Potential barriers and tunnelling

Examples

\[ E < U_o \] Scanning Tunelling Microscope
\[ E > U_o \] Ramsauer-Townsend Effect

Angular Momentum

- Orbital
- Spin

Pauli exclusion principle
potential barrier ($E < U_0$)

Recall step-up potential, $E < U_0$: particle penetrates into wall. But if the wall is finite width $L$…?

Solve SSSE:

For region I, solution is complex $k_1x$ exponentials: ($A \rightarrow$, $B \leftarrow$)
For region II, solution is real $k_2x$ exponentials: ($C \rightarrow$, $D \leftarrow$)
For region III, solution is complex $k_1x$ exponentials: ($F \rightarrow$, $G \leftarrow$)

Particle transmission through barrier! More parameters in solution
Particle transmission

Recall Reflection Coefficient \( R = \frac{B*B}{A*A} \)
Transmission Coefficient \( T = \frac{F*F}{A*A} \)
(with \( k_1 = k_{III} \) - modified if \( U_I \neq U_{III} \))

If assume that \( E \ll U_o \) the maths simplifies and

\[
T \approx \frac{16}{4 + \left( \frac{k_2}{k_1} \right)^2} \exp(-2k_2L) \quad \text{or} \quad T \approx \exp(-2k_2L)
\]

Square bracket is of order unity. cf strong dependence in \( x \! \)!
Decay constant \( k_2 \) related to height of barrier \( (U_o - E) \)

Examples: Radioactive decay, scanning tunneling microscope…..
boundary matching and $|\psi|^2$ plot

(1) exclude $G \exp(-k_1 x)$ - no movement in -ve $x$ in region III ($G=0$)

(2) two boundaries $x = 0$ and $x = L$

(3) $|\psi|^2$ plot
region I: mix of travelling/standing - partial reflection
region II: exponential decay profile
region III: pure travelling wave (transmitted particles)
Scanning Tunneling Microscope (STM)

Sharp point (tip) close (~ 1 nm) to surface; under bias electrons tunnel across the gap (barrier potential width $z$)
Because of exponential dependence on $z$ (factor of ~10 for 1Å change when $U_o$ ~ 4 eV), tunnel current is very sensitive to variations in $z$ as tip is scanned across surface.
Keep current constant $\Rightarrow z$ const. $\Rightarrow$ tip height = image
Also, exponential dependence restricts to narrow region of tunneling, giving “atomic” resolution. $\Rightarrow$ Imaging atoms…
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 \(- p 11 \text{ of lecture 6} \)

\[
\psi = A \exp\left(-\frac{iEt}{\hbar} + \frac{ipx}{\hbar}\right) = Ae^{-iEt/\hbar} e^{ipx/\hbar}
\]

Now consider partial differential with \(x\)

\[
\frac{\partial \psi}{\partial x} = Ae^{-iEt/\hbar} \cdot \frac{ip}{\hbar} e^{ipx/\hbar} = \frac{ip}{\hbar} \psi
\]

Re-arranged: \(
\frac{\hbar}{i} \frac{\partial}{\partial x} \psi = p \psi
\)

Or: \(-i\hbar \frac{\partial}{\partial x} \psi = p \psi\)

\text{i.e.} \text{ if we “operate” on } \psi \text{ with } -i\hbar \delta/\delta x \text{ get the value of momentum } p \text{ multiplied by } \psi \quad \text{So } -i\hbar \delta/\delta x \text{ is the momentum ‘operator’ } \hat{p}\)

Expect Kinetic Energy operator \(\frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}\)

Total Energy Operator (Hamiltonian) \(\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x) \text{ and } \hat{H} \psi = E \psi\)

General Equation: \(\text{Operator on } \psi = \text{value } \times \psi\)
Know (Bohr model) that angular momentum is quantised in levels separated by $\hbar$.

By analogy with linear momentum, can define an angular momentum operator

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

So eigenvalue equation is $L_z\psi = b\psi$

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

BUT… cannot determine any pair of these $L_i$ together — there exists an uncertainty relation between any pair of $L_{xyz}$ (also next lecture)

However, total Angular momentum must be conserved.

Define total angular momentum operator $L^2$

Can determine this plus any single $L_i$ without uncertainty

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

Eigenvalue equation $\hat{L}^2\psi = a\psi$
Solving \( L_z \psi = b \psi \) gives...
a set of eigenvalues \( b \) each separated by \( \hbar \) (cf Bohr)

and that \( b \) can have values between \(+n\hbar/2\) and \(-n\hbar/2\)
where \( n \) is an integer. Write \( n\hbar/2 = l\hbar \)

If \( n \) is an even number then \( b \) has values \( n/2...2,1,0,-1,-1,-2...-n/2 \)
This is same as orbital angular momentum, seen before.

Solving for total angular momentum gives \( \hat{L}^2 \psi = a \psi = l(l+1)\hbar^2 \psi \)
and \( \hat{L}_z \psi = m\hbar \psi \quad |m| \leq l \quad l \) is the angular quantum number

But...What if \( n \) is an odd number?
⇒ an angular momentum of \( ...+\hbar/2, -\hbar/2... \)

‘Spin’ Angular momentum – no classical equivalent!
Spin angular momentum

Spin angular momentum is an inherent, quantum property of particles.

Particles having half-integral spin are Fermions \((\text{electron etc.})\)

Particles having integral spin are Bosons \((\text{photon etc.})\)

Now consider a quantum state with two particles:

Suppose we have two quantum states \(a(x)\) and \(b(x)\) each with a distinguishable particle in it.

*For example we might have an electron in state \(a\) and a proton in state \(b\).*

Now the probability of finding the electron in position \(x_1\) in state \(a\) is \(|a(x_1)|^2\) and likewise the probability of finding the proton at position \(x_2\) in state \(b\) is \(|b(x_2)|^2\).

If the two particles are not interacting then these probabilities are quite independent, so the joint probability of both is simply their product.

That means the composite state \(\psi\) describing both is given by

\[
\psi = A \ a(x_1) \ b(x_2)
\]

where \(A\) is a normalising constant

This is fine for *distinguishable* particles…. 
Identical particles

BUT: Electrons (and other particles) are NOT distinguishable - there are no identifying 'tags' on individual electrons!
- so the above argument about probabilities is incomplete.

*We need to allow for the probabilities that particle 1 might be in states a OR b, and vice versa for particle 2.*

**Composite state** should be \[ \psi = A \ a(x_1) \ b(x_2) + B \ a(x_2) \ b(x_1) \]

and \[ |A|^2 = |B|^2 \]

If we exchange the particles twice, we return to original state

*OK irrespective of signs of A or B*

But if **exchange once**, for A +ve, B could be +ve or –ve….

**Reality:** It’s –ve for Fermions and +ve for Bosons!

Means that if we try to get fermions 1 and 2 into same state then \[ \psi \rightarrow 0 \] !!!!

This is the **Pauli Exclusion Principle:**

No two fermions (electrons) can have the same quantum state.

⇒ **Can only have a spin up and a spin down electron in any atomic state**

*N.B. in contrast, Bosons ‘like’ to be in same state! (laser cavity etc.) “Exchange’ interaction – no classical equivalent*
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 $\pi/a$
(c.f. diagram from black body radiation - Lecture 5)

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

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

So total number of electrons up to $k_F$ is

$$N = \frac{2}{(\pi/a)^3} \frac{4 \pi k_F^3}{8}$$

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

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 – Lecture 11 - 12