PX101: Quantum Phenomena

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1 Introduction

Please note that this Quantum Mechanics revision guide is not intended as a stand alone publication and there is no substitute for hard graft and thorough thought (i.e. going to the lectures and doing the work sheet problems and practicing exam papers.) Having said that I hope any bits of the subject you may be unsure about are clarified and your understanding enriched by reading this.

2 The State of Affairs at the End of the 19th Century

This section explains what was held to be common belief at the end of the 19th Century when some believed the unified universal theorem was close at hand. This section should help to show why we need a quantum mechanical description of the universe.

- Wave behaviour was understood as a spatial pattern that fills all available space, a travelling wave would be described as:

$$u(\vec{x},t) = Acos(kx \pm \omega t) = Re[Ae^{i(kx-\omega t)}]$$

- Newton mechanics were established.
- Electricity and magnetism were summed up in Maxwell's Equations
- Thermodynamics was well understood - each degree of freedom contributes $\frac{kt}{2}$ energy to the system

I will now list the main characteristics of particles and waves and the way they were believe to behave at the time, hopefully highlighting their differences to you to show what an intellectual leap Quantum Mechanics was.
Particles

- Exist at a single location in space
- Are physical objects
- Only do one thing at a time
- Scatter off each other

Waves

- Fill all available space
- Are patterns of variations with a variable
- Encompasses many types of motion all at the same time
- Interact by interference

3 Light and all that Jazz

This section explains the formulation of a quantum description of light. This has a lot to do with thermal physics also since the primary source of light is from thermally excited electrons. More precisely light is emitted due to thermal excitations of the electric and magnetic fields associated with these particles.
Quite a lot of this uses the idea of a black body which is a perfect absorber and emitter of radiation. That is to say that it radiates all the power possile at a given temperature, T, and it emits and radiates all wavelengths of EM radiaion leading to a continuous spectrum.
Wien came up with this law:

$$I(\lambda) = \frac{ae^{-\frac{\sigma}{\lambda t}}}{\lambda^5}$$

where $I(\lambda)$ is the spectral emittence and the intensity $I = \int_0^\infty I(\lambda)d\lambda$
Now the important result that comes from this is that:

$$\lambda_m \Gamma = 2.9 \times 10^{-3} mK$$

where λ_m is the peak wavelength in the spectrum, Γ is temperature of the blackbody.
ie. The wavelength λ_m at which a black body radiates most strongly is inversely proportional to Γ
Another important formula to be aware of is the Rayleigh-Jeans formula which is:

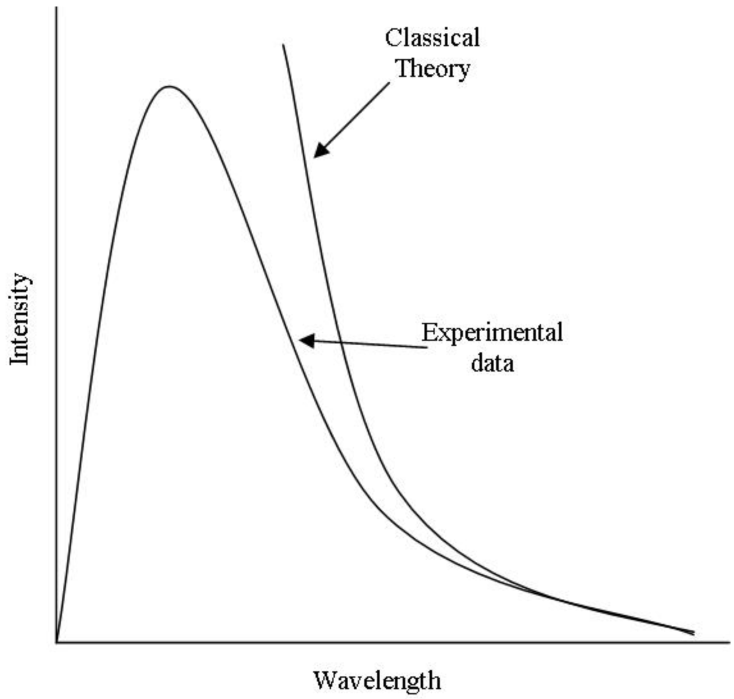
$$E(\lambda, \Gamma) = \frac{2Lk\Gamma\delta\lambda}{\lambda^2} \qquad \text{Where } n >> 1$$

$$I(\lambda, \Gamma) = \frac{2\pi lkT}{\lambda^4} \qquad \text{Where } \lambda << 2L$$

You should have a derivation for this in your notes, so I will not repeat it but the basic ideas is that we are summing the energy per mode for all modes between λ and $\lambda + \delta\lambda$
Where the contribution per mode is given by kT
Now the important thing to realise is that as we decrease λ, we have more modes per $\delta\lambda$ and thus more energy.
In a rather unrigorous way I think of this as assuming energies of the standing waves associated with the black body. ie. The modes are the associated standing waves.

