})^2 \tag{64}$$

where $n_x = 0,1,2...$, $n_y = 0,1,2...$ and $n_z = 1,2,3....$ So the total energy is given by

$$E = E_x + E_y + E_z = (n_x+n_y+1)\hbar\omega + \frac{\hbar^2}{2m^\star}(\frac{n_z\pi}{a})^2 \tag{65}$$

For typical a E_z is much larger than $\hbar\omega$.
Our ground state is $(n_x,n_y,n_z) = (0,0,1)$. T he first excited state is $(1,0,1)$ or $(0,1,1)$ which has the same energy. Thanks to Spin we can fit 4 electrons in this state. So there is a degeneracy of 4. This is a one phonon state. The second exited level is then $(2,0,1)(1,1,1)(0,2,1)$; a two phonon state with a degeneracy of 6.

Level	# electrons in level	# electrons in dot
Ground	$2 \times 1 = 2$	2
1st	$2 \times 2 = 4$	$2 + 4 = 6$
2nd	$2 \times 3 = 6$	$6 + 6 = 12$
3rd	$2 \times 4 = 8$	$12 + 8 = 20$

This means that plotting the ionisation energy would give something like in 3. There will be jumps in ionisation energy. The numbers at which these jumps occur are called magic numbers. This is similar to magic numbers in atomic and nuclear physics.

7 Conduction in a semi conductor quantum dot

Consider a quantum dot as shown in 4. V_g is tuned so that E_1 lies between the Fermi levels of the source and the drain. That way electrons can tunnel from the drain into the dot to occupy E_0 but can't get out. They can't jump to E_2 without extra energy. E_1 is the interesting level, as electrons can tunnel in from drain and out into an empty state in the source. In fact, between states of the same energy resonant tunnelling occurs. So the transmission probability is large and current flows through two insulator layers!

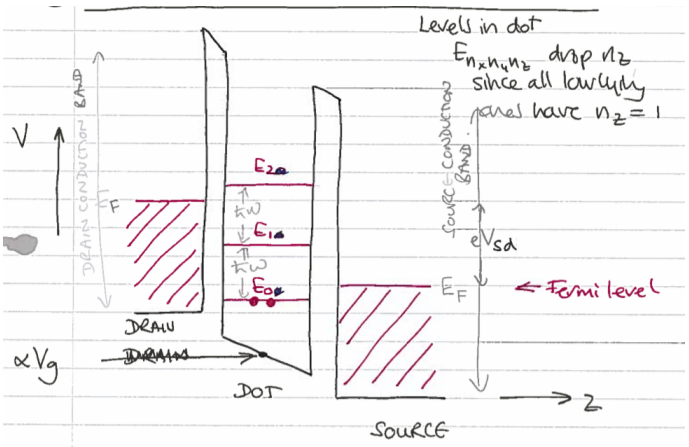
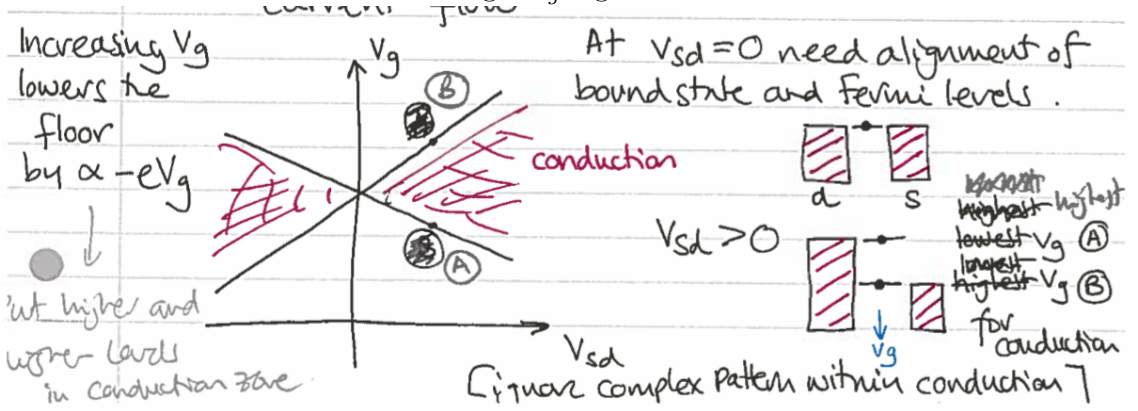


Figure 4: Potential landscape of a quantum dot

The conduction only happens when V_g is tuned so that an electron states lies in the window between Fermi levels.

Let's call the difference in Fermi levels V_{sd}. Now if $V_{sd} = 0$, V_g needs to be tuned so that it exactly lines up with the Fermi levels for tunnelling to occur. The system then conducts electricity otherwise it doesn't. Increasing V_g gives a broader conduction band:



Different conduction diamonds are formed when different bound states are in the V_{sd} window, i.e. when V_g has shifted the floor by $\hbar\omega$.

These conduction areas can be observed in experiment (see end of this chapter), however they do not follow the regular $\hbar\omega$-ladder. This can be explained by coulomb repulsion between electrons that we have ignored so far. Let's look at one electron in E_{00}, then $E = E_{00}$. For two electrons $E = E_{00} + \Delta E_e$. More electrons means less attraction which results in a system at a higher energy. It is often referred to

as a *Coulomb blockade* and lifts the degeneracy of multi-electron states. However it is very hard to calculate.
Uses of Quantum Dots include

- artificial atoms
- Qbits in quantum computers.
- electron traps
- electron pair traps
- biological labelling

Now as promised the measured conduction bands in a quantum dot:

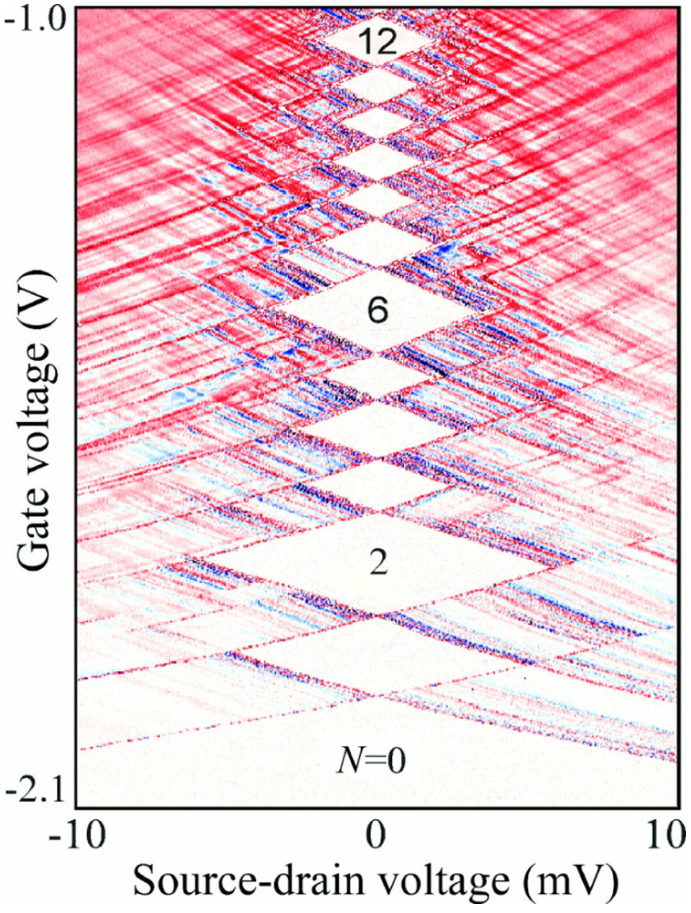


Figure 5: Conductions Bands in a Quantum Dot

8 Orthogonality, Basis states and Dirac notation

An operator is said to be hermitian if

$$\int f\hat{A}gd^3\vec{r} = \int g\hat{A}^\star fd^3\vec{r} \tag{66}$$

Its eigenvalues then are real:

$$\hat{A}\phi_n = a_n\phi_n \quad a_n \in \mathbb{R} \tag{67}$$

Another property of an hermitian operator is that its eigenfunctions are orthogonal:

$$\int \phi_m^\star(\vec{r})\phi_n(\vec{r})d^3\vec{r} = \delta_{mn} \tag{68}$$

This doesn't necessarily apply to eigenfunctions with degenerate eigenvalues. But it turns out that you can always construct orthogonal eigenfunctions if you choose to.
For example the general solution of the TDSE is

$$\Psi(\vec{r},t) = \sum_n c_n e^{-\frac{iE_nt}{\hbar}}\phi_n(\vec{r}) \tag{69}$$

