Quantum Physics PY1T20/PYU11P20

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1

Quantum Physics Lecture 13

Potential barrier of finite width

- $E > U_o$ Resonant tunneling (non-exam)
- *Example: Ramsauer-Townsend Effect (non-exam)*

Angular Momentum

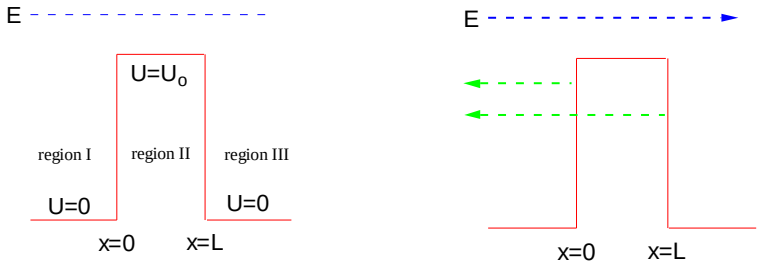
- Reminder: operators and eigenfunctions
- Angular momentum operator(s) in quantum mechanics
- Eigenvalues of angular momentum
- Spin
- Fermions and bosons

The Pauli exclusion principle

Commutators and the uncertainty principle (non-exam)

2

potential barrier ($E > U_o$)



Recall step-up or down potential, $E > U_o$: some reflection at the boundary; here there are 2 boundaries!
For certain wavelengths, $\lambda = 2L/n$, the two reflected waves (green) interfere destructively and transmission $T = 1$

- 'Resonant' Tunnelling

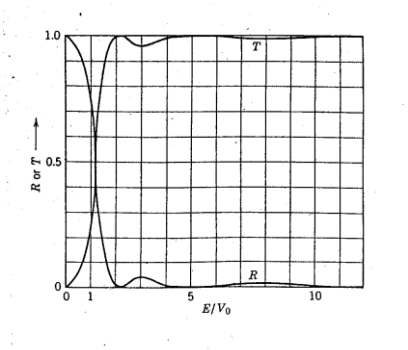
Also true of "down" potential barrier, *ie potential well*

Basis of Ramsauer-Townsend and other effects…..

Ramsauer-Townsend effect

Scattering of low energy electrons by helium atoms (SF lab)

Observe one (or more?) minima in scattered electron current, corresponding to unity transmission!



Free particle functions and operators

$$\psi = A\exp(-iEt/\hbar + ipx/\hbar) = Ae^{-iEt/\hbar}e^{ipx/\hbar}$$

Now consider partial differential with x

$$\frac{\partial\psi}{\partial x} = A^{-iEt/\hbar}\frac{ip}{\hbar}e^{ipx/\hbar} = \frac{ip}{\hbar}\psi$$

Re-arranged: $\frac{\hbar}{i}\frac{\partial}{\partial x}\psi = p\psi$ Or: $-i\hbar\frac{\partial}{\partial x}\psi = p\psi$

i.e. if we "operate" on ψ with $-i\hbar\delta/\delta x$ get the value of momentum p multiplied by ψ
$-i\hbar\delta/\delta x$ *is the momentum 'operator'* $\hat{p}$ *and*
the free particle function ψ *is an eigenfunction of* $\hat{p}$ *with eigenvalue p.*

General Equation for an eigenfunction: Operator on eigenfunction ψ = *eigenvalue* $\times\ \psi$

5

Other operators and eigenfunctions

We can use the momentum operator to construct operators for other observable properties e.g.:

Kinetic energy operator

$$\hat{T} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

Total energy operator = "Hamiltonian"

$$\hat{H} = \frac{\hat{p}^2}{2m} + U(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)$$

Key facts:

- the eigenvalues of an operator are the possible results of a measurement
- the eigenfunctions are those states where there is no uncertainty ('measure $\hat{p}$ get p').

