Quantum Mechanics

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15th December 2006

1 Introduction

Lecturer is Jon Billowes. All of his slides are on www.man.ac.uk/dalton/phys30101 Motivation to spot mistakes, he hands out Guest list places for Rock Kitchen. Again see Blue book for syllabus.

After talking through his hand out we now get going.

2 Review of QM

A wave-function contains all possible information about a state or system. ψ is single-valued, continuous and differentiable. $|\psi(x,\ t)|^2 dx$ gives the probability of finding the particle between x and dx, if the wave-function is normalised. Normalised is when $\int_{-\infty}^{+\infty} |\psi(x,\ t)|^2 dx = \int_{-\infty}^{+\infty} |\psi(\underline{r},\ t)|^2 = 1$, same for more dimensions.

Time-dependent Schrödinger Eqn. Gives the time evolution of the wave-function for particles in a potential V

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(x,\ t) = i\hbar\frac{\partial \Psi}{\partial t}$$

Time-independent Schrödinger Eqn. If V(x) is not a function of time and energy is constant we apply separation of variables. Use $\Psi(x,\ t) = U(x)T(t)$, substitute into TDSE and divide by Ψ.

$$-\frac{\hbar^2}{2m}\frac{1}{U}\frac{\partial^2 U}{\partial x^2} + V(x) = i\hbar\frac{1}{T}\frac{\partial T}{\partial t} = E$$

Both sides can either be equal to a constant or zero. This gives the well know solution for RHS $T = const \times \exp(-\frac{iEt}{\hbar}) = const \times \exp(-i\omega t)$. This leaves the LHS as the TISE

$$-\frac{\hbar^2}{2m}\frac{\partial^2 U}{\partial x^2} + V(x)U = EU$$

or written with operators $\hat{H}U = EU$, where $\hat{H}$ is the Hamiltonian operator. This gives the stationary states of the system.

If $V(x) = 0$ solutions for U are $U = const \times \exp(ikx)$ where $E = \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m}$. The full solution is the product of $U(x)$ and $T(t)$

$$\Psi(x,\ t) = const \times \exp(i(kx - \omega t))$$

Insert picture of finite square well(with outside at potential V=V_0, energy of particle $E < V_0$, well centered on origin, left of well region I, inside well region II, right of well region III.

2.1 The infinite square well

Insert picture of a square well(from -a to +a, V=0 inside). In the forbidden region the wave-function is zero $U_I(x) = 0$ and in the inside of the well $U_{II}(x)$ must satisfy $-\frac{\hbar^2}{2m}\frac{d^2U_{II}}{dx^2} = EU_{II}$. Solutions are of the form

$$U_{II}(x) = A\cos(kx) + B\sin(kx) \tag{1}$$

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

The boundary conditions are $U_{II}(x = +a, -a) = 0 = U_I(x = -a, +a)$. Substituting boundary conditions into Eqn. 1 gives

$$A\cos(ka) + B\sin(ka) = 0 \tag{2}$$

$$A\cos(ka) - B\sin(ka) = 0 \tag{3}$$

There are two types of solution, either Eqn. 2 + Eqn. 3 (implies $B = 0$)

$$2A\cos(ka) = 0 \; with \; A = 0 \; or \; ka = \frac{n\pi}{2} \; with \; n = 1, 3, 5, ...$$

or Eqn. 2- Eqn. 3(implies $A = 0$).

$$2B\sin(ka) = 0 \; with \; B = 0 \; or \; ka = \frac{n\pi}{2} \; with \; n = 2, 4, 6, ...$$

From this we get $E = \frac{\hbar^2 n^2 \pi^2}{8ma^2}$. Make sure to look at his pictures in notes for lecture 2. They show sketches of wave-functions for infinite square well.

2.2 Finite square-well – 1-D

Again look at his notes for sketches of the wave functions.

Boundary conditions In region II, $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}U_{II} = EU_{II}$ with $U_{II} = A\cos(kx) + B\sin(kx)$, as for infinite well($k^2 = \frac{2mE}{\hbar^2}$). In region I $\frac{\hbar^2}{2m}\frac{d^2}{dx^2}U_I = (V_0 - E)U_I$, with solutions $U_I = C\exp(+\mu x) + D\exp(-\mu x)$ with

$$\mu^2 = \frac{2m(V_0 - E)}{\hbar^2} \tag{4}$$

but as U_I must remain finite for $x \to -\infty \Rightarrow D = 0$. Similarly for region III, but this time $C = 0$.

Additional boundary conditions are that $U(x)$ is continuous at $x = +a, -a$ and $\frac{dU}{dx}$ is also continuous at $x = +a, -a$. So at boundary $x = a$.

$$A\cos(ka) + B\sin(ka) = D\exp(-\mu a) \tag{5}$$

$$-Ak\sin(ka) + Bk\cos(ka) = -D\mu\exp(-\mu a) \tag{6}$$

At boundary $x = -a$

$$A\cos(ka) - B\sin(ka) = C\exp(-\mu a) \tag{7}$$

$$-Ak\sin(ka) + Bk\cos(ka) = -C\mu\exp(-\mu a) \tag{8}$$

Both times this shows first how $U(x)$ is continuous and then how $\frac{dU}{dx}$ is continuous.

To find solutions we first subtract Eqn 8 from Eqn 6 then divide by Eqn 5 added to Eqn 7, this gives as solution $\tan(ka) = \frac{\mu}{k}$ or $D = -C$ and $A = 0$.

Similarly another set of solutions is found from Eqn (8+6)/(5-7). This gives $\cot(ka) = \frac{-\mu}{k}$.

Consider first solution Solve this graphical and remember(see equation. 4 and 2) that

$$\mu^2 = \frac{2m(V_0 - E)}{\hbar^2} = \frac{2mV_0}{\hbar^2} - k^2 = \frac{1}{a^2}[\frac{2mV_0a^2}{\hbar^2} - k^2a^2]$$

define $\lambda = \frac{2mV_0a^2}{\hbar^2}$. Thus $\frac{\mu}{k} = \frac{\sqrt{\lambda - k^2a^2}}{ka}$. These functions are plotted in his notes of lecture 2. λ tells you how many solutions there are for your given square well, the bigger λ the more solutions. When λ is small there is at least one bound state. This is not always true once we get to 3D.

2.3 Finite square well in 3D

This is problem 3.5 in Rae.See figure 2-10–1 for a plot of well. This means we have to solve

$$[-\frac{\hbar^2}{2m}\nabla^2 + V]U = EU \tag{9}$$

We assume a spherically-symmetric wavefunction(independent of θ, ϕ), so no angular momentum. We will try solutions of form $U = \frac{1}{r}\phi(r)$, then $\nabla^2 u \rightarrow \frac{1}{r}\frac{\partial^2\phi}{\partial r^2}$ so equation 9 becomes

$$-\frac{\hbar^2}{2m}\frac{\partial^2\phi}{\partial r^2} + V\phi = E\phi$$

for region I, where $V = 0$ solutions are $\phi_I = A\cos(kr) + B\sin(kr)$ with $k^2 = \frac{2mE}{\hbar^2}$. In region II, where$V = V_0$ solutions are $\phi_{II} = C\exp(-\mu r) + D\exp(\mu r)$ with $\mu^2 = \frac{(V_0-E)2m}{\hbar^2}$. As we require $U_{II} = \frac{\phi_{II}}{r}$ to be finite as $r \rightarrow \infty$ we need $D = 0$. Similarly we need $U_I = \frac{\phi_I}{r}$ to be finite as $r \rightarrow 0$ so we need $A = 0$. Our solutions are then

$$U_I = \frac{B\sin(kr)}{r}\ U_{II} = \frac{C\exp(-\mu r)}{r}$$

The wavefunction has to be continuous at $r = a$ so $U_I(a) = U_{II}(a)$, also need the derivative to be continuous $\frac{dU_i(a)}{dr} = \frac{dU_{II}(a)}{dr}$. This gives $\cot(ka) = -\frac{\mu}{k} = -\sqrt{\frac{2mV_0}{\hbar^2k^2} - 1}$. See fig 2-10–2 for a plot. If $k^2a^2 = \frac{2mV_0a^2}{\hbar^2} < (\frac{\pi}{2})^2$ there are no bound states. From this it follows that $V_0 > \frac{\pi^2\hbar^2}{8ma^2}$.