This is just a linear superposition of energy eigenfunctions. At $t = 0$:

$$\Psi(\vec{r},0) = \sum_n c_n\phi_n(\vec{r}) \tag{70}$$

This looks like a Fourier series. To find the c_n we need to multiply $\Psi(\vec{r},0)$ by $\phi_m^\star$ and then integrate over all space. Then all terms where $n \neq m$ vanish by orthogonality leaving

$$\int \phi_m^\star(\vec{r})\Psi(\vec{r},0)d^3\vec{r} = c_m\int |\phi_m(\vec{r})|^2d^3\vec{r} = c_m \tag{71}$$

if the eigenfunctions are normalised. These coefficients c_n are probability amplitudes with $|c_n|^2$ being the probability of measuring the energy to be E_n.
Eigenfunctions must be orthogonal otherwise quantum mechanical probabilities wouldn't work.

Example:
Consider a particle in an infinite square well (so the particle is confined to

$0 < x < a$) in the ground state

$$\phi(x) = \sqrt{\frac{2}{a}} \sin \frac{\pi x}{a} \tag{72}$$

Suddenly the right wall moves to $2a$. Now $\phi(x)$ is no longer an eigenfunction.

What is the probability of measuring the particle to have an energy corresponding to the first excited state of the new system?

The eigenfunction of the first excited state of the new system is

$$\psi_2 = \sqrt{\frac{1}{a}} \sin \frac{\pi x}{a} \tag{73}$$

Now

$$c_2 = \int \psi_2^\star \phi_1 dx = \frac{\sqrt{2}}{a} \int_0^a \sin^2 \frac{\pi x}{a} dx 0 \frac{1}{\sqrt{2}} \tag{74}$$

So the probability of measuring is

$$|c_2|^2 = \frac{1}{2} \tag{75}$$

Hermitian operators have a further property called completeness. Any well behaved function can be expanded in terms of their eigenfunctions.

Dirac notation:

We can denote states by $|\psi\rangle$ and its hermitian conjugate as $\langle\psi| = |\psi\rangle^\dagger$.

The probability of finding a system that is described by $|\psi\rangle$ in the state $|\chi\rangle$ is given by

$$\langle\chi|\psi\rangle = \int \chi^\star \psi d^3\vec{r} \tag{76}$$

9 (First-order, time independent) Perturbation Theory

If a complicated problem is very similar to a known system we can sometimes approximate the Hamiltonian by the Hamiltonian of the known system plus a small perturbation:

$$\hat{H} = \hat{H}_0 + \hat{H}' = \hat{H}_0 + \lambda \hat{H}_1 \tag{77}$$

where we know the (unperturbed) eigenstates $|\phi_n\rangle$ and eigenvalues $E_n^{(0)}$ of $\hat{H}_0$.
We can use the simple exact eigenfunctions to solve the full problem

$$\hat{H} |\phi_n\rangle = E_n |\phi_n\rangle \tag{78}$$

If λ is small we can call it a perturbation and $E_n \approx E_n^{(0)} + \lambda E_n^{(1)}$ and

$$|\psi_n\rangle \approx |\phi_n\rangle + \lambda \sum_{m \neq n} c_{nm} |\phi_m\rangle \tag{79}$$

Now

$$\hat{H} |\psi_n\rangle = E_n^{(0)} + \lambda \sum_{m \neq n} c_{nm} E_m^{(0)} |\phi_m\rangle + \lambda \hat{H}_1 |\phi_n\rangle \tag{80}$$

And

$$E_n |\psi_n\rangle = (E_n^{(0)} + \lambda E_n^{(1)})(|\phi_n\rangle + \lambda \sum_{m \neq n} c_{nm} |\phi_m\rangle) \tag{81}$$

$$= E_n^{(0)} |\phi_n\rangle + \lambda E_n^{(1)} |\phi_n\rangle + \lambda E_n^{(0)} \sum_{m \neq n} c_{nm} |\phi_m\rangle + \mathcal{O}(\lambda^2) \tag{82}$$

These two things must be equal, so

$$\lambda E_n^{(1)} |\phi_n\rangle + \lambda \sum_{m \neq n} (E_n^0 - E_m^{(0)}) c_{nm} |\phi_m\rangle = \lambda \hat{H}_1 |\phi_n\rangle \tag{83}$$

Multiplying with $\langle \phi_n |$ from the left gives

$$\lambda E_n^{(1)} = \lambda \langle \phi_n | \hat{H}_1 |\phi_n\rangle = \text{ Expectation Value for } \hat{H}' \tag{84}$$

So there is a shift in levels by $\lambda \langle \phi_n | \hat{H}_1 |\phi_n\rangle = \langle \phi_n | \hat{H}' |\phi_n\rangle$.

Example: Quantum dot with tilted bottom

$$V(x) = e\epsilon(x - \frac{a}{2}) \tag{85}$$

for $0 < x < a$ and ∞ elsewhere.
An infinite square well is solved by

$$\phi_n(x) = \sqrt{\frac{2}{a}} \sin\Big(\frac{n\pi x}{a}\Big) \tag{86}$$

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2} \quad n = 1, 2, .. \tag{87}$$

Note that the eigenfunctions are normalised; this is essential!
Our perturbation is

$$\hat{H}' = e\epsilon(x - \frac{a}{2}) \tag{88}$$

Our shift in energy levels is

$$\delta E_n = \langle \phi_n | \, \hat{H}' \, | \phi_n \rangle \tag{89}$$

$$= \frac{2e\epsilon}{a} \int_0^a (x - \frac{a}{2}) \sin^2(\frac{n\pi x}{a}) dx = 0 \tag{90}$$

because $x - \frac{a}{2}$ is odd and $\sin^2$ is even about $x = \frac{a}{2}$ so the product is odd.
So the tilted bottom has no effect in first order! This means that we were justified in ignoring it earlier.

For the eigenfunctions one finds

$$|\psi_n\rangle = \sum_{k \neq n} \frac{\langle \phi_k | \, \hat{H} \, | \phi_n \rangle}{E_n^{(0)} - E_k^{(0)}} \, |\phi_k\rangle \tag{91}$$

This obviously leads to problems for degenerate levels. But in the degenerate case any linear combination of degenerate eigenfunctions is also an eigenfunction. It is always possible to choose some combination that doesn't get mixed by $\hat{H}'$, i.e. $\langle \phi_k | \, \hat{H}' \, | \phi_n \rangle = 0$ if $E_n^{(0)} = E_k^{(0)}$ for $n \neq k$. Then we can calculate δE as above.

10 Quantum Wires and Nanotubes

In this section we want to talk about electrons in long narrow wires where the width of the conductor is small enough to expect quantum behaviour.

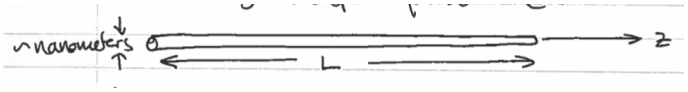


Figure 6: Quantum Wire

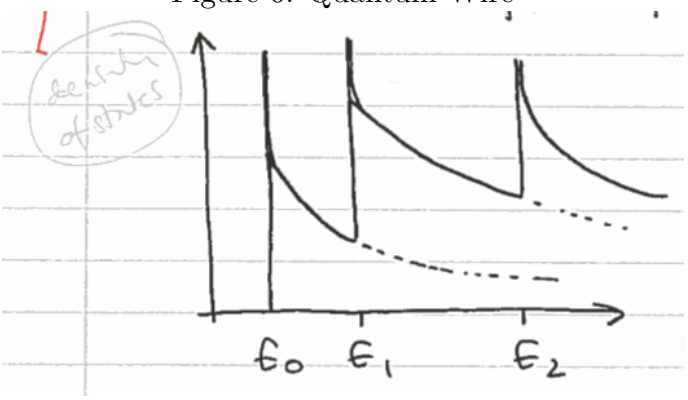


Figure 7: Density of states in a quantum wire

$\hat{H}$ splits into z and $r\phi$ components (because of the structure of the Laplacian in cylindrical coordinates), giving electron energies:

$$E = \frac{\hbar^2 k_z^2}{2m^\star} + E_p \qquad (92)$$

where E_p is the eigenvalue associated with the xy motion.