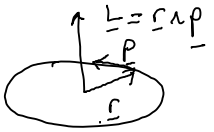
Recall: steady-state Schrodinger equation $\hat{H}\psi = E\psi$ - solving this gives us the possible results of measuring energy

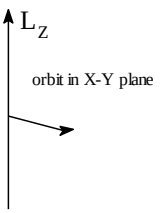
We've seen there are lots of these, labelled by some 'quantum number', e.g. for the harmonic oscillator n=0, 1, 2, 3 .., and the allowed $E = E_n = \hbar\omega(n + 1/2)$

6

Angular momentum revisited

Classical angular momentum is a vector $\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p} = \begin{vmatrix} \boldsymbol{i} & \boldsymbol{j} & \boldsymbol{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}$





So for an orbit in the x-y plane the only component is $L_z = xp_y - yp_x$

Know *(Bohr model)* that there is a quantisation of angular momentum 'possible values separated by $\hbar$'

⇒Need to construct operators for angular momentum and find their eigenvalues (=allowed values in a measurement)

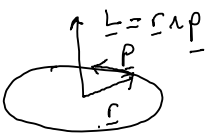
To do this we replace x, y, z and p_x, p_y, p_z by the corresponding operators, e.g. :

$$\hat{L}_z = \hat{x}\hat{p}_y - y\hat{p}_x = x\left(-i\hbar\frac{\partial}{\partial y}\right) - y\left(-i\hbar\frac{\partial}{\partial x}\right) = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

This is around z-axis. Similarly there exist L_x and L_y for x and y axes.

7

Angular momentum: eigenvalues and uncertainty



⇒Need to construct operators for angular momentum and find their eigenfunctions+values

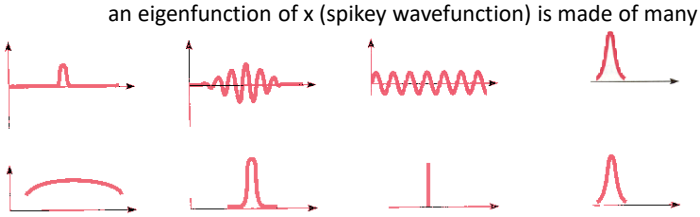
$$\hat{L}_z = \hat{x}\hat{p}_y - y\hat{p}_x = x\left(-i\hbar\frac{\partial}{\partial y}\right) - y\left(-i\hbar\frac{\partial}{\partial x}\right) = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

This is around z-axis. Similarly there exist L_x and L_y for x and y axes.

Can we find eigenfunctions of all the components of angular momentum? I.e. solve: $\hat{L}_x\phi = l_x\phi, \hat{L}_y\phi = l_y\phi, \hat{L}_z\phi = l_z\phi$

Not necessarily!

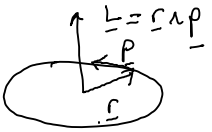
We've seen that we cannot make a state with no uncertainty in x and no uncertainty in p –
these quantities are connected by an uncertainty principle – if we know x exactly, p_x is uncertain, and v.v.
an eigenfunction of p (definite p) is made of many different eigenfunctions of x (spread out in x)
an eigenfunction of x (spikey wavefunction) is made of many different eigenfunctions of p (spread out in p).



Similar thing happens with L_x, L_y, and L_z:
can find eigenfunctions of one of these three,
but they are not eigenfunctions of the others.

8

Angular momentum: eigenvalues and uncertainty



⇒Need to construct operators for angular momentum and find their eigenfunctions+values

$$\hat{L}_z = \hat{x}\hat{p}_y - y\hat{p}_x = x\left(-i\hbar\frac{\partial}{\partial y}\right) - y\left(-i\hbar\frac{\partial}{\partial x}\right) = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

We can though find eigenfunctions of one component + magnitude of the a.m. vector $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$

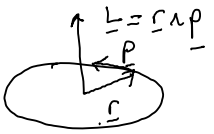
- i.e. functions which solve $\hat{L}_z\phi = b\phi$ $\hat{L}^2\phi = c\phi$ - with eigenvalues 'b' for $\hat{L}_z$
  'c' for $\hat{L}^2$

Solving these we find that the eigenvalues of the z-component are : $b = m\hbar$, where m is an integer -3, -2, -1, 0, 1, 2...
(Similar to Bohr assertion but note *m*=0 is allowed, contrary to Bohr assumption).