Examples Consider deuteron, a neutron plus a proton. This has a binding energy of 2.23MeV.See figure 2-10–3 for a plot of the well. The neutron-neutron system is just unbound by 0.06MeV, this is also true for the proton-proton system. A ${}^{9}Li$ "well" binding a neutron pair is only just bound. Look at lecture notes form lecture 3/week 2.

2.4 Tunneling

Draw a graph of "tunneling" potential, fig 2-10–4. We will consider a flux of particles of momentum $\hbar k$, energy $E = \frac{\hbar^2 k^2}{2m}$, approaching a barrier, height $V_0 > E$ and width a.

$$U_I = A\exp(ikx) + B\exp(-ikx)$$
$$0 < x < a \; U_{II} = C\exp(\mu x) + D\exp(-\mu x)$$
$$x > a \; U_{III} = F\exp(ikx)$$

Boundary conditions U and $\frac{du}{dx}$ are continuous at $x = 0$ and $x = a$.
Consider $x = 0$ first:

$$U_I(0) = U_{II}(0) \Rightarrow A + B = C + D \tag{10}$$

$$U_I' = U_{II}' \Rightarrow A - B = \frac{\mu}{ik}(C - D) \tag{11}$$

and at $x = a$:

$$U_{II}(a) = U_{III}(a) \Rightarrow Ce^{\mu a} + De^{-\mu a} = F\exp(ika) \tag{12}$$

$$U_{II}' = U_{III}' \Rightarrow Ce^{\mu a} - De^{-\mu a} = \frac{ik}{\mu}F\exp(ika) \tag{13}$$

Equations 10 + 11 give

$$2A = (1 + \frac{\mu}{ik})C + (1 - \frac{\mu}{ik})D \tag{14}$$

Equations 12 + 13 give

$$2Ce^{\mu a} = (1 + \frac{ik}{\mu})F\exp(ika) \tag{15}$$

Equations 12 - 13 give

$$2De^{-\mu a} = (1 - \frac{ik}{\mu})F\exp(ika) \tag{16}$$

.Substitution from equation 15 and 16 into equation 14 allows F to be related to A, this gives an equation of the form

$$\frac{F}{A} = \frac{4i\mu k}{(2i\mu k + \mu^2 - k^2)\exp(-\mu a) + (2i\mu k - \mu^2 + k^2)\exp(\mu a)}\exp(-ika) \tag{17}$$

If the tunneling probability is small, we can ignore the term in $\exp(-\mu a)$ in Equation 17, then equation 17 becomes

$$\frac{|F|^2}{|A|^2} = \frac{16\mu^2 k^2}{(\mu^2 + k^2)^2}\exp(-2\mu a) = \frac{16E(V_0 - E)}{V_0^2}\exp(-2\mu a)$$

this is the "tunneling probability". The tunneling probability is largely dominated by the exponential decay within barrier $\exp(-const \times width \times height)$.

2.5 The postulates of quantum mechanics

Postulate 1 We have a wavefunction $\Psi = \Psi(parameters\ of\ system,\ time)$. Parameters are for example: particle co-ords, "internal" variables like spin and such. Ψ is the general solution to TDSE, U, U_n time independent part of Ψ and ψ is the general wavefunction whose time-dependence is not being considered. ϕ, ϕ_n eigenfunctions of an operator(not necessarily energy operator).

Postulate 2 "Dynamical variable" is a measurable quantity such as momentum, position etc. Operators $\hat{H} = \frac{p^2}{2m} + V = -\frac{\hbar^2}{2m}\nabla^2 + V$.

Hermitian operator is defined as: If $f(\underline{r})$ and $g(\underline{r})$are functions of $\underline{r}$ which vanish at infinity, then $\hat{Q}$ is Hermitian if and only if

$$\int_{all\ space} f\hat{Q}g d\tau = \int_{all\ space} g\hat{Q}^* f d\tau \tag{18}$$

Consider the operator $\hat{p}_x = -i\hbar\frac{\partial}{\partial s}$, show this is Hermitian. LHS of Eqn 18 is

$$-i\hbar\int_{-\infty}^{+\infty} f\frac{\partial g}{\partial x}dx = -i\hbar[[fg]_{-\infty}^{+\infty} - \int g\frac{\partial f}{\partial x}dx]$$

yada yada yada yada, it turns out to be just the RHS of Eqn 18.

Eigenvalues of Hermitian operators are real This is a necessary feature if they are physically measurable quantities. To show let $\hat{Q}\phi_n = q_n\phi_n$ then $Q^*\phi_n^* = q_n^*\phi_n^*$ is the complex conjugate. Then $\int \phi_n^*\hat{Q}\phi_n d\tau = q_n\int \phi_n^*\phi_n d\tau = q_n\int |\phi_n|^2 d\tau$ and so $\int \phi_n\hat{Q}^*\phi_n^* d\tau = q_n^*\int |\phi_n|^2 d\tau$. These two equations are equal by definition 18. From this it follows that the eigenvalues are always real. Two important properties of eigenfunctions of Hermitian operators

1. Orthonormality, expressed by $\int \phi_n^*\phi_m d\tau = \delta_{nm}$. there are cases for which our eigenfunctions have degenerate eigenvalues which will give $q_m = q_n\ for\ m \neq n$.

2. Completeness, any well behaved function ψ can be expressed as a linear combination of the eigenfunctions ϕ_n, which are said to form a complete set. Mathematically

$$\psi = \sum_{n=1}^{\infty} a_n\phi_n$$

to determine the co-efficients we consider the overlap between any eigenfunction ϕ_m and the general wave function ψ.

$$\int \phi_m^*\psi d\tau = \int\sum_n a_n\phi_m^*\phi_n d\tau = \sum a_n\delta_{nm} = a_m = \int \phi^*\psi d\tau$$

Postulate 3 If the eigenfunction is to represent the wavefunction of a particle at $x = x_0$ immediately after a position measurement , then $|\phi|^2$ at $x = x_0$ must be large and zero elsewhere with the normalization $\int |\phi|^2 dx = 1$. The eigenfunction thus has the form of the Dirac delta function $\phi(x) = \delta(x - x_0)$. Then $\hat{X}\delta(x - x_0) = x_0\delta(x - x_0)$. This is satisfied by $\hat{X} = x$. Trying to explain why $\hat{X} = x$.

Postulate 4 Consider the normalization of $\psi = \sum a_n \phi_n$.

$$\int |\psi|^2 d\tau = \int (a_1^* \phi_1^* + a_2^* \phi_2^* + ...)(a_1 \phi_1 + a_2 \phi_2 + ...) d\tau = \sum a_n^* a_n \int \phi_n^* \phi_n d\tau$$

All cross terms are equal to zero. This gives

$$\sum |a_n|^2 = 1$$

where $|a_n|^2$ is the probability of finding ψ in a state ϕ_n. Quantum mechanics exactly predicts the average values returned in many measurements of a dynamical variable of the same wave function ψ. Expectation value of operator $\hat{Q}$ given by $< \hat{Q} >= \sum |a_n|^2 q_n$. Consider

$$\int \psi \hat{Q} \psi d\tau = \int (\sum_m a_m^* \phi_m^*)(\sum_n a_n q_n \phi_n) d\tau = \sum_{n,m} q_n \int a_m^* a_n \phi_m^* \phi_n d\tau$$

which is zero unless $n = m$(when $\phi_m^* \phi_n = 1$) so

$$= \sum_n |a_n|^2 q_n =< \hat{Q} >$$

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Continuous eigenvalues So far we have consider discrete eigenvalues but some dynamic variables have a continuous range of eigenvalues(momentum, position). We write the general eigenvalue equation as $\hat{Q}\phi(k,\ x) = q(k)\phi(k,\ x)$, where the index n has been replaced by a continuous variable, k. We now have

$$\psi(x) = \int a(k)\phi(k,\ x) dk$$

where $|a(k)|^2 dk$ is the probability of a result in the range between k and $k + dk$. The amplitudes $a(k)$ are given by

$$a(k) = \int \phi^*(k,\ x)\psi(x) dx$$

Example with momentum eigenfunctions $\phi(k,\ x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$, so a general wavefunction looks like $\psi = \frac{1}{\sqrt{2\pi}} \int a(k) e^{ikx} dk$, this looks like a Fourier transform, so $a(k)$ given by $a(k) = \frac{1}{\sqrt{2pi}} \int \psi e^{-ikx} dx$, which is just a inverse Fourier transform. The inverse transform is the wavefunction in k-space(momentum space).