If the ends are insulating the wavefunction will vanish at $z = 0$ and $z = L$. So it will be sinusoidal and

$$k_z = \frac{n\pi}{L} \quad n = 1, 2, 3... \qquad (93)$$

(It turns out that the choice of boundary conditions doesn't matter if L is very long.)

Plotted against k_z, the states are evenly spaced (always π/L apart). How many states are there in a region k_z and $k_z + \delta k_z$? Factoring in spin

$$2 \times \frac{\delta k_z}{\pi/L} = \frac{2L}{\pi}\delta k_z \qquad (94)$$

Now $\delta k_z \to dk_z$

$$\frac{dn}{dk_z} = \frac{2L}{\pi} \text{ density of states} \qquad (95)$$

Or in terms of energy $k_z = \sqrt{\frac{dm^\star}{\hbar^2}(E - E_p)}$

$$\frac{dk_z}{dE} = \frac{1}{2}(\frac{2m^\star}{\hbar^2})^{1/2}\frac{1}{\sqrt{E - E_p}} \qquad (96)$$

So for electrons in a particular xy state

$$\frac{dn}{dE} = \frac{dn}{dk_z}\frac{dk_z}{dE} = \frac{L}{\pi}(\frac{2m^\star}{\hbar^2})^{1/2}\frac{1}{\sqrt{E - E_p}} \qquad (97)$$

This is the density of states in one dimension. Plotted this looks something like in 7Overall the number of states from different E_m add up. This is very different from a bulk conductor where $\frac{dn}{dE} \propto \sqrt{E}$ and smooth with E.
It turns out that radial excitations are only several eV. This is especially true for thin walled tubes.
The angular TISE is

$$-\frac{\hbar^2}{2m^\star R^2}\frac{d^2\phi}{d\phi^2} = E\phi \tag{98}$$

or

$$\frac{d^2\phi}{d\phi^2} = -p^2\phi \text{ where } p^2 = \frac{2m^\star R^2 E}{\hbar^2} \tag{99}$$

This is solved by

$$\phi = Ae^{ip\phi} \tag{100}$$

with the periodic boundary condition

$$\psi(\phi) = \psi(\phi + 2\pi) \rightarrow p \text{ is an integer} \tag{101}$$

The eigenvalues are

$$E_0 = 0 \tag{102}$$

$$E_1 = \frac{\hbar^2}{2m^\star R^2} \tag{103}$$

$$E_2 = \frac{4\hbar^2}{2m^\star R^2} \tag{104}$$

etc.. These are all doubly degenerate in spin.
We can expect spike in conductance when the potential driving the current is such that the electron energy matches one of these due to the large density of states available to carry the current. This gives an ability to check our understanding. What nanotubes are available to check this?

- Silicon/germanium nanowires: Conducting cylinders with walls that are about one atom thick. These are important as they could improve the capacity of Li-ion batteries by increasing the electrode area.

  $$R \approx 20nm \quad m^\star = 0.2m_e \quad E_1 = \frac{\hbar^2}{2m^\star R^2} \approx 4.75 \times 10^{-4} eV \tag{105}$$

  This is to small to resolve. So they are not helpful in testing our calculations.

- Carbon nanotubes: These occur naturally when wood burns. They are a sheets of graphene rolled up into a tube. But electrons have zero mass in graphene. So they behave relativistic.The limiting velocity is the Fermi velocity $v_F \approx 10^6 m/s$. Their relativistic energy is $E = v_F|\vec{p}|$ (this is similar to $E = cp$ for

photons). Fitting the wavefunction to the boundary conditions give

$$\lambda = \frac{2\pi R}{n} \quad n \text{ is an integer} \tag{106}$$

so $k = \frac{2\pi}{\lambda} = \frac{n}{R}$. So

$$E_n = \frac{\hbar v_F}{R} n \tag{107}$$

So we should expect equally spaced spikes in conductance which can be observed ($E_1 \approx 0.94eV$).

11 Angular Momentum

Quick recap:
Position and momentum are incompatible observables. They can't both be known with infinite precision. Their operators don't commute

$$\hat{p}_x = i\hbar\frac{\partial}{\partial x} \quad \hat{x} = x \tag{108}$$

$$[\hat{p}_x, \hat{x}] = -i\hbar \tag{109}$$

The operator for orbital angular momentum is

$$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}} \tag{110}$$

It turns out that

$$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z \tag{111}$$

the components of the angular momentum do not commute however they do commute with $\hat{\vec{L}}^2$.
It turns out that the eigenfunctions of $\hat{L}^2$ and $\hat{L}$ are spherical harmonics Y_{lm} with eigenvalues $\hbar^2 l(l+1)$ and $m\hbar$ respectively, where $l \geq 0$ and $-l \leq m \leq +l$.
We want to derive these eigenvalues in a neat way. So we are looking for α and β in

$$\hat{L}^2\phi = \alpha\phi \quad \hat{L}_z\phi = \beta\phi \quad \alpha \geq \beta^2 \tag{112}$$

To do that we define two new operators that are called ladder operators:

$$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y \tag{113}$$

We find the commutator relations

$$[\hat{L}_+, \hat{L}_-] = 2\hbar\hat{L}_z \tag{114}$$

$$[\hat{L}_z, \hat{L}_\pm] = \pm\hbar\hat{L}_\pm \tag{115}$$

These ladder operators have the cool property that if ψ is an eigenfunction of $\hat{L}_z$ with eigenvalue β, then $\hat{L}_\pm\psi$ is a new (non normalised) eigenfunction with eigenvalue $\beta \pm \hbar$. So $\hat{L}_\pm$ raise and lower the eigenfunctions up and down the ladder of $\hat{L}_z$ eigenvalues (β) corresponding to the $\hat{L}^2$ eigenvalues (α) in steps of $\hbar$. At the top/bottom of the ladder ϕ_b and ϕ_t

$$\hat{L}_+\phi_t = 0 \quad \hat{L}_-\phi_b = 0 \tag{116}$$

We can use that to derive that $\alpha = \beta_t(\beta_t + \hbar)$ and $\alpha = \beta_b(\beta_b - \hbar)$. So $\beta_b = -\beta_t$. But $\beta_t - \beta_b = n\hbar$. So

$$\beta_t = \frac{1}{2}n\hbar \quad \beta_b = -\frac{1}{2}n\hbar \tag{117}$$

And using $\alpha = \beta_t(\beta_t + \hbar)$ we find

$$\alpha = \hbar^2\frac{n}{2}(\frac{n}{2} + 1) \tag{118}$$

If n is an even integer we can set $\frac{n}{2} = l$ and we have our familiar equations $\alpha = \hbar l(l+1)$ and $-l\hbar \leq \beta \leq l\hbar$. But if n is odd, this implies the possibility of a half integer angular momentum.
So there are two types of angular momentum orbital and intrinsic spin.