3.1 The Ultraviolet Catastrophe - 1st Problem

Now these approximations lead to the first major problem for classical physics - the ultraviolet catastrophe, which is summed up in the graph below.



Essentially the Rayleigh-Jeans formula agrees with the observed intensity for large λ but as λ decreases the intensity tends to infinity, which does not agree with the observed intensity (and also implies an infinite amount of energy). This happens at ultra-violet wavelengths, hence the origin of the name "Ultra-Violet Catastrophe".

Planck came along to sort this out by hypothesising that energy could only be added in discrete amounts, $\Delta E = hf$. (This was pretty radical - but you already knew that). This leads to a suppression of energy per mode as λ decreases.

He also discovered a correspondence between energy of radiation and cavity walls as they are in equilibrium with one another and that atoms behave like simple harmonic oscillators.

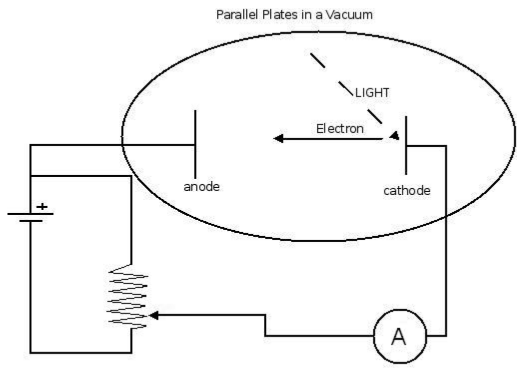
These led to Planck's law

$$I(\lambda) = \frac{2\pi hc^2}{\lambda^5} \frac{1}{e^{\frac{hc}{\lambda kt}} - 1}$$

which fits observed spectra and agrees with Rayleigh-Jeans formula for large λ.

3.2 Photo-Electric Effect - 2nd Problem

Setup:



The idea is that the incoming light gives energy to the cathode causing electrons to be released. By "making the anode negative", it can oppose e^- and stop current flowing. The minimum voltage required to do this gives a measure of the kinetic energy of the electrons.

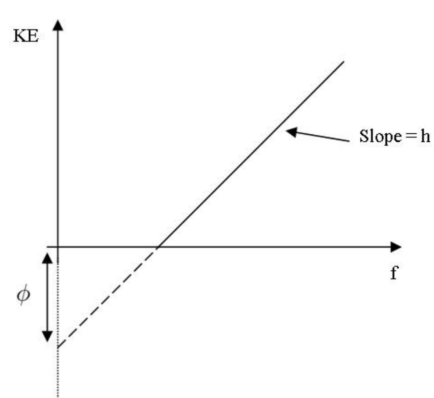
3.2.1 Observations

1. Varying cathode material at a fixed wavelength varies the stoppping voltage.
2. Maximum KE depends on λ (or f) of light, not intensity as proposed by Maxwell's classical wave theory.
3. No electrons emitted for a frequency less than a particular value (called the threshold frequency).

2 and 3 are problems for classical physics, which Einstein solved by extending Planck's idea to say that light travelled in distinct packets with energy $E = hf$ Giving us:

$$KE = hf - \phi$$

Where ϕ is the work function (amount of energy required to move an electron from surface of material).

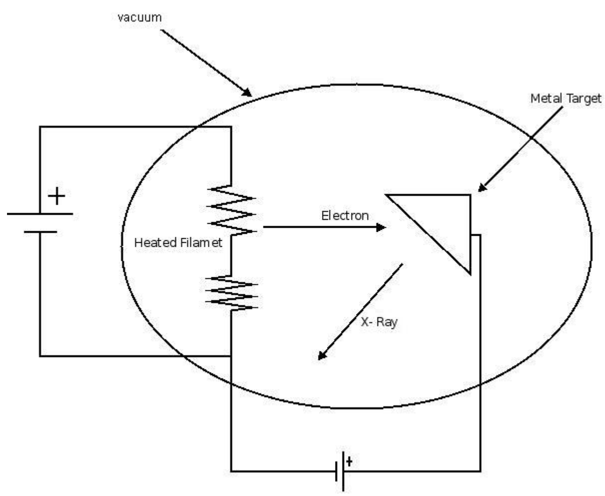


This had 2 major side effects when combined with special relativity, namely that for light with $v = c$ we obtain:

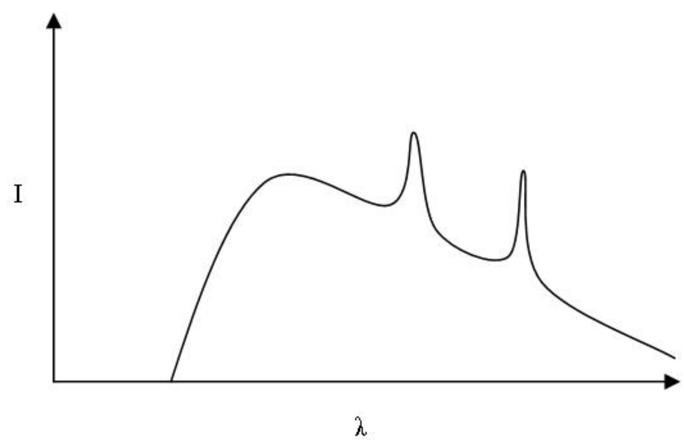
$$E = \gamma mc^2 = \frac{1}{\left(1 - \frac{v^2}{c^2}\right)^2} mc^2$$

This implies infinite energy unless $m = 0$, in turn impling that $p = \frac{E}{c} = \frac{h}{\lambda}$. I.e. a particle with zero mass can have momentum.

3.3 X-ray generation - 3rd Problem



The idea - Electrons are boiled off the filament and hit the target causing transfer of energy and emission of X-rays.
Observations



1. Minimum wavelength, below which no X-rays produced (Bremstralung radiation)
2. Characteristic lines of increased intensity at certain λ

These were both problems for classical physics. Number 1 is easily explained away by the photon model $E = hf$, as it corresponds to all the incoming electrons energy being converted into energy of the X-ray photon.

2 is explained by the allowed atomic energy transitions, specifically those which cause an X-ray photon to be produced, ie a photon of energy $E = hf = \left(\frac{hc}{\lambda}\right)$ is produced when electrons change energy levels, but only certain values of E are allowed within the atom. These energy differences correspond to the wavelengths of the spectral peaks and the characteristic lines of the graph.

3.4 Compton Effect - 4th Problem

Set up - see your handouts.

3.4.1 The Idea

We fire X-rays at a carbon target where the X-rays scatter, some elastically, and others inelastically. Then we measure the wavelength of both the elastically and inelastically scattered x-rays at various angles.

3.4.2 Observation

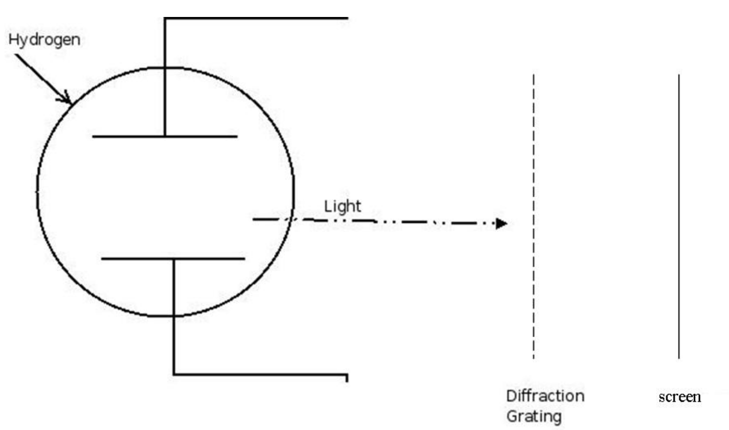
Difference between wavelengths of elastic and inelastic scatter peaks increase with increasing scattering angle.

$$\lambda' - \lambda = \frac{h}{mc}(1 - cos\theta) = \lambda_c(1 - cos\theta) \qquad \text{Where } \lambda_c = \text{Compton wavelength}$$

However our new quantum-mechanical description of light can use wave-particle duality to describe the diffraction in the monochromiter[1] (and the fact we have a monochromatic source) in terms of waves and the scattering at the taarget in terms of particles.