2.6 Commutation Relations

The order of QM operators is important because we can get different results if we change the order of operations. Consider sequential operations on ψ,

$$\begin{aligned}
(\hat{p}_x \hat{x} - \hat{x} \hat{p}_x)\psi &\equiv [\hat{p}_x,\ \hat{x}]\,\psi \\
. &= -i\hbar \frac{\partial}{\partial x}\psi - \left(-x i\hbar \frac{\partial}{\partial x}\psi\right) \\
. &= -i\hbar\psi - i\hbar x \frac{\partial \psi}{\partial x} + i\hbar x \frac{\partial \psi}{\partial x} \\
. &= -i\hbar\psi \neq 0
\end{aligned}$$

This is independent of the form of ψ and so we write $[\hat{p}_x,\ \hat{x}] = -i\hbar$. Obviously we could show $[\hat{p}_y,\ \hat{y}] = [\hat{p}_z, \hat{z}]$and $-[\hat{p}_x,\ \hat{x}] = [\hat{x},\ \hat{p}_x]$.

Compatibility If $\left[\hat{Q},\ \hat{R}\right] = 0$ the physical observables they represent are said to be compatible. The operators $\hat{Q}, \hat{R}$ have a common set of eigenfunctions. Thus a measurement of $\hat{Q}$ on ψwill collapse the state into a common eigenfunction ϕ_n. A subsequent measurement of other quantity represented by $\hat{R}$ will have an exactly predictable result. Operators of compatible observables commute, if $\psi = \sum a_n\phi_n$ then

$$\begin{aligned}
\left[\hat{Q},\ \hat{R}\right]\psi &= \sum_n a_n\left(\hat{Q}\hat{R}\phi_n - \hat{R}\hat{Q}\phi_n\right) \\
&= \sum_n a_n\left(\hat{Q}r_n\phi_n - \hat{R}q_n\phi_n\right) \\
&= \sum_n a_n\left(q_n r_n\phi_n - r_n q_n\phi_n\right) = 0
\end{aligned}$$

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The Uncertainty Principle If two operators, $\hat{Q}, \hat{R}$ do not commute there is a fundamental limit of the products of the r.m.s deviations associated with a measurement of q and r. If $\Delta q, \Delta r$ are the RMS deviations of any particular set of measurements then $\Delta q\Delta r \geq \frac{1}{2}\left|< i\left[\hat{Q}, \hat{R}\right] >\right|$. It does not mean

1. A measurement of p_x affects the subsequent measurement of x. (The first measurement of ψ collapses ψ into a momentum eigenstate, so we can not even make the x measurement on ψ.

2. If two operators commute, $\left[\hat{Q}, \hat{R}\right] = 0$ then the product of their uncertainties must be zero. Consider a measurement of x and y for a hydrogen atom. Both have uncertainties, however if ψ is already in one of the common eigenfunctions then both observables are exactly determined.

Look at handout about *Uncertainty principle*. We now look at an example of the uncertainty principle, for a sketch of the setup see his lecture notes on the Internet. Basically it is particles with $p = \hbar k$ going through a slit(width a) and then hitting a screen. The x direction is along plane of slit and z is towards screen. For a screen at $z \approx 0$ we would not get a very interesting distribution, everything would be between $\pm\frac{a}{2}$, standard deviation on x given by $\Delta x \approx \pm\frac{a}{3}$.

In order to measure the transverse momentum we would move the screen further away. We will now get a single slit interference pattern. Where the first minimum will occur at $\sin\theta = \frac{\lambda}{a}$. Most particles are in central maximum, we have $p_x = P\sin\theta$ (P incoming momentum), so error $\Delta p_x = \pm\hbar k\frac{\lambda}{a} = \pm\hbar\frac{k2\pi}{ka}$. The error on both x and p_x is then $\Delta x\Delta p_x = \frac{a}{3}\frac{h}{a} = \frac{h}{3} \geq \frac{\hbar}{2}$.

2.7 Time-dependence of Ψ

Postulate 5 The development of the wavefunction between measurements is governed by the time Dependant Schrödinger equation. We will consider case where $\hat{H}$ is time-independent(i.e. energy is conserved). Expand Ψ in eigenfunctions of $\hat{H}$

$$\Psi\left(\vec{r},\ t\right)=\sum_{n}a_{n}\left(t\right)u_{n}\left(\vec{r}\right)$$

all time dependence is in the amplitudes a_n so eigenfunctions of $\hat{H}$ must be time-independent.Substitute into TDSE, 25.10.2006

$$\begin{aligned} i\hbar\sum_{n}\frac{\partial a_{n}}{\partial t}u_{n} &= \hat{H}\sum_{n}a_{n}u_{n}=\sum a_{n}E_{n}u_{n} \\ \Rightarrow 0 &= \sum\left(i\hbar\frac{da_{n}}{dt}-a_{n}E_{n}\right)u_{n} \end{aligned}$$

last line must be true for all points in space, so each coefficient must separately be zero

$$\begin{aligned} \frac{da_{n}}{a_{n}} &= \frac{E_{n}}{i\hbar}dt \\ \Rightarrow a_{n}(t) &= a_{n}(t=0)\exp\left(\frac{iE_{n}t}{\hbar}\right) \end{aligned}$$

the amplitudes oscillate independently with frequency $\omega_n=\frac{E_n}{\hbar}$. This gives as the general solution to the TDSE

$$\Psi\left(\vec{r},\ t\right)=\sum_{n}a\left(t=0\right)u_{n}\left(\vec{r}\right)e^{-i\omega_{n}t}$$

Consider energy measurement at time t=0, the answer must be one of the eigenvalues of $\hat{H}$. If E_m is measured then $a_m\left(t=0\right)=1$, $a_n\left(t=0\right)=0,\ n\neq m$. States collapse in u_m and TDSE will now be $\Psi\left(\vec{r},\ t\right)=u_m\exp\left(-\frac{iE_mt}{\hbar}\right)$ where the time dependent value is like a phase factor which allows time evolution of Ψ. Subsequent measurement of energy will again give result E_m, as expected.

2.8 Quantum beats

Consider an initial state which is a linear combination of ϕ_q and ϕ_2, where ϕ_1& ϕ_2 are real, e.g. particle in a box. The difference of the two energy levels is $\Delta E=E_2-E_1=\hbar\omega$. The general wavefunction of this is given by

$$\begin{aligned} \Psi\left(\vec{r},\ t\right) &= \phi_{1}\exp\left(-\frac{iE_{1}t}{\hbar}\right)+\phi_{2}\exp\left(-\frac{iE_{2}t}{\hbar}\right) \\ &= \exp\left(-\frac{iE_{2}t}{\hbar}\right)\left[\phi_{1}e^{i\omega t}+\phi_{2}\right] \end{aligned}$$

the probability distribution is then just

$$\begin{aligned} \psi\psi^{*} &= \left(\phi_{1}^{*}e^{-i\omega t}+\phi_{2}^{*}\right)\left(\phi_{1}e^{i\omega t}+\phi_{2}\right) \\ &= \left|\phi_{1}\right|^{2}+\left|\phi_{2}\right|^{2}+\phi_{1}^{*}\phi_{2}e^{-i\omega t}+\phi_{2}^{*}\phi_{1}e^{i\omega t} \\ \left|\psi\right|^{2} &= \phi_{1}^{2}+\phi_{2}^{2}+2\phi_{1}\phi_{2}\cos\omega t \end{aligned}$$

The interference between the two phase factors creates a time-dependence of the probability distribution that has the appearance of motion. Important example is precession of spin in a magnetic field.