12 Intrinsic Spin

$$\hat{S}^2\chi = \hbar^2 s(s+1)\chi \tag{119}$$

$$\hat{S}_z\chi = m_s\hbar \tag{120}$$

Here we want to focus on $s = \frac{1}{2}$, so $m_s = \pm\frac{1}{2}$. No spatial wave functions have the right properties. This forces us into a different mathematical language.
We want to use column vectors to denote the states

$$m_s = +\frac{1}{2} \to \alpha_z = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad m_s = \frac{1}{2} \to \beta_z = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{121}$$

These are examples of spinors. They are orthonormal:

$$\alpha_z^\dagger\alpha_z = \begin{pmatrix} 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = 1 \quad \text{and} \quad \beta_z^\dagger\alpha_z = \begin{pmatrix} 0 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0 \tag{122}$$

A general spinor can be expressed using α_z and β_z.
Now we want to find an explicit form for the spin operators. We now that

$$[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z \tag{123}$$

and

$$[\hat{S}^2, \hat{S}_z] = 0 \tag{124}$$

Let's introduce the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{125}$$

Remember that matrix products are not commutative. It turns out that defining

$$\hat{S}_x = \frac{\hbar}{2}\sigma_1 \quad \hat{S}_y = \frac{\hbar}{2}\sigma_2 \quad \hat{S}_z = \frac{\hbar}{2}\sigma_3 \tag{126}$$

satisfies the commutator relations and gives α_z and β_z as their eigenstates. Also, defining

$$\hat{S}^2 = \frac{3\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{127}$$

works.

13 Magnetic Moments

Circulating charges generate magnetic moments. A classically orbiting charge q around the z axis with a radius of r and a momentum of p has a magnetic moment of

$$\mu = IA = \frac{q}{2m}pr = \frac{q}{2m}L_z \tag{128}$$

In a magnetic field the energy of this system will depend on its orientation.

$$E_{pot} = -\vec{\mu} \cdot \vec{B} \tag{129}$$

i.e. $\vec{\mu}$ prefers to be parallel to the field.
In quantum mechanics we can wirte

$$\hat{\vec{\mu}} = \frac{q}{2m}\hat{\vec{L}} \tag{130}$$

Let's take $\vec{B}$ to be in z direction and consider an electron $q = -e$.

$$\hat{H} = \hat{\vec{\mu}} \cdot \vec{B} = \frac{e}{2m}\hat{\vec{L}} \cdot \vec{B} = +\frac{eB}{2m}\hat{L}_z \tag{131}$$

The eigenenergies are

$$\mu_m = \frac{eB}{2M}m_l = \mu_B B m_l \hbar \quad m_l = -l, ... + l \tag{132}$$

where the Bohr magneton is defined as

$$\mu_B = \frac{e\hbar}{2m_e} \approx 5.8 \times 10^{-5} eV/T \tag{133}$$

The electron also has intrinsic angular momentum (spin) which contributes to the magnetic moment. Assuming that there is an proportionality to the angular mometum we gan write

$$\hat{\mu}_S = -g\frac{e\hat{S}}{2m} \tag{134}$$

For an electron $g \approx 2$. In general

$$\hat{\vec{\mu}} = \hat{\vec{\mu}}_L + \hat{\vec{\mu}}_S \tag{135}$$

But for now we want to assume that $l = 0$. So an electron that's just sitting in a magnetic field has a Hamiltonian

$$\hat{H} = -\hat{\vec{\mu}}_S \cdot \vec{B} = \frac{eg}{2m}\hat{\vec{S}} \cdot \vec{B} = \frac{egB}{2m}m_S\hbar = \pm\frac{g}{2}\mu_B B \tag{136}$$

if the magnetic field is in z direction. This means a (tiny) splitting of the energy eigenvalues.
Let's look at the time evolution of this system. The TDSE is

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi \tag{137}$$

Our $\hat{H}$ is not time dependent so we can separate $\psi = \chi T(t)$, where $T(t) \propto e^{i\omega t}$ and we can use α_z and β_z from last lecture to write down the spin part. The general solution is

$$\psi(t) = a_1 e^{i\omega t}\alpha_z + a_2 e^{i\omega t}\beta_z = \begin{pmatrix} a_1 e^{-i\omega t} \\ a_2 e^{i\omega t} \end{pmatrix} \tag{138}$$

If the system is initially in α_z then $a_1 = 1$ and $a_2 = 0$:

$$\psi(t) = \alpha_z e^{-i\omega t} \tag{139}$$

This is a stationary state with $< S_z >= \frac{\hbar}{2}$ and $< S_x >=< S_y >= 0$.
Let's compare that with an initial state of $\alpha_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$. The time evolution now looks like this:

$$\psi(t) = \frac{1}{\sqrt{2}}\alpha_z e^{-i\omega t} + \frac{1}{\sqrt{2}}\beta_z e^{i\omega t} = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i\omega t} \\ e^{i\omega t} \end{pmatrix} \tag{140}$$

Now the expectation values become more interesting:

$$< \hat{S}_z >= \psi^\dagger \hat{S}_z \psi = \frac{1}{2}\frac{\hbar}{2}\begin{pmatrix} e^{i\omega t} & e^{-i\omega t} \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} e^{-i\omega t} \\ e^{i\omega t} \end{pmatrix} = \frac{\hbar}{4}(1-1) = 0 \tag{141}$$

$$< \hat{S}_x >= \frac{\hbar}{4}\begin{pmatrix} e^{i\omega t} & e^{-i\omega t} \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} e^{-i\omega t} \\ e^{i\omega t} \end{pmatrix} = \frac{\hbar}{2}\cos 2\omega t \tag{142}$$

$$< \hat{S}_y >= \frac{\hbar}{2}\sin 2\omega t \tag{143}$$

So the spin vector is precessing around the z axis. The rate of precession is

$$\omega_p = 2\omega = \frac{g\mu_B B}{\hbar} = \frac{egB}{2m} \tag{144}$$

This is the **Larmor frequency**.
After $\omega_p t = 2\pi$ we are back to where we started. So it takes a 4π rotation to return to the same state.

14 Adding Angular Momentum

In quantum mechanics adding angular momenta is not as easy as just adding vectors together. We want to start by adding the spin of two spin $\frac{1}{2}$ particles. For each particle we can write down ladder operators:

$$\hat{S}_+ = \hat{S}_x + i\hat{S}_y = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \hat{S}_- = \hat{S}_x - i\hat{S}_y = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{145}$$

Let's again use $\alpha = \alpha_z = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\beta = \beta_z = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ to refer to the top and the bottom of the ladder. So

$$\hat{S}_+\alpha = 0 \quad \hat{S}_-\beta = 0 \tag{146}$$

$$\hat{S}_-\alpha = \hbar\beta \quad \hat{S}_+\beta = \hbar\alpha \tag{147}$$

The operator for the total spin of our two particle system is

$$\hat{\vec{S}} = \hat{\vec{S}}^{(1)} + \hat{\vec{S}}^{(2)} \tag{148}$$

There are 4 possible combinations of eigenstates (in z direction):

combination	$\alpha(1)\alpha(2)$	$\alpha(1)\beta(2)$	$\beta(1)\alpha(2)$	$\beta(1)\beta(2)$
$m_1 + m_2$	+1	0	0	-1

We can try to define a ladder operator for the total angular momentum:

$$\hat{S}_\pm = \hat{S}_\pm^{(1)} + \hat{S}_\pm^{(2)} \tag{149}$$

If a system has two types of angular momentum described by operators $\hat{J}_1$ and $\hat{J}_2$ with quantum numbers J_1 and J_2, a total angular momentum operator can be defined as $\hat{J}$.
The eigenvalues of $\hat{J}^2$ are $J(J+1)\hbar^2$ where

$$J = |J_1 - J_2|, |J_1 - J_2| + 1, J_1 + J_2 \tag{150}$$

The eigenvalues of $\hat{J}_z$ are $M_J\hbar$ where

$$M_J = -J, -J+1, ...J \tag{151}$$

So every J value has $2J+1$ substates.
The eigenstates with quantum number J and M are constructed from superpositions of products of those with M_{J1} and M_{J2}. The coefficients of the products in the superposition are called Clebsch-Gordan coefficients. The total number of eigenstates of J and M must be the same as the total number of possible products of M_{J1} and M_{J2}, i.e.

$$\sum_{J=|J_1-J_2|}^{J_1+J_2} = (2J_1+1)(2J_2+1) \tag{152}$$

To construct eigenfunctions, either look up the Clebsch-Gordan coefficients, or start with the product of the eigenfunctions of the maximum J and the maximum M_J and use ladder operators to run down the ladder of associated M_J values. Use orthogonality to consturct the state corresponding to $M_J = M_{J1} + M_{J2} - 1$ and run down a second ladder with the ladder operators. Repeat until finished.