And the eigenvalues of the magnitude squared are : $c = \hbar^2 l(l+1)$ where l = 0, 1, 2, 3,...

With the restriction that for each l ('magnitude quantum number') the value of m must be $-l \leq m \leq l$

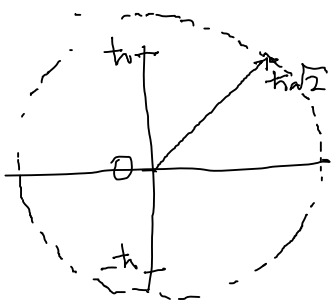
Angular momentum: cartoon interpretation



$\hat{L}_z\phi = \hbar m\phi$ $\hat{L}^2\phi = \hbar^2 l(l+1)\phi$
m is an integer ('magnetic quantum number' or 'ang. momentum projection quantum number')
l is a positive integer or zero ('magnitude of angular momentum quantum number')
For each l, allowed values of m are $-l \leq m \leq l$

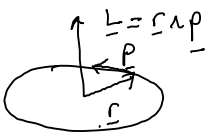
In quantum mechanics a particle can have quantised values of 'magnitude of angular momentum', and for each of these, it has a range of quantised values of any one component of angular momentum.

Sometimes depicted as a 'smeared out' vector with the right projections :



$l=1 \quad L^2\phi = \hbar^2 \cdot 1 \cdot 2 \cdot \phi$

Spin angular momentum



$\hat{L}_z\phi = \hbar m\phi \quad \hat{L}^2\phi = \hbar^2 l(l+1)\phi \qquad l = 0, 1, 2 \ldots \quad -l \leq m \leq l$

In quantum mechanics a particle can have quantised values of 'magnitude of angular momentum', and for each of these, it has a range of quantised values of any one component of angular momentum.

So far: have been talking about angular momentum due to motion of particle through space. 'Orbital angular momentum'.

Experimental fact: particles can also have angular momentum in and of themselves, called 'spin angular momentum'.

This works quite like orbital angular momentum:

- there is a quantum number for the magnitude of spin (like *l* but now called *s*), such that the observed value(s) of the total-spin-squared are $\hbar^2 s(s+1)$
- there is a quantum number for the z-component of spin (like *m* but now called m_s), such that the observed value of the z-component of spin is $\hbar m_s$

But differently:

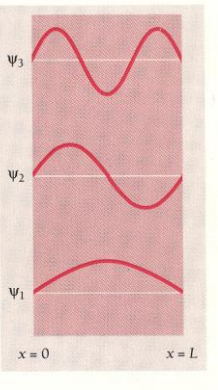
- s is a property of the particle and cannot be changed
- s can be half-integer – for an electron, s=1/2
- m_s goes from –s to +s in integer steps ⇒ if s=half-odd-integer then m_s is half-odd-integers, e.g. s=1/2, m_s=+1/2 or -1/2

'Spin up' 'Spin down'

Fermions and bosons

- There are two classes of particle in the universe:
  - Fermions, with half-odd-integer spin (e.g. electrons, protons, neutrons)
  - Bosons, with integer spin (e.g. photons, alpha particles = 2 protons+2 neutrons).
- Fermions and bosons have different forms for the 'many-particle' wavefunction
- e.g. two particles, wavefunction depends on coordinates of both, x_1 and x_2, $\psi(x_1, x_2, t)$
- If the particles are indistinguishable (e.g. two electrons) then the predictions of quantum mechanics from the wavefunction $\psi(x_1, x_2)$ ought to be the same as those for $\psi(x_2, x_1)$.
- This is only true if we insist (and we do!) that $\psi(x_1, x_2) = \pm\psi(x_2, x_1)$
- Sign is a property of the type of particle:
- for bosons it is always the + sign, for fermions it is always a – sign.