See Rae p160 for an example of this

2.9 Degeneracy

Same eigenvalues for two or more eigenfunctions. We assumed in proof of orthonormality that if $\hat{Q}\phi_n = q_n\phi_n$then ,$q_n \neq q_m$ for all $n \neq m$, this was also assumed in discussion of compatibility, but now if $q_n = q_m$ a measurement of q_n would not tell us which eigenfunction the state had collapsed into.

Orthonormality It is always possible to construct a set of orthonormal eigenfunctions from a set of non-orthonormal eigenfunctions. Consider

$$\begin{aligned} \hat{Q}\phi_1 &= q\phi_1 \\ \hat{Q}\phi_2 &= q\phi_2 \end{aligned}$$

Any linear combination is also an eigenfunction, $\hat{Q}\left(\alpha\phi_1 + \beta\phi_2\right) = q\left(\alpha\phi_1 + \beta\phi_2\right)$ and then construct $\phi_2' = S_{12}\phi_1 - \phi_2$ where $S_{12} = \int \phi_1^*\phi_2 d\tau$ then

$$\int \phi_1^*\phi_2' d\tau = S_{12}\int \phi_1^*\phi_1 d\tau - \int \phi_1^*\phi_2 d\tau = S_{12} - S_{12} = 0$$

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Compatibility If $\left[\hat{Q},\ \hat{R}\right] = 0$ then a common set of eigenfunctions exist. If there is a degeneracy $\hat{Q}\phi_1 = q\phi_1,\ \hat{Q}\phi_2 = q\phi_2$ then any combination $\phi' = \alpha\phi_1 + \beta\phi_2$ is also an eigenfunction of $\hat{Q}$, but not necessarily of $\hat{R}$:

$$\begin{aligned} \hat{R}\phi' &= \left(\alpha r_1\phi_1 + \beta r_2\phi_2\right) \\ &\neq const\left(\alpha\phi_1 + \beta\phi_2\right) \end{aligned}$$

never the less a set of eigenfunctions can be found that are common to both operators.

Measurement of $\hat{Q}$ on ψwill collapse to ϕ_n and measure the result q_n, but ϕ_n may not be eigenfunction of $\hat{R}$.

Measurement with $\hat{R}$ on ϕ_n will collapse into one of the common eigenfunctions leaving q_n unchanged and giving result r_n.

Subsequent measurement of $\hat{Q},\ \hat{R}$ always return $q_n,\ r_n$. As an example of this consider the $n = 2$ energy levels of hydrogen atom. This has two possible values for l(angular momentum), remember m_l. We use

$$\begin{aligned} \hat{Q} &= \hat{l}^2 \\ \hat{R} &= \hat{l}_z \end{aligned}$$

when we measure with $\hat{l}^2 = l\left(l+1\right)\hbar^2$ we can get two answers, $\left\{2\hbar^2,\ 0\right\}$. If we get non zero answer the atom can be in three different states(different values of m_l). We now measure $\hat{l}_z = m\hbar$, this can give three answers, $\{+1,\ 0,\ -1\}$.

We now know which state the atom is in and further measurements of $\hat{l}^2$ or $\hat{l}_z$ give exactly predictable results.

Gives summary of course so far, which is on the web as pdf

3 Angular momentum

One of them most important aspects of QM with implications in particle, nuclear, atom, etc physics. Angular momentum is always quantised because of periodic boundary conditions. Remind yourself that $\hat{L} = \hat{R} \times \hat{P}$ and $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$. One might wonder how these two operators commute, is there a set of common eigenfunctions? What happens for $\left[\hat{L}_x,\ \hat{L}_y\right]$etc. This is rather tedious algebra, look it up in any introductory book. The result is $\left[\hat{L}_x,\ \hat{L}_y\right] = i\hbar\hat{L}_z$. We can cyclically swap the subscripts to get similar results for other combinations of $x,\ y,\ z$. Now try 8.11.2006

$$\begin{aligned}
\left[\hat{L}^2, \hat{L}_x\right] &= \left[\hat{L}_x^2, \hat{L}_x\right] + \left[\hat{L}_y, \hat{L}_x\right] + \left[\hat{L}_z, \hat{L}_x\right] \\
\left[\hat{L}_y^2, \hat{L}_x\right] &= \hat{L}_y^2\hat{L}_x - \hat{L}_x\hat{L}_y^2 \\
&= \hat{L}_y\left(\hat{L}_x\hat{L}_y - i\hbar\hat{L}_z\right) - \left(i\hbar\hat{L}_z + \hat{L}_y\hat{L}_x\right)\hat{L}_y \\
&= -i\hbar\left(\hat{L}_y\hat{L}_z + \hat{L}_z\hat{L}_y\right)
\end{aligned}$$

similarly we can obtain $\left[\hat{L}_z^2, \hat{L}_x\right] = -i\hbar\left(\hat{L}_y\hat{L}_z + \hat{L}_z\hat{L}_y\right)$ and we can now safely say that

$$\begin{aligned}
\left[\hat{L}^2, \hat{L}_x\right] &= 0 \\
\left[\hat{L}^2, \hat{L}_y\right] &= 0 \\
\left[\hat{L}^2, \hat{L}_z\right] &= 0
\end{aligned}$$

Thus there exists a common set of eigenfunctions of $\hat{L}^2$ and $\hat{L}_x$(and the others). By convention we will work with the last set of eigenfunctions of $\hat{L}^2, \hat{L}_z$. We can always describe an eigenfunction of $\hat{L}_x$, say by a linear combination of $\hat{L}_z$ eigenfunctions.

3.1 $\hat{L}^2$, $\hat{L}_z$ operators in spherical polar co-ords

Recall that $\hat{L} = \hat{R} \times \hat{P} = -i\hbar\vec{r} \times \nabla$. From this it follows that

$$\hat{L} = -i\hbar\left(\frac{\partial}{\partial\theta}\hat{\phi} - \frac{1}{\sin\theta}\frac{\partial}{\partial\phi}\hat{\theta}\right)$$

since $\hat{z} = \cos\theta\hat{r} - \sin\theta\hat{\theta}$ we can write $\hat{L}_z = \hat{z} \cdot \hat{L} = -i\hbar\frac{\partial}{\partial\phi}$ and with more effort we can find $\hat{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$. The eigenfunctions of $\hat{L}^2$ are called "spherical harmonics" $Y(\theta,\phi)$. To find them we use separation of variables, $Y(\theta,\phi) = \Theta(\theta)\Phi(\phi)$, for which we get $\Theta = \sum_l a_l \cos^l\theta$ with $l = 0, 1, 2, 3, ...$ with constraints on a_l to make series terminate. For Φ we get $\Phi = \frac{1}{\sqrt{2\pi}}e^{im\phi}$ where $|m| \leq l$, both m and l are integers, e.g. $m = +l, l-1, ..., 0, ..., -l$. So final solutions have the form normalization times associated Legendre polynomial($Y_{l,m}$) times $e^{im\phi}$. The eigenvalues of $Y_{l,m}$ are given by

$$\begin{aligned}
\hat{L}^2 Y_{l,m} &= l(l+1)\hbar^2 Y_{l,m} \\
\hat{L}_z Y_{l,m} &= m\hbar Y_{l,m}
\end{aligned}$$

3.2 The ladder operators

We can find eigenvalues and develop the complete set of eigenfunctions of $\hat{L}^2, \hat{L}_z$ by using what are known as "Ladder operators", $\hat{L}_+, \hat{L}_-$ defined thus:

$$\begin{aligned}\hat{L}_+ &= \hat{L}_x + i\hat{L}_y \\ \hat{L}_- &= \hat{L}_x - i\hat{L}_y\end{aligned}$$

These are not Hermitian operators and do not represent any dynamical variable. They change $Y_{l,m}$ to $const \times Y_{l,m\pm1}$. We establish some commutation relations: 10.11.2006

$$\begin{aligned}\hat{L}_+\hat{L}_- &= \underbrace{\hat{L}_x^2 + \hat{L}_-^2} -i\left[\hat{L}_x, \hat{L}_y\right] \\ &= \hat{L}^2 - \hat{L}_z^2 \ + \hbar\hat{L}_z \qquad (19)\end{aligned}$$

similarly

$$\hat{L}_-\hat{L}_+ = \hat{L}^2 - \hat{L}_z^2 - \hbar\hat{L}_z \qquad (20)$$

thus we get $\left[\hat{L}_+, \hat{L}_-\right] = 2\hbar\hat{L}_z$ and also

$$\begin{aligned}\left[\hat{L}_z, \hat{L}_+\right] &= \left[\hat{L}_z, \hat{L}_x\right] + i\left[\hat{L}_z, \hat{L}_y\right] \\ &= i\hbar\left(\hat{L}_y - i\hat{L}_x\right) = \hbar\hat{L}_+ \qquad (21)\end{aligned}$$

similarly we get $\left[\hat{L}_z, \hat{L}_-\right] = -\hbar\hat{L}_-$.