Example: electron with $L = 3$ and $S = \frac{1}{2}$
This forms states with

$$J_1 = 3 - \frac{1}{2}, 3 + \frac{1}{2} = \frac{7}{2}, \frac{5}{2} \tag{153}$$

If we add a second electron with $J_2 = \frac{1}{2}$ the combined system can have

$$J = 2, 3, 4 \tag{154}$$

Notice that there are two ways to make 3.

Always be careful with fermions. The Pauli principle can make some combinations impossible.

Example: Two electrons with $J = \frac{3}{2}$

m_1	m_2	M
$3/2$	$3/2$	X
	$1/2$	2
	$-1/2$	1
	$-3/2$	0
$1/2$	$3/2$	X
	$1/2$	X
	$-1/2$	0
	$-3/2$	-1
$-1/2$	$3/2$	X
	$1/2$	X
	$-1/2$	X
	$-3/2$	-2
$-3/2$	$3/2$	X
	$1/2$	X
	$-1/2$	X
	$-3/2$	X

So the only possible M values are

$$M_{J=2} = \pm 2, \pm 1, 0 \tag{155}$$

$$M_{J=0} = 0 \tag{156}$$

15 Two State Systems

Two state systems are important because they arise in many areas of physics. They are particulary important in a new field called quantum computing to generate qbits.

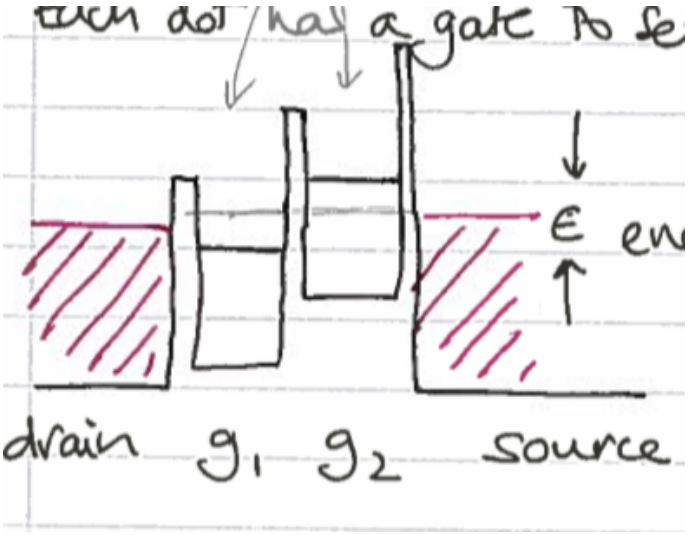


Figure 8: Double quantum dot

Classical bits can either be 0 or 1 (usually represented by voltage levels). A quantum bits can be in a superposition of both.
A random classical bit has a 50% chance of being either 1 or 0 and holds no information. A qbit is a two level system. For example a spin 1/2 particle has the two states $\alpha_z =: 1$ and $\beta_z =: 0$. We can also use this to code information like with classical bits. But unlike classical bits, we could form superpositions of eigenstates eg. $\frac{1}{\sqrt{2}}(|\alpha_z\rangle + |\beta_z\rangle)$. So there is a 50% chance of measuring 1 or 0. But this contains additional information (for which there is no classical analogue) because $\alpha_x = \frac{1}{\sqrt{2}}(\alpha_z + \beta_z)$. More on this later.
Another example for a two state system is linear polarisation of photons. The

$$\begin{pmatrix} E_{0x}e^{i\phi_x} \\ E_{0y}e^{i\phi_y} \end{pmatrix} \tag{157}$$

Linear polarisation along the axes:

$$|H\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |V\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{158}$$

or at 45˙ (diagonal and antidiagonal):

$$|D\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad |A\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{159}$$

Circular polarisation:

$$|R\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} \qquad |L\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} \tag{160}$$

Photons are important for quantum information as they are easily transported without loss of polarisation.
Some systems are approximately two state, if other levels are at high energy and are inaccessible. An example would be a double quantum dot, where we want ϵ to be the difference between V_{g1} and V_{g2} and $V_{g1} > V_{g2}$.

$$|L\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |R\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{161}$$

If we measure the energy relative to the midpoint between states, the Hamiltonian is

$$\hat{H} = \frac{1}{2} \begin{pmatrix} \epsilon & 0 \\ 0 & -\epsilon \end{pmatrix} \tag{162}$$

The eigenvalues are $\pm\frac{\epsilon}{2}$.
There is a complication, which is that states can tunnel between the two. To work with that we define a Hamiltonian

$$\hat{H} = \frac{1}{2} \begin{pmatrix} \epsilon & -\Delta \\ -\Delta & -\epsilon \end{pmatrix} = \frac{1}{2}(\epsilon\sigma_3 - \Delta\sigma_1) \tag{163}$$

where $-\frac{\Delta}{2}$ is called the mixing energy. (Notice the similarities with a spin 1/2 particle in a magnetic field.)
In situations where $\Delta = 0$ we get the same as above. In situations where $\epsilon = 0$

$$\hat{H} = \frac{1}{2} \begin{pmatrix} 0 & -\Delta \\ -\Delta & 0 \end{pmatrix} \tag{164}$$

The eigenvectors are $\chi_{12} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$ with eigenvalues $\pm\frac{\Delta}{2}$.
If you prepare an electron in $|L\rangle$ and adjust $\epsilon = 0$ it evolves via the TDSE

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi = \frac{1}{2} \begin{pmatrix} 0 & -\Delta \\ -\Delta & 0 \end{pmatrix} \psi \tag{165}$$

The general solution is

$$\psi(t) = c_1 e^{\frac{i\delta t}{2\hbar}} \chi_1 + c_2 \chi_2 e^{-\frac{i\delta t}{2\hbar}} \tag{166}$$

16 Manipulating Spins with oscillating fields

The TDSE is

$$i\hbar\frac{d\psi}{dt} = \hat{H}\psi \tag{167}$$

If the Hamiltonian is not a function of time we can use separable solutions

$$\psi = T(t)\chi \quad \text{with} \quad T \propto e^{i\omega t} \quad \omega = \frac{E}{\hbar} \tag{168}$$

An example would be an electron in constant B_0 in z direction. The time evolution would look like this

$$\psi = a_1 e^{i\omega_0 t}\alpha_z + a_2 e^{i\omega_0 t}\beta_z \quad \omega_0 = \frac{eg}{4m}B_0 \tag{169}$$

The motion is a precession of the spin around $\vec{B}_0$ at $2\omega_0$.
When $\hat{H} = \hat{H}(t)$ we can not separate the TDSE and for most problems the problem is no longer analytically solvable. We can however do it for a spin 1/2 particle (with g factor $g = 2$) in a time dependent field.

$$\vec{B} = \begin{pmatrix} B_1\cos\omega t \\ B_1\sin\omega t \\ B_0 \end{pmatrix} \quad \vec{S} = \frac{\hbar}{t}\begin{pmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\end{pmatrix} \tag{170}$$

This can be thought of as a polarised light shining on the electron from z direction ($\omega > 0$ means right handed circular polarisation and $\omega < 0$ means left handed).
Now

$$\hat{H} = -\vec{\mu}\cdot\vec{B} = \frac{eg}{2m}\hat{\vec{S}}\cdot\hat{\vec{B}} \tag{171}$$

$$= \frac{eg\hbar}{4m}[\sigma_1 B_1\cos\omega t + \sigma_2 B_1\sin\omega t + \sigma_3 B_0] \tag{172}$$

$$= \frac{eg\hbar}{4m}\begin{pmatrix} B_0 & B_1(\cos\omega t - i\sin\omega t) \\ B_1(\cos\omega t + i\sin\omega t) & -B_0 \end{pmatrix} \tag{173}$$

$$= \frac{eg\hbar}{4m}\begin{pmatrix} B_0 & B_1 e^{-i\omega t} \\ B_1 e^{i\omega t} & -B_0 \end{pmatrix} \tag{174}$$