The exclusion principle



Consider a potential with stationary states ϕ_n, so that for one particle

$$H_1(x_1)\phi_n(x_1) = E_n\phi_n(x_1)$$

Suppose two particles move in this potential and do not interact.
Total energy : $H_2 = H(x_1) + H(x_2)$

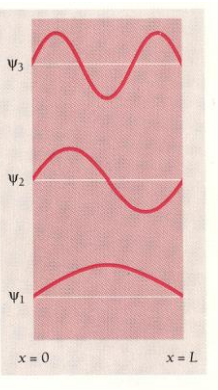
Stationary states of the two particle Hamiltonian are products : e.g. $\psi_2(x_1)\psi_3(x_2)$

This is fine for distinguishable particles in quanum mechanics. But for fermions/bosons it is wavefunction, because it treats the two particles (supposed to be indistinguishable) differently

To fix this we note that if $\psi_2(x_1)\psi_3(x_2)$ is a stationary state of energy E, so is $\psi_2(x_2)\psi_3(x_1)$

So another stationary state, of the same energy, but suitable for fermions : $N[\psi_2(x_1)\psi_3(x_2) - \psi_2(x_2)\psi_3(x_1)]$

The exclusion principle



General case, 1 fermion with quantum number n and 1 with quantum number m :

$$N[\psi_n(x_1)\psi_m(x_2) - \psi_n(x_2)\psi_m(x_1)]$$

What happens if n=m, i.e. both particles occupy the same energy level?

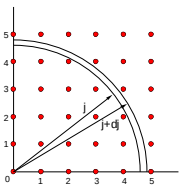
Pauli exclusion principle:
no two electrons can have the same quantum numbers.

But electrons have spin-1/2, so actually there are two quantum numbers for the state of each:
n (level in well) and m_s (spin projection, 'up' or 'down')

So each 'orbital' (state of the orbital motion, here labelled n) can hold up to 2 electrons.

Pauli exclusion principle & filling up quantum states

Example: Free electrons in a metal



States are waves in 3-D box of side a, spacing of states in k-space is π/a
(c.f. diagram from black body radiation - Lecture 6)

Exclusion principle – not more than 2 electrons per state
Electrons fill up states to a maximum level – the Fermi level k_F

$$k^2 = k_x^2 + k_y^2 + k_z^2 \qquad E = \hbar^2 k^2 / 2m$$

So total number of electrons up to k_F is

$$N = \frac{\text{spins}}{\text{vol. of single state}} \; \frac{\text{vol. of sphere in } k-\text{space}}{\text{positive octant only}} = \frac{2}{(\pi/a)^3} \; \frac{\frac{4}{3}\pi k_F^3}{8}$$

$$\Rightarrow \quad k_F = \left(\frac{3\pi^2 N}{V}\right)^{\frac{1}{3}} \qquad E_F = \frac{\hbar^2}{2m}\left(3\pi^2 \frac{N}{V}\right)^{\frac{2}{3}}$$

Another example: Atoms having Z > 1 Can fill quantum states with max. 2 electrons each
Gives the basic structure of the **Periodic Table** of the elements – *next Lectures!*

Commutators and uncertainty

We've seen that we cannot make a state with no uncertainty in x and no uncertainty in p –
an eigenfunction of p (definite p) is made of many different eigenfunctions of x ('spread out in x')
an eigenfunction of x (spikey wavefunction) is made of many different eigenfunctions of p.

But for other quantities we can do this –
we can make a state with no uncertainty in p_x and no uncertainty in p_y
we can make a state with no uncertainty in L^2 and no uncertainty in L_z

This is related to the fact that in the first case the order of the operators matters:

applying the operator p_x to a wavefunction and then applying the operator x
gives a different result to
applying the operator x to a wavefunction and then applying the operator p_x

whereas in the second case it does not. *'x and p_x do not commute whereas p_x and p_y commute'.*

General principle: non-commuting operators: no eigenfunctions of both & uncertainty principle restrictions on accuracy
commuting operators: eigenfunctions of both & no fundamental restrictions on accuracy

Commutators: example of x and p.

The effect of two operators on a function often depends on their order.
Difference between applying operators in one order vs another is another operator, called the commutator :

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

Let's work this out for x and p – we need to think about the commutator acting on an arbitrary function $\phi(x)$:

$\Rightarrow [\hat{x}, \hat{p}_x] = i\hbar \neq 0$ 'they don't commute (this is not zero)'.