Now consider the eigenvalue equation

$$\hat{L}_z\phi = \beta\phi$$

now operate with $\hat{L}_+$

$$\hat{L}_+\hat{L}_z\phi = \beta\hat{L}_+\phi$$

using Eqn 21 we get $\hat{L}_z\hat{L}_+\phi = \beta\hat{L}_+\phi + \hbar\hat{L}_+\phi = (\beta + \hbar)\left(\hat{L}_+\phi\right)$. Similarly we can show that $\hat{L}_z\left(\hat{L}_-\phi\right) = (\beta - \hbar)\left(\hat{L}_-\phi\right)$. Thus $\hat{L}_+\phi$ and $\hat{L}_-\phi$ are (unnormalized) eigenfunctions of $\hat{L}_z$ with eigenvalues $\beta + \hbar$ and $\beta - \hbar$.

Now we can do the same with $\hat{L}^2\phi = \alpha\phi$. We would expect that α does not change.

$$\begin{aligned}\hat{L}_+\hat{L}^2\phi &= \alpha\hat{L}_+\phi \\ \hat{L}_-\hat{L}^2\phi &= \alpha\hat{L}_-\phi\end{aligned}$$

since $\hat{L}^2$ commutes Whit all components of angular momentum, it also commutes with $\hat{L}_+$ and $\hat{L}_-$. Thus $\hat{L}^2\left(\hat{L}_+\phi\right) = \alpha\left(\hat{L}_+\phi\right)$ and $\hat{L}^2\left(\hat{L}_-\phi\right) = \alpha\left(\hat{L}_-\phi\right)$, the eigenfunction changes but the eigenvalue stays the same, recall that $\alpha =$l$(l+1)\,\hbar^2$.

Eventually repeated applications of $\hat{L}_+$ will reach a maximum projection β_1, repeated applications of $\hat{L}_-$ will reach minimum β_2, where $\beta_1^2 < \alpha$ and $\beta_2^2 < \alpha$.

So

$$\hat{L}_+\phi_1 = 0 \qquad (22)$$

and

$$L_-\phi_2 = 0 \tag{23}$$

Operate on Eqn 22 with $\hat{L}_-$ and use Eqn 20, we get $\hat{L}_-\hat{L}_+\phi_1 = \left(\hat{L}^2 - \hat{L}_z^2 - \hbar\hat{L}_z\right)\phi_1 = \left(\alpha - \beta_1^2 - \hbar\beta_1\right)\phi_1 = 0$, solving for $\alpha = \beta_1\left(\beta_1 + \hbar\right)$ and from Eqn 23 we get $\alpha = \beta_1\left(\beta_1 - \hbar\right)$, thus

$$\beta_1 = -\beta_2 \tag{24}$$

Since β changes by one unit of $\hbar$ in raising and lowering operations it follows $\beta_1 - \beta_2 = n\hbar$, where n is an integer. If arrangement of states is symmetric about $L_z = 0$(no hat), then it follows that $n = even = 2l$. Consider though that so far there is nothing to stop n being odd-integer, which would lead to $\frac{1}{2}$-spin.

Thus from Eqn 24 $\alpha = l\left(l+1\right)\hbar^2$ and $\beta = m\hbar$ with $-l \leq m \leq +l$.

3.3 Axial symmetry of $\widehat{L}_z$ eigenvalues

We show $< \hat{L}_y >= 0 =< \hat{L}_x >$. Since $\hat{L}_+ = \hat{L}_x + i\hat{L}_y$, $\hat{L}_- = \hat{L}_x - i\hat{L}_y$ we get $\hat{L}_x = \frac{1}{2}\left(\hat{L}_+ + \hat{L}_-\right)$. Let ϕ_m be an eigenstate of $\hat{L}_z$, then

$$\begin{aligned} < \hat{L}_x > &= \int \phi_m^* \hat{L}_x \phi_m d\tau \\ &= \frac{1}{2}\int \phi^* \left(\hat{L}_+ + \hat{L}_-\right)\phi_m d\tau \\ &= \frac{1}{2}\int c_1\phi_m^*\phi_{m+1} + c_2\phi_m^*\phi_{m-1} d\tau = 0 \end{aligned}$$

where c_1 and $c_2$are constants.

Insert Monday, 13.11.2006 lecture notes.

3.4 What is the co-efficient c_1 in $L_+\phi_m = c_1\phi_{m+1}$?

14.11.2006

We need this relationship (remember both L_x and L_y are hermitian[1]). Consider

$$\begin{aligned} \int f\hat{L}_- g d\tau &= \int f\left(L_x - iL_y\right) g d\tau \\ &= \int g\left(L_x^* - iL*_y\right) f d\tau \\ &= \int g\left(L_x + iL_y\right)^* f d\tau \\ & \int g L_+^* f d\tau \end{aligned}$$

[1] $\int f\hat{Q}g d\tau = \int g\hat{Q}^* f d\tau$

Now using normalised wave functions ϕ_m we have

$$\begin{aligned}
|c_1|^2 \underbrace{\int \phi_{m+1}\phi^*_{m*1}d\tau}_{} &= \int \left(L_+\phi_m\right) L^*_+\phi^*_m d\tau \\
& \quad gL^*_+ f d\tau \\
|c_1|^2 \quad 1 &= \int \phi^*_m L_- L_+ \phi_m d\tau \\
& \quad \int \phi^*_m \left(L^2 - L_z^2 - \hbar L_z\right) \phi_m d\tau \\
& \quad l\left(l+1\right)\hbar^2 - m^2\hbar^2 - m\hbar^2
\end{aligned}$$

Thus $L_+\phi_m = \sqrt{l\left(l+1\right) - m\left(m+1\right)}\hbar\phi_{m+1}$ and similarly $L_-\phi_m = \sqrt{l\left(l+1\right) - m\left(m-1\right)}\hbar\phi_{m-1}$. This shows us what happens if we try and apply L_+or L_- to often, ie beyond available m.

4 Spin

Appears naturally in the relativistic Dirac equation, corrected Schroedinger equation There is no classical analog(Dirac particles are point like, have no structure) and no differential operator exists. Nevertheless the same algebra can be used as for orbital angular momentum.

Electron is a spin-1/2 particle which means $s = \frac{1}{2}\hbar$, $m_s = \pm\frac{1}{2}$. Spin angular momentum operators $\hat{S} = \left(\hat{S}_x, \hat{S}_y, \hat{S}_z,\right)$ and $\hat{S}^2$.

4.1 Commutation relations

We have $\left[S_x, S_y\right] = i\hbar S_z$(and similar for cyclic exchange of x,y,z). Also have $\left[S^2, S_x\right] = \left[S^2, S_y\right] = \left[S^2, S_z\right] = 0$, by convention we work with the common set of eigenfunctions of $\hat{S}^2$, $\hat{S}_z$. We call the eigenfunctions α and β.