The TDSE is

$$i\hbar\frac{d}{dt}\begin{pmatrix}c_1\\c_2\end{pmatrix} = \frac{eg\hbar}{4m}\begin{pmatrix} B_0 & B_1 e^{-i\omega t} \\ B_1 e^{i\omega t} & -B_0 \end{pmatrix}\begin{pmatrix}c_1\\c_2\end{pmatrix} \tag{175}$$

This is solved by

$$\psi = a_1(t)e^{-i\omega_0 t}\alpha_z + a_2(t)e^{i\omega_0 t}\beta_z = \begin{pmatrix} a_1(t)e^{-i\omega_0 t} \\ a_2(t)e^{i\omega_0 t} \end{pmatrix} \tag{176}$$

Substituting this into the TDSE, using $\alpha_z = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\beta_z = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ and tidying everything up gives

$$i\hbar \frac{d}{dt} \begin{pmatrix} a_1(t) \\ a_2(t) \end{pmatrix} = \frac{eg\hbar}{4m} \begin{pmatrix} 0 & B_1 e^{i(2\omega_0 - \omega)t} \\ B_1 e^{-i(2\omega_0 - \omega)t} & 0 \end{pmatrix} \begin{pmatrix} a_1(t) \\ a_2(t) \end{pmatrix} \tag{177}$$

These are two equations for a_1 and a_2. So we can solve this problem now. Notice that we can already see that there could be a resonant effect when $\omega = 2\omega_0$, i.e. when the time varying field rotates around with the Larmor precession of the spin, i.e. from the point of view of the spin it looks like B_1 is a constant field. So it will precess around that. So in the lab frame for $\omega = 2\omega_0$ the spin and B_1 will both process at $2\omega_0$ around z. The spin will additionally precess around B_1 at $2\omega_1$, where $\omega_1 = \frac{eg}{4m}B_1$. This looks like an oscillation of $< \hat{S}_z >$ between $\pm\frac{\hbar}{2}$ at a frequency of $2\omega_1$. But at $+\frac{\hbar}{2}$ the system has a higher energy than $-\frac{\hbar}{2}$ due to the presence of B_0. So the electron absorbs energy from the oscillating field as $< \hat{S}_z >$ increases and radiates it as $< \hat{S}_z >$ decreases. This is called stimulated emission ($\rightarrow$ Rabi Oscillation).
If the electron is in $< \hat{S}_z >= \frac{\hbar}{2}$ the state could be made into a $-\frac{\hbar}{2}$ state by exposure to the right sort of electromagnetic radiation for a set duration.
For complicated solids $g_e \neq 2$ (due to similar effects as $m^\star$). So the absorption/radiation of microwaves acts as a signature. You can measure ω_1 and determine g.
This effect is also the idea behind nuclear magnetic imagery.
For $\omega \neq 2\omega_0$ we need to solve for $a_1(t)$ and $a_2(t)$.

17 Spin Orbit Coupling

We know that the hydrogen atom has energy eigenvalues of $E = \frac{E_R}{(n_r+l+1)^2} = -\frac{E_r}{n^2}$. In a $n = 2$ shell we could either have

$$n_r = 1 \quad l = 0 \quad m_l = 0 \quad m_l = \pm\frac{1}{2} \tag{178}$$

($2s$ can host 2 electrons) or

$$n_r = 0 \quad l = 1 \quad m_l = \pm 1, 0 \quad m_s = \pm\frac{1}{2} \tag{179}$$

($2p$ can host 6 electrons)
These levels are not perfectly degenerate due to fine and hyper fine structure effects. One of these effects is spin-orbit coupling. For the electron the proton is moving and creating a magnetic field

$$\vec{B} = \frac{1}{2}\frac{\mu_0 I\hat{z}}{2r} = \frac{\mu_0 e}{8\pi m r^3}\vec{L} \tag{180}$$

The factor of a half is called the Thomas precession factor. It is needed to account for switching between accelerating frames.
We want to treat this as a perturbation problem. The interaction Hamiltonian is

$$\hat{H}_{SO} = -\hat{\vec{\mu}} \cdot \hat{\vec{B}} = f(r)\hat{\vec{L}} \cdot \hat{\vec{S}} \tag{181}$$

There will be an overall positive sign, because the system is in lower energy when $\vec{S}$ and $\vec{L}$ are antiparallel.
The total angular momentum is

$$\hat{\vec{J}} = \hat{\vec{L}} + \hat{\vec{S}} \quad \rightarrow \quad \hat{J}^2 = \hat{L}^2 + \hat{S}^2 + 2\hat{\vec{L}} \cdot \hat{S} \tag{182}$$

so we can write

$$\hat{\vec{L}} \cdot \hat{\vec{S}} = \frac{1}{2}(\hat{J}^2 - \hat{L}^2 - \hat{S}^2) \tag{183}$$

Using first order perturbation theory

$$\Delta E_j =< \hat{H}_{SO} >= \langle nljm| f(r)\hat{\vec{L}} \cdot \hat{\vec{S}} |nlsjm\rangle \tag{184}$$

$$= \frac{1}{2}\langle nlsjm| f(r)(\hat{J}^2 - \hat{L}^2 - \hat{S}^2) |nlsjm\rangle \tag{185}$$

$$= \frac{\hbar^2}{2}(j(j+1) - l(l+1) - s(s+1)) < f(r) > \tag{186}$$

$$= \epsilon_{nl}(j(j+1) - l(l+1) - s(s+1)) \tag{187}$$

So for our $n = 2$ shell this would have no effect on $2s$ but $2p$ will split up in $2p_{1/2}$ and $2p_{3/2}$. For $2p_{1/2}$ the energy shift will be $\Delta E_{1/2} = -\epsilon_{21}$ and for $2p_{3/2}$ it will be $\Delta E_{3/2} = \frac{\epsilon_{21}}{2}$. This splitting is only a 0.0004% effect.

These ideas can be extended to multi-electron atoms with few valence electrons by starting with a central field approximation. That however is not very good at dealing with electron electron repulsion.

If the e-e correction is bigger than spin-orbit interaction you get what is called **LS coupling**. You can form $\hat{S} = \sum \hat{S}_i$ and $\hat{L} = \sum \hat{L}_i$ separately and couple them to a J. This effect is predominant in low-Z atoms.

If on the other hand the spin-orbit interaction is stronger than the e-e correction **jj coupling** happens. This is more common in high-Z atoms. Here the spin and orbital angular momentum couple for each electron

$$\vec{j_i} = \vec{l_i} + \vec{s_i} \tag{188}$$

and then they all couple to

$$\vec{J} = \sum \vec{j} \tag{189}$$

Atom nuclei have magnetic moments too, which can interact with the electrons magnetic field. This causes changes in atomic levels that are 10^3 times smaller then from fine structure effects $\rightarrow$ **Hyperfine Structure**.

18 Atoms in Magnetic Fields: Zeeman Effect

Let's now stick an LS coupled atom in a weak magnetic field. So the Hamiltonian now can be written as

$$\hat{H} = \hat{H}_{central} + \hat{H}_{SO} + \hat{H}_{mag} \tag{190}$$

where (if B is along the z axis and with $g_S \approx 2$ and $g_L = 1$)

$$\hat{H}_{mag} = \frac{e}{2m}(\hat{\vec{L}} + 2\hat{\vec{S}}) \cdot \vec{B} \tag{191}$$

$$= \frac{eB}{2m}(\hat{L}_z + 2\hat{S}_z) = \frac{eB}{2m}(\hat{J}_z + \hat{S}_z) \tag{192}$$

If $\hat{H}_{mag}$ is small compared to $\hat{H}_{SO}$ we can use perturbation theory

$$\Delta E_{mag} =< \hat{H}_{mag} >= \frac{eB}{2m}[m_j\hbar + < \hat{S}_z >] \tag{193}$$

We need to find $< \hat{S}_z >$. This is very complicated but we can make a few assumptions to make it a bit easier. The uncertainty of $\vec{S}$ around $\vec{J}$ means that only the component of $\vec{S}$ along $\vec{J}$ will be non zero if we take the average. But the uncertainty of $\vec{J}$ around z means that only the z projection of $\vec{S}_J$ will be non zero.
So we decompose $\vec{S}$ into a part that is perpendicular and a part that is parallel to $\vec{J}$. The direction of $\vec{J}$ we will now call $\vec{n} = \frac{\vec{J}}{|\vec{J}|} = \frac{\vec{J}}{\hbar\sqrt{j(j+1)}}$.