Consider $S_z\alpha = +\frac{1}{2}\hbar\alpha$ and $S_z\beta = -\frac{1}{2}\hbar\beta$, alpha and beta are orthonormal. Applying $S^2\alpha = \frac{1}{2}\left(\frac{1}{2}+1\right)\hbar^2\alpha$, for β its the same just with $-\frac{1}{2}$.

A general spin wavefunction, χ (eg a spin polarized along the x-axis), may be expressed as a linear combination of the S^2,S_z eigenfunctions.

$$\chi = a\alpha + b\beta$$

where a,b are coefficients which determine relative population and relative phase of the α and β eigenfunctions.

Ladder operators are defined as

$$\begin{aligned}
\hat{S}_+ &= \hat{S}_x + i\hat{S}_y \\
\hat{S}_- &= \hat{S}_x - i\hat{S}_y
\end{aligned}$$

thus $\hat{S}_x = \frac{1}{2}\left(\hat{S}_+ + \hat{S}_-\right)$ and $\hat{S}_y = \frac{1}{2i}\left(\hat{S}_+ - \hat{S}_-\right)$, same as before. So we get

$$\begin{aligned}
\hat{S}_+\chi &= \sqrt{s\left(s+1\right) - m_s\left(m_s+1\right)}\hbar\chi_{m_s+1} \\
\hat{S}_-\chi &= \sqrt{s\left(s+1\right) - m_s\left(m_s-1\right)}\hbar\chi_{m_s-1}
\end{aligned}$$

if we now operate $\hat{S}_+\chi_{\frac{1}{2}} = 0$ but $\hat{S}_+\chi_{-\frac{1}{2}} = \sqrt{\frac{3}{4}+\frac{1}{4}}\hbar\chi_{+\frac{1}{2}} = \hbar\alpha$ where we used/defined $\chi_{-\frac{1}{2}} = \beta$. We can do the same for $\hat{S}_-\alpha = \hbar\beta$. So we can use the raising and lowering operators to go from one state to the other.

17.11.2006

Eigenfunctions of S_x We can write $S_x\alpha = \frac{1}{2}(S_+ + S_-)\alpha = \frac{1}{2}\hbar\beta$ and similarly $S_x\beta = \frac{1}{2}(S_+ + S_-)\beta = \frac{1}{2}\hbar\alpha$ if we add these two we get

$$S_x(\alpha+\beta) = \frac{1}{2}\hbar(\alpha+\beta)$$

if we use $\frac{1}{\sqrt{2}}(\alpha+\beta)$ as the eigenfunction with eigenvalue $\frac{1}{2}\hbar$. If we subtract we get $S_x(\alpha-\beta) = \frac{1}{2}(\beta-\alpha) = -\frac{1}{2}(\alpha-\beta)$, with eigenfunction $\frac{1}{\sqrt{2}}(\alpha-\beta)$ and eigenvalue of $-\frac{1}{2}\hbar$.

If we do this for S_y when adding we get eigenfunctions $\frac{1}{\sqrt{2}}(\alpha+i\beta)$ with eigenvalue $\frac{1}{2}\hbar$ and when subtracting we get eigenfunctions $\frac{1}{\sqrt{2}}(\alpha-i\beta)$ with eigenvalue $-\frac{1}{2}\hbar$.

4.2 Dirac Notation

How do we write a wavefunction ϕ in this notation? Just write $|\phi>$, this is a "Ket" or "state vector". The complex conjugate ϕ^* is just $<\phi|$, this is called a "Bra". Instead of writing $\phi_{n,L,m}$ we write $|n,l,m>$. Basically read your average Quantum Mechanics book for more details.

For a spin-1/2 particle we write up state α as $|\alpha>$ or $|+\frac{1}{2}>$and down state β as $|\beta>$ or $|-\frac{1}{2}>$. With $<\alpha|\alpha>=1$ and $<\beta|\beta>=1$ but $<\alpha|\beta>=<\beta|\alpha>=0$. A general state ψ made up of these two is $|\psi>=a|\alpha>+b|\beta>$ where $a=<\alpha|\psi>$ and $b=<\beta|\psi>$.

4.3 Matrix representation of QM

We can work with ϕ_n set of eigenstates. Again read your average book. In general this approach has the problem that our matrix Q has an infinite amount of elements. Luckily when we talk about spin we only need a 2x2 matrix.

We take

$$\sum a_n\hat{Q}\phi_n = q\sum a_n\phi_n$$

basically we expanded a wave function Ψ in terms of ϕ, $\Psi = \sum a_n\phi_n$. If we now multiply by ϕ_m^* and integrate over all space. This gives

$$\begin{aligned}\sum a_n\int\phi_m^*\hat{Q}\phi_n d\tau &= q\sum a_n\int\phi_m^*\phi_n d\tau\\ \sum Q_{nm}a_n &= qa_m\end{aligned}$$

because of orthogonality and δ_{nm}. Here Q_{nm} is a matrix. 22.11.2006

This gives us a matrix equation, it is like a normal "operator" equation, but with a matrix operator. It looks like

$$[Q]\begin{pmatrix}a_1\\a_2\\\vdots\end{pmatrix} = q\begin{pmatrix}a_1\\a_2\\\vdots\end{pmatrix}$$

we fix $a_1, a_2, ...$ by requiring that the determinant of Q is zero.

The matrix $[Q]$ is Hermitian, this means that $[Q] = [Q^{+}]$, this means that take complex conjugate and transpose it. This guarantees all q are real.

Suppose we choose to work in a basis composed of its own eigenfunctions $Q_{mn} = \int \Psi_m^* \hat{Q} \Psi_n d\tau = \int q_n \Psi_m^* \Psi_n d\tau = q_n \delta_{mn}$. Which means that matrix Q_{mn} is diagonal. The size of the matrix is determined by the number of eigenvalues, this leads to many of them being infinite.

But in cases with angular momentum the number is restricted, eg $Y_{lm}(\theta, \phi)$, with $2l+1$ eigenvalues for a particular l.

4.3.1 Matrix representation of spin

Choose to represent using eigenfunctions of s_z. If we use Dirac notation the matrix looks like

$$\begin{aligned} S_{11} = & < \alpha|\hat{s}_z|\alpha >= & \frac{\hbar}{2} \\ S_{12} = & < \alpha|\hat{s}_z|\beta > & = 0 \\ S_{21} = & < \beta|\hat{s}_z|\alpha > & = 0 \\ S_{22} = & < \beta|\hat{s}_z|\beta > & = -\frac{\hbar}{2} \end{aligned}$$

we end up with

$$\left(\begin{array}{cc} \frac{\hbar}{2} & 0 \\ & -\frac{\hbar}{2} \end{array} \right) \left(\begin{array}{c} a_1 \\ a_2 \end{array} \right) = \frac{\hbar}{2} \sigma_z \left(\begin{array}{c} a_1 \\ a_2 \end{array} \right) = q \left(\begin{array}{c} a_1 \\ a_2 \end{array} \right)$$

we get the eigenvalues from the determinant of something. The diagonal elements of the matrix Q are the eigenvalues.

4.3.2 Matrix representation of s_x

24.11.2006

Matrix representation of $\hat{s}_x$in α, β basis. We have shown $s_x \alpha = \frac{\hbar}{2}\beta$ and $s_x|\beta >= \frac{\hbar}{2}|\alpha >$. So we can write

$$\begin{aligned} [s_x] & = \left(\begin{array}{cc} s_{11} & s_{12} \\ s_{21} & s_{22} \end{array} \right) \\ = \left(\begin{array}{cc} < \alpha|s_x|\alpha > & < \alpha|s_x|\beta > \\ < \beta|s_x|\alpha > & < \beta|s_x|\beta > \end{array} \right) & = \frac{\hbar}{2} \left(\begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right) \end{aligned}$$

We could demonstrate all commutation relations by matrix multiplication, eg.

$$[s_x, s_y] = \frac{\hbar^2}{4} (\sigma_x \sigma_y - \sigma_y \sigma_x) = \frac{i\hbar^2}{2} \sigma_z = i\hbar s_z$$

we can also find $s^2 = s_x^2 + s_y^2 + s_z^2$. It turns out that $\left[s^2\right] = \frac{3}{4}\hbar^2 \left(\begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right)$. Any spin-1/2 vector $\left(\begin{array}{c} a \\ b \end{array} \right)$, representing a state like $a|\alpha > +b|\beta >$, is an eigenfunction of s^2:

$$\frac{3}{4}\hbar^2 \left(\begin{array}{cc} 1 & \\ & 1 \end{array} \right) \left(\begin{array}{c} a \\ b \end{array} \right) = q \left(\begin{array}{c} a \\ b \end{array} \right)$$

where $q = \frac{3}{4}\hbar^2 = s\,(s+1)\,\hbar^2$. Make sure to check the website about correspondence of Dirac notation and these matrices.

4.3.3 Matrix representation of spin-1 system

We can find the matrix representations of all the operators of all operators that one would need to describe a spin-1 particle.

We will work in the basis of eigenfunctions of L^2, L_z which we denote by $|m>$, $m = \pm 1, 0$. Matrix elements of $[L_x]$ can be found thus:

Write $L_x = \frac{1}{2}(L_+ + L_-)$, find $L_x|n >= a|n+1> + b|n-1>$, then find $< m|L_x|n >= a < m|n+1> + b < m|n-1>$, where $< m|n-1 >= \delta_{m(n-1)}$ an orthonormal set.

Example, description of l=1 spin polarized in $m_x = \hbar$ eigenstate of L_x. We need eigenvector

$$[L_x]\,[a] = \hbar\,[a]$$

which gives $[a] = \frac{1}{2}\begin{bmatrix} 1 \\ \sqrt{2} \\ 1 \end{bmatrix}$.

4.4 Measuring a spin component

Charged particles with intrinsic spin or orbital angular momentum have a magnetic dipole moment $\vec{\mu}$. He does lots of talking about gyromagnetic ratios and such. Look at hyperphysics or so if you don't remember. Important part is

$$\mu = g_l l \mu_B$$

with Bohr magneton. 29.11.2006

The electron also has an intrinsic moment – like a bar magnet – along direction of spin $\vec{s}$. This is given by $\mu_s = g_s s \mu_B$, with $s = \frac{1}{2}$. Simple Dirac theory gives $g_s = -2$.

The Stern Gerlach apparatus measures one component of spin by detecting the direction a particle is pulled in a magnetic field gradient. Since force on a particle in a magnetic field is given by $F = -\nabla\left(-\vec{\mu}\cdot\vec{B}\right)$. If $\vec{B}$ changes in the z direction we have $F = +\vec{\mu}\frac{\partial B_z}{\partial z} = \mu_z\frac{\partial B_z}{\partial z}$. A beam of particles is deflected "up" or "down" depending on the sign of the component of $\vec{\mu}$ along z-axis ($m_s = \pm\frac{1}{2}$).

We will discuss successive measurements on spin-1/2 particles. We start with an unpolarized beam, 50% spin up $|\alpha>$ & 50% spin down, $|\beta>$. Measuring $s_x$in x-direction, we need to describe $|\alpha>$ in terms of eigenstates of $\hat{s}_x$. Since $|m_x = \frac{1}{2} >= \frac{1}{\sqrt{2}}(|\alpha> + |\beta>)$ and $|m_x = -\frac{1}{2} >= \frac{1}{\sqrt{2}}(|\alpha> - |\beta>)$, so adding them we get $|\alpha >= \frac{1}{\sqrt{2}}\left(|m_x = \frac{1}{2}> + |m_x = -\frac{1}{2}>\right)$.

After second measurement(in the x direction now) we have 1/4 of original beam in $|m_x = +\frac{1}{2}>$ state. All memory is lost of the state before the magnet, if we were to measure in z-direction again we would find 50% in up state and 50% in down state, as in the first measurement. So after third measurement we are left with 1/8 of the original beam.

5 Addition of angular momentum

We consider vector addition of two angular momenta in this example adding the electron spin and orbital angular momentum. The algebra below can be applied to any angular momenta, eg spin and spin.

Vector equation

$$\vec{J} = \vec{L} + \vec{S}$$

if we square this we get $\vec{J}\vec{J} = J^2 = L^2 + S^2 + 2\vec{L}\vec{S}$, with $J_z = L_z + S_z$. IN QM we can write this as $\hat{J}^2 = \hat{L}^2 + \hat{S}^2 + 2\hat{\vec{L}}\hat{\vec{S}}$ and $\hat{J}_z = \hat{L}_z + \hat{S}_z$.

It is easy to show that $\left[J^2, L^2\right] = 0$, $\left[J^2, S^2\right] = 0$ but J^2 does not commute with L_z or S_z due to $\vec{L} \cdot \vec{S}$ term. We can show this by writing $L \cdot S = L_x S_x + L_y S_y + L_z S_z$.

5.1 Spin orbit coupling & "fine structure"

6.12.2006

Each l-state is $2\,(2l+1)$ degenerate. We can lift this by applying a magnetic field.

Classically an electron orbiting a nucleus, $+Ze$, "sees" the nucleus orbiting around it, this looks like a current loop around the electron. As we know current loops create a magnetic field. The field at the electron(center of loop) is given by

$$B = \frac{\mu_0 I}{2r}$$

where all symbols have the usual meaning. The nucleus is orbiting with angular velocity ω. Hence the current is given by $I = \frac{Ze\omega}{2\pi}$. Getting ω from the classical angular momentum $\vec{L} = m_e \omega r^2$ so we can write

Interaction energy with the electron's magnetic moment is

$$E = \frac{1}{2}\vec{\mu}_s \cdot \vec{B}$$

where the factor of $1/2$ come from relativistic effects called "Thomas precession", we just accept it. Using $\vec{\mu}_s = -\frac{e\hbar}{2m_e} = -\mu_B = -\frac{e}{m_e}\vec{s}$. So if we put it all together we get the interaction energy E to be given by

$$E = A\vec{L} \cdot \vec{S}$$

where $A = \frac{\mu_0 Ze^2}{8\pi m_e^2 r^3}$. The Hamiltonian now includes a correction

$$\hat{H}_{so} = A\hat{L} \cdot \hat{S}$$

called the spin-orbit interaction. We have seen $\hat{L}\cdot\hat{S}$ commutes with $\hat{J}^2$, $\hat{J}_z$, $\hat{L}^2$, $\hat{S}^2$. So the states $|j, m_j, l, s>$ are eigenfunctions of $\hat{H}_{so}$. The spin-orbit coupling results in the states with $l \neq 0$ being split into two components, one with $\vec{s}$ parallel to $\vec{L}$ and one with $\vec{s}$ anti parallel.

The splitting of energy levels(energy shift) with $l \neq 0$ due to the corrections to the Hamiltonian $\hat{H}_{so}$ can be calculated as follows:

$$\vec{J} = \vec{L} + \vec{S} \rightarrow J^2 = \vec{J}\vec{J} = L^2 + S^2 + 2\vec{L}\vec{S}$$

and we can write the Hamiltonian as

$$H_{so} = A\vec{L}\cdot\vec{S} = \frac{A}{2}\left[J^2 - L^2 - S^2\right]$$

if we write this in Dirac notation we get $,H_{so}|j, m_j, l, s>$ which equals

$$\underbrace{\frac{A}{2}\left(j\left(j+1\right) - l\left(l+1\right) - s\left(s+1\right)\right)\hbar^2}_{=\Delta E}|j, m_j, l, s>$$

8.12.2006

Magnitude of spin-orbit-interaction. Consider a state with $l = 1$, the energy difference,gap, shift, is then

$$gap = \frac{3}{2}A\hbar^2 = \frac{3}{2}\frac{\mu_0 e^2}{8\pi m_e^2 r^3}\hbar^2$$

we will use $r = a_0$, Bohr radius, and fact that we can write $R_\infty = \frac{e^2}{2\cdot 4\pi\epsilon_0 a_0}$, using $c^2 = \frac{1}{\mu_0\epsilon_0}$ we find that

$$\frac{3}{2}A\hbar^2 = \frac{3}{2}R_\infty\frac{\hbar^2}{c^2 a_0^2 m_e^2} = \frac{3}{2}R_\infty\alpha^2$$

where α is the fine-structure constant. This gives us a gap, splitting, shift of about 1.1×10^{-3}eV.