$$\vec{S} = (\vec{S} \cdot \vec{n})\vec{n} + \vec{S}_{perpendicular} \tag{194}$$

$$\hat{S} = \frac{\hat{\vec{S}} \cdot \hat{\vec{J}}}{j(j+1)\hbar^2}\hat{\vec{J}} + \hat{\vec{S}}_{perpendicular} \tag{195}$$

Using the scalar product trick

$$\hat{\vec{L}}^2 = (\hat{\vec{J}} - \hat{\vec{S}})^2 \rightarrow \hat{\vec{S}} \cdot \hat{\vec{J}} = \frac{1}{2}(\hat{\vec{J}}^2 + \hat{\vec{S}}^2 - \hat{\vec{L}}^2) \tag{196}$$

we find

$$\hat{\vec{S}} = \frac{\hat{J}^2 + \hat{S}^2 - \hat{L}^2}{2j(j+1)\hbar^2} \cdot \hat{\vec{J}} + \hat{\vec{S}}_{perpendicular} \tag{197}$$

On average $< \hat{S}_{perpendicular} >= 0$ so

$$< \hat{S}_z >= [\frac{< \hat{J}^2 > + < \hat{S}^2 > - < \hat{L}^2 >}{2j(j+1)\hbar^2}] < \hat{J}_z > \tag{198}$$

$$= \frac{\hbar^2(j(j+1) + s(s+1) - l(l+1))}{2j(j+1\hbar^2}m_j\hbar \tag{199}$$

So we can finally use that to find

$$\Delta E_{mag} = \frac{e\hbar}{2m} B m_j (1 + \frac{j(j+1) + s(s+1) - l(l+1)}{j(j+1)}) = g_J \mu_B m_j B \tag{200}$$

for the energy shift. So the m_j degeneracy will be lifted.

> **Example**: 2p levels in hydrogen
> $n = 2$, $l = 1$, $s = \frac{1}{2}$ and therefore $j = \frac{1}{2}, \frac{3}{2}$.
> For $j = 1/2$ turns out to be $g_J = 2/3$ and for $j = 3/2$ $g_J = 4/3$. So this one will split twice as much(, because the moments are adding in parallel).

So we should expect a splitting of the lines in the hydrogen spectrum, which we do find. However we won't see all imaginable transitions. We need to obey the **selection rules for dipole transitions**:

$$\Delta l = 1 \qquad \Delta m = 0, \pm 1 \tag{201}$$

For a strong magnetic field we will need to switch around the order of the perturbation (magnetic then spin orbit). Now

$$\hat{H}_{mag} = \frac{e}{2m} B(\hat{L}_z + 2\hat{S}_z) \tag{202}$$

$$\Delta E_{mag} = \frac{e\hbar}{2m} B(2m_l + 2m_s) \tag{203}$$

This is the **Paschen Back effect**.

At hyperfine level the spin of the nucleus will couple with the $\hat{J}$ f the electrons and this will also cause a splitting in a magnetic field.

19 Entanglement and Identical Particles

Consider a 2-state system, e.g a spin 1/2 particle with the two possible spin eigenstates $\alpha_z \equiv 1$ and $\beta_z \equiv 0$ or a polarised photon with $H \equiv 1$ and $V \equiv 0$ or $L \equiv 1$ and $R \equiv 0$. This can be a qbit. A qbit operation could be achieved by exploiting the Faraday effect (rotates polarisation of light) or by manipulating spin with magnetic fields.

Collapse of a wavefunction

Consider a wavefunction

$$\chi = c_1\alpha_z + c_2\beta_z \tag{204}$$

If we measure (z component of) the spin we can find $\pm\frac{\hbar}{2}$ with probability $|c_1|^2$ and $|c_2|^2$ respectively. If we measure it to be $+\frac{\hbar}{2}$ the wave function collapses to α_z. The original wavefunction χ is lost and with it all information that it encoded.

Entanglement

Two things are said to be entangled if the probabilities of outcomes of measurements on one are changed by measurements of the other.

> **Example**: Entangled system
> Consider pair of spin-1/2 particles with $S = 0$ in the state
>
> $$\psi(1,2) = \frac{1}{\sqrt{2}}[\alpha_z(1)\beta_z(2) - \beta_z(1)\alpha_z(2)] \tag{205}$$
>
> Now we measure the spin (in z direction) of particle 1.
> If the answer is $+\frac{\hbar}{2}$ the wavefunction after the measurement will be $\psi(1,2) = \alpha_z(1)\beta_z(2)$. No a measurement of the spin (in z direction) of electron 2 will always yield $-\frac{\hbar}{2}$
> If the answer is $-\frac{\hbar}{2}$ the wavefunction after the measurement will be $\psi(1,2) = \beta_z(1)\alpha_z(2)$. So now the spin of particle 2 will always be $+\frac{\hbar}{2}$.
> So this system is entangled.

We can also prepare an unentangled pair:

> **Example**: Unentangled system
> Now consider a pair in the state
>
> $$\psi(1,2) = \frac{1}{\sqrt{2}}[\alpha_z(1)\alpha_z(2) + \beta_z(1)\alpha_z(2)] \tag{206}$$

Now whatever we measure for particle 1 a second measurement of the spin of particle 2 will always give $+\frac{\hbar}{2}$.

Let's go back to the entangled pair

$$\psi(1,2) = \frac{1}{\sqrt{2}}[\alpha_z(1)\beta_z(2) - \beta_z(1)\alpha_z(2)] \tag{207}$$

Using $\alpha_z = \frac{1}{\sqrt{2}}(\alpha_x + \beta_x)$ and $\beta_z = \frac{1}{\sqrt{2}}(\alpha_x - \beta_x)$ we can rewrite this as

$$\psi(1,2) = \frac{1}{\sqrt{2}}[\beta_x(1)\alpha_x(2) - \alpha_x(1)\beta_x(2)] \tag{208}$$

The system is still entangled after a change of basis. This will become important in the next lecture.

Identical particles:
Two quantum mechanical particles of the same sort are absolutely identical. (You cannot put labels on electrons.) This means that $\psi(1,2)$ and $\psi(2,1)$ must lead to the same physical properties. We introduce an operator $\hat{P}$ that swaps particles

$$\psi(2,1) = \hat{P}\psi(1,2) \qquad \hat{P}\psi(1,2) = p\psi(1,2) \tag{209}$$

p must ensure that $|\psi(2,1)|^2 = |\psi(1,2)|^2$. This means that $p^2 = 1 \rightarrow p = \pm 1$. Either

- $p = +1$: The wavefunction is symmetric under particle exchange ($\psi(1,2) = \psi(2,1)$). Such particles are called **bosons**. They have integer spin.
- $p = -1$: The wavefunction is antisymmetric under particle exchange ($\psi(1,2) = -\psi(2,1)$. This is the case for **fermions** . They have half integer spin.

This connection between symmetry of the wavefunction and spin is the spin statistics theorem. It is a consequence of relativistic quantum field theory.
If there are two particles in different states ϕ_n and ϕ_m then for a boson pair the wave function would be

$$\psi_{sym}(1,2) = \frac{1}{\sqrt{2}}[\phi_n(1)\phi_m(2) + \phi_m(1)\phi_n(2)] \tag{210}$$

whereas for a fermion pair

$$\psi_{antisym}(1,2) = \frac{1}{\sqrt{2}}[\phi_n(1)\phi_m(2) - \phi_m(1)\phi_n(2)] \tag{211}$$

20 Quantum Key Distribution

Many secure coding protocols use algorithms that require the exchange of a secret key.

Alice and Bob want to exchange information securely. Eve tries to intercept the information. Most security protocols can usually be cracked via brute force algorithms. The security comes from this taking a very, very long time. If we use quantum mechanics to encode information the interception would be a measurement and would therefore change the information. This allows interception to be detected.