5.2 Zeeman Effect

If a magnetic field B is applied to an atom along the z–axis then an extra term must be included in the Hamiltonian of the form $-\vec{\mu}\cdot\vec{B}$. For a single electron the Hamiltonian will look as follows

$$\begin{aligned}\hat{H} &= \hat{H}_0 + \hat{H}_{so} + \hat{H}_{mag} \\ &= \left(\frac{p^2}{2m} + V\right) + \frac{A}{2}\left(J^2 - L^2 - S^2\right) - \frac{\mu_B}{\hbar}\left(g_l\hat{L}_z + g_s\hat{S}_z\right)B\end{aligned}$$

where the last term is the new one added due to the magnetic field. We now have a problem as $\hat{H}_{mag}$ does not commute with $\hat{J}^2$. Aside: It would work if $g_l = g_s$, but they are not. On the other hand the spin-orbit term $\hat{H}_{so}$ does not commute with $\hat{L}_z$ or $\hat{S}_z$. Eigenfunctions of $\hat{H}$ are a linear combination of either $|j,\ m_j,\ l,\ s>$ set of eigenstates or $|l,\ m_l,\ s,\ m_s>$. The first one is a better set for weak fields and latter basis is better for strong fields.

We will look at the weak field where $H_{mag} \ll H_{so}$ and use $|j,\ m_j,\ l,\ s>$ as appropriate eigenfunctions. Here $\vec{J}$ precesses about the field B, J_z is a constant, but S_z and L_z are not.

We will also look at strong fields for which H_{mag} dominates and interaction is much stronger than spin-orbit interaction($H_{mag} \gg H_{so}$). In this case $\vec{L}$ and $\vec{S}$ independently precess about B. In this case S_z and L_z are constants, as is J_z but not $\vec{J}$. As $\vec{S}$ might be pointing to the left and $\vec{L}$ pointing to the right, which is different to both pointing in the same direction.

Weak field Zeeman effect The atomic state $\vec{J}\left(=\vec{L}+\vec{S}\right)$ has a composite magnetic moment made up of orbital and intrinsic spin contributions

$$\mu_J = g_J j \mu_B$$

where g_j is the Lande g-factor. 13.12.2006

Thus in a weak magnetic field, energy=

$$\begin{aligned} -\vec{\mu}_J \cdot \vec{B} &= -g_J \mu_B \vec{j} \cdot \vec{B} \\ &= -g_J \mu_B m_J B \end{aligned}$$

where B is component of magnetic field along z axis. The spacing between adjacent energy levels is given by $\Delta E = g_J \mu_B B$.

Strong Field We now have $H_{mag} \gg H_{so}$, so we ignore it for now. Our Hamiltonian now looks like

$$H = H_0 - \frac{\mu_B}{\hbar}\left(g_l L_z + g_s S_z\right) B$$

All terms in this H commute with L^2, L_z, S^2, S_z and $J_z = L_z + S_z$.

Eigenfunctions of H are $|l, m_l, s, m_s>$. We can find the energy shift due ti H_{mag} of each state

$$H_{mag}|l, m_l, s, m_s >= -\frac{e\hbar}{2m}\left(g_l m_l + g_s m_s\right) B |l, m_l, s, m_s >$$

Intermediate fields We have to include both H_{so} and H_{mag}. This makes finding eigenstates rather complicated. They can be expressed as a linear combination of either $|l, m_l, s, m_s>$ basis or the $|j, m_j, s, m_s>$ basis.

Note though that $|j, m_j = \pm j >= 1 \cdot |l, m_l = \pm 1, s, m_s = \pm\frac{1}{2}>$. These states are eigenfunction of both H_{so} and H_{mag}.

6 Time-independent perturbation theory

Consider the effect of a weak perturbation $\hat{H}\prime$, eg an external field acting on an atom, that would otherwise have eigenstates and energies given by

$$\hat{H}_0 u_n = E_n^0 u_n$$

where E_n^0 is the unperturbed energy of the n-th state. Let new Hamiltonian $\hat{H} = \hat{H}_0 + \beta \hat{H}\prime$ where β is a label which will allow us to identify 1st order (linear in β) and 2nd order β^2 terms.

Let the new eigenstates & energies be

$$\hat{H}\psi_n = E_n \psi$$

we write the higher order corrections to $E_n^0,\ u_n$

$$\begin{aligned} E_n &= E_n^0 + \beta E_n' + \beta^2 (...) \\ \psi_n &= u_n + \beta u_n' + \beta^2 (...) \end{aligned}$$

Finding correction E_n'. Substituting in the previous equations we obtain

$$\hat{H}_0 + \beta\hat{H}'\left(u_n + \beta u_n'\right) = \left(E_n^0 + \beta E_n'\right)\left(u_n + \beta u_n'\right)$$

if we look at the zeroth-order term we don't learn anything new, its just the old eigenvalue equation.

If we look at the first order terms, ie terms in β, we get

$$H_0 u_n' + H' u_n = E_n^0 u_n' + E_n' u_n$$

we can always write u_n' as

$$u_n' = \sum_m a_m u_m$$

Multiply by u_n^* and integrate over all space.

$$\underbrace{\int u_n^* H_0 \left(\sum a_m u_m\right) d\tau}_{\underbrace{\int u_n^* \sum a_m E_m^0 u_m d\tau}_{=a_n E_n^0}} + \underbrace{\int u_n^* H' u_n d\tau}_{RHS} = \underbrace{\int u_n^* E_n^0 \left(\sum a_m u_m\right) d\tau}_{=a_n E_n^0} + \underbrace{\int u_n^* E_n' u_n d\tau}_{E_n'}$$

Thus we get

$$E_n^{'} = \int u_n^* H' u_n d\tau$$

where E_n' is the energy shift.

Look at Hydrogen atom with finite size proton. We usually use a Coulomb potential like $V = -\frac{e^2}{4\pi\epsilon_0 r}$ which is $= \infty$ at $r = 0$. Now consider a proton with finite size. Let all charge be on the surface of a small sphere, radius $R \approx 10^{-15}m$. Outside the sphere the potential is still $V = -\frac{e^2}{4\pi\epsilon_0 r}$. Inside the sphere things are different, $V = -\frac{e^2}{4\pi\epsilon_0 R}$, it is constant. The perturbation we consider is only due the difference in potential between point like distribution and finite size one $\hat{H}' = \Delta V$. For $r > R$, $\hat{H}' = 0$, for $r < R$ we have

$$H' = \frac{e^2}{4\pi\epsilon_0 r} - \frac{e^2}{4\pi\epsilon_0 R}$$

So we get the energy shift from

$$E = \int \psi^* \left(\frac{e^2}{4\pi\epsilon_0 r} - \frac{e^2}{4\pi\epsilon_0 R}\right) \psi \underbrace{4\pi r^2 dr}_{=d\tau}$$

simplify this even further, for a 1s electron $|\psi|^2 = \frac{1}{\pi a_0^3}\exp\left(-\frac{r}{a_0}\right) \approx \frac{1}{\pi a_0^3}$ for $r \ll a_0$. So we get

$$E = \frac{4\pi e^2}{4\pi\epsilon_0} \int |\psi|^2 \left(r - \frac{r^2}{R}\right) dr = \frac{1}{\pi a_0^3}\frac{e^2}{\epsilon_0}\frac{1}{6}R^2$$

As a fraction of the 1s energy $R_\infty = \frac{1}{2}\frac{e^2}{4\pi\epsilon_0 a_0}$, we get

$$\frac{\Delta E}{E_{1s}} = \frac{4}{3}\frac{R^2}{a_0^2} \approx 10^{-10}$$

Alan Aspect knows how to disprove hidden variable theory.