There are several Quantum Information protocols for exchanging a key. We will be using a two state system

$$\alpha_z = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \beta_z = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{212}$$

$$\alpha_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \beta_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{213}$$

or more generally, without choosing a basis

$$\alpha_z = \frac{1}{\sqrt{2}}[\alpha_x + \beta_x] \qquad \beta_z = \frac{1}{\sqrt{2}}[\alpha_x - \beta_x] \tag{214}$$

$$\alpha_x = \frac{1}{\sqrt{2}}[\alpha_z + \beta_z] \qquad \beta_x = \frac{1}{\sqrt{2}}[\alpha_z - \beta_z] \tag{215}$$

A and B receive one of a pair of entangled particles in a state, say

$$\psi = \frac{1}{\sqrt{2}}[\alpha_z(1)\alpha_z(2) - \beta_z(1)\beta_z(2)] \tag{216}$$

Each makes a measurement using S_z or S_x. They agree to measure N events and randomly switch between S_x or S_x. Along either axis $\alpha \equiv 1$ and $\beta \equiv 0$ in binary.

If they have their analysers aligned, then if A measures $+\frac{\hbar}{2}$ then B has to get $+\frac{\hbar}{2}$ as well.

If they use a different axis, they don't have to find the same value. So if A measures along z and gets $+\frac{\hbar}{2}$ then B can still get both values along x with equal probability.

Now A and B publicly exchange the knowledge of their sequence of axes (e.g. $S_x, S_z, S_x, S_x ...$) but not the measurements. They discard events where they used different axes. They are now left with about $N/2$ events where they used the same axis. In those events they should have measured the same information which they can use as their key.

Why is this secure?

If E intercepts particles going to B, E needs to pass something onto B, otherwise she will get noticed. The best thing she can do is pass on the information E measures. But E doesn't know along which axis she has to use. So let's assume she randomly switches between x and z. Consider now the $N/2$ key events where A and B have used the same axis. Out of these E will by chance get about $N/4$ right (i.e. used the same axis as B). But the rest of the time she gets it wrong so she won't get the key. A and B can find out, that E messed around with the communication.
e.g. if A and B used S_z in some event and E used S_x. Then E's measurement along x collapses the wavefunction

$$\psi = \frac{1}{\sqrt{2}}[\alpha_z(1)\alpha_z(2) - \beta_z(1)\beta_z(2)] \tag{217}$$

$$= \frac{1}{\sqrt{2}}[\alpha_x(1)\alpha_x(2) + \beta_x(1)\beta_x(2)] \tag{218}$$

into either $\alpha_x(1)\beta_x(2)$ which we can write as

$$\alpha_x(1)\beta_x(2) = \frac{1}{2}[\alpha_z(1) + \beta_z(1)][\alpha_z(2) - \beta_z(2)] \tag{219}$$

$$= \frac{1}{2}(\alpha_z(1)\alpha_z(2) - \beta_z(1)\beta_z(2) + \beta_z(1)\alpha_z(2) - \alpha_z(1)\beta_z(2)) \tag{220}$$

or $\beta_x(1)\alpha_x(2)$ which is the same as

$$\beta_x(1)\alpha_x(2) = \frac{1}{2}[\alpha_z(1) - \beta_z(1)][\alpha_z(2) + \beta_z(2)] \tag{221}$$

$$= \frac{1}{2}(\alpha_z(1)\alpha_z(2) - \beta_z(1)\beta_z(2) - \beta_z(1)\alpha_z(2) + \alpha_z(1)\beta_z(2)) \tag{222}$$

Both times the first two terms describe a scenario where A and B do measure the same result and the last two terms describe one where they do not.
Now A and B won't necessarily get the same information any more. So if E is there, out of the $\approx N/2$ events where A and B should have the same information $\approx N/8$ times they will be different. So by sharing publicly some of the $N/2$ they can be find out if E intercepted.
Practically this is easier with photon polarisation.

21 Quantum Teleportation and Computing

No cloning theorem:

> *It is impossible to transfer the quantum state of a reference system to a target system, without relying on prior knowledge of the reference state without disturbing it in the process.*

Quantum teleportation is the transfer of the known quantum state of a reference system to a target system. This will inevitably change the reference system.
Alice has a known reference state based on a spin 1/2 particle qbit

$$\psi(3) = A\alpha(3) + B\beta(3) \tag{223}$$

In this lecture we will only work along one axis so we can omit the subscript. Alice wants to transfer that state to a target qbit (1) and send it to Bob. To do this Alice will

- make particle (1) part of an entangled pair with qbit (2)

$$\psi(1,2,3) = \frac{1}{\sqrt{2}}[A\alpha(3) + B\beta(3)][\alpha(1)\beta(2) - \beta(1)\alpha(2)] \tag{224}$$

  This is algebraically identical to

$$\psi(1,2,3) = -\frac{1}{2}[A\alpha(1) + B\beta(1)]\psi_1(2,3) + \frac{1}{2}[A\alpha(1) - B\beta(1)]\psi_2(2,3) \tag{225}$$

$$-\frac{1}{2}[A\beta(1) + B\alpha(1)]\psi_3(2,3) - \frac{1}{2}[A\beta(1) - B\alpha(1)]\psi_4(2,3)$$

  where

$$\psi_1(2,3) = \frac{1}{\sqrt{2}}[\alpha(2)\beta(3) - \beta(2)\alpha(3)] \tag{226}$$

$$\psi_2(2,3) = \frac{1}{\sqrt{2}}[\alpha(2)\beta(3) + \beta(2)\alpha(3)] \tag{227}$$

$$\psi_3(2,3) = \frac{1}{\sqrt{2}}[\alpha(2)\alpha(3) - \beta(2)\beta(3)] \tag{228}$$

$$\psi_4(2,3) = \frac{1}{\sqrt{2}}[\alpha(2)\alpha(3) + \beta(2)\beta(3)] \tag{229}$$

  are Bell's states. They are the maximally entangled spin 1/2 particles.

- Alice sends qbit (1) to Bob
- Alice then makes a measurement on qbits (2) and (3) to find out which Bell state they are in. So $\psi(1,2,3)$ will collapse into the appropriate term.

- Alice phones Bob and tells him the result of her measurement.

If Alice's measurement was in Bell state 1:

$$\psi(1,2,3) \to [A\alpha(1) + B\beta(1)]\psi_1(2,3) \tag{230}$$

So now (1) is in the same state as (3) was initially. Note that we had to destroy the initial state to achieve this.
If the answer was one of the other Bell states, e.g. $\psi_2(2,3)$

$$\psi(1,2,3) \to [A\alpha(1) - B\beta(1)]\psi_2(2,3) \tag{231}$$

then Alice tells Bob that he has to turn on a magnetic field for a certain amount of time. Exploiting Lamor precession Bob can turn the system into the desired one.

A classical computer (CC here for short) turns classical bits into other classical bits using a set of rules to manipulate bits. A quantum computer (QC) evolves (often entangled) qbits by the TDSE (unitary evolution). A read out happens via a measurement of the qbits. In principle all CC operations can be realised in a QC. For example

NOT	input	output
	0	1
	1	0

a NOT gate could be implemented using

$$0 \equiv \alpha_z \qquad 1 \equiv \beta_z \tag{232}$$

by applying a filed in y direction for $\omega t = \frac{\pi}{2}$. On a more complicated state we can do two basic operations in only one physical operation, e.g.

$$A\alpha_z + B\beta_z \to A\beta_z - B\alpha_z \tag{233}$$

One qbit in a general state has 2 terms. A general state for two entangled qbits looks like this

$$a_1\alpha(1)\alpha(2) + a_2\alpha(1)\beta(2) + a_3\beta(1)\alpha(2) + a_4\beta(1)\beta(2) \tag{234}$$

So we can do 4 operations in one physical operation. N entangled pairs 2^N computer operations in one physical step. So for computing problems that scale rapidly in size QC have a big advantage. The measurement limits the amount of output.

22 Recommended Literature

- AIM Rae, Quantum Mechanics, Chapman-Hall
- Gasiorowicz, Quantum Physics, Wiley
- Phillips, Introduction to QM, Wiley