3.5 Lines of hydrogen - 5th problem

Set up



3.6 The idea

We heat up the hydrogen electrically and this causes it to emit light. We then analyse the "spectral emission".

[1]Calcite crystal

3.7 Observations

There are discrete spectral lines, i.e light is only emitted at certain well defined wavelengths (frequencies) given by Rydberg formula

$$\frac{1}{\lambda} = R(\frac{1}{m^2} - \frac{1}{n^2})$$

This was a problem for classical physics due to their "plum pudding" model of the atom so Bohr wandered in and used these discrete spectral lines and Rutherford Scattering[2] to propose a new model of the atom.
He proposed discrete energy level orbits of the electrons around the nucleus, implying the spectral lines were transitions between states.
He assumes circular orbits with angular momentum[3] [4]:

$$L_n = \frac{nh}{2x} \implies r_n = \frac{n^2}{z} a_0$$

Where the electrons are held in orbit by the electrostatic force, and a_0 is the Bohr radius.
This gives us $E_n = -\frac{1}{8}\frac{me^4z^2}{\epsilon_0^2 b^2 h^2}$ for the energies of the electrons in hydrogen like atoms with angular momentum $\frac{nh}{2\pi}$
At this point I feel it is a good time to mention Bohr's correspondence priniciple:

Quantum Physics should give the same results as classical physics in the limit of large quantum numbers.

This forms one of the postulates of the whole of quantum theory and is (pretty much) common sense. It says that everything you have found from experiments to be true (testing classical mechanics) must still be true if we use quantum mechanics.
Now this explains our discrete spectral lines for hydrogen as the lines we see are the wavelengths corresponding to the allowed transitions between orbits.
This also explains our characteristic lines in the X-ray generation. An electron is "knocked out" of its orbit by an incoming high energy electron. This leaves a "core hole" which another electron falls into whilst emitting a photon; whose energy corresponds to the difference in the energy of that electrons orbit and the energy of the orbit of the core hole.

4 De Broglie Hypothesis

De Broglie extended the idea of wave particle duality by saying all particles had an associated wavelength and in certain circumstances behaved like a wave.

$$\lambda = \frac{h}{p} \implies Ln = \frac{nh}{2\pi} = r_n p = \frac{r_n h}{\lambda}$$
$$\implies 2\pi r_n = n\lambda$$

I.e:the orbits of the electron can be thought of as standing waves occurring only when an integer number of wavelengths fit into 2π multiplied by the orbit.

[2]Rutherford scattering experiment was to fire α particles at a target. Most were scattered by small angles but some were deflected by large angles implying a dense positive charged nucleus of small diameter containing most of the mass of the atom.

[3]n runs like $1, 2, 3$...for future reference it is called the principle quantum number.

[4]

$$a_0 = \frac{\epsilon_0 h^2}{\pi m e^2}$$

for those who want to know!

5 Time dependent Schrödinger equation (TDSE)

All of the above leads us to the need of a wave equation which schrodinger gave us.
In 1D:

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = i\hbar\frac{\partial\psi}{\partial t}$$

In 3d:

$$\frac{-\hbar^2}{2m}\nabla^2\psi = i\hbar\frac{\partial\psi}{\partial t}$$

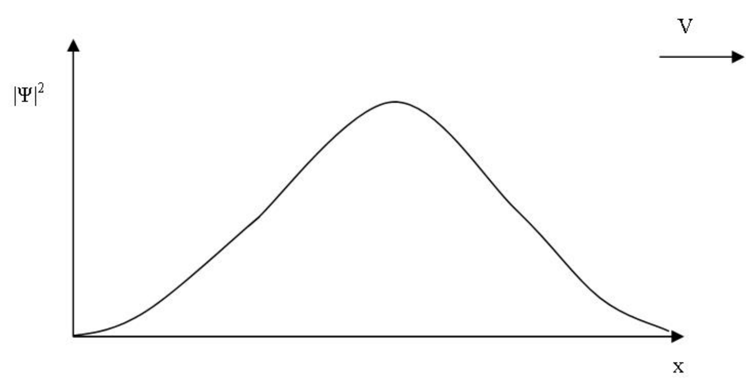
Which are valid for a free particle with mass m.
So the plane wave $e^{i(kx-\omega t)}$ is a solution although beware since $\cos(kx-\omega t)$ (without the imaginary part $i\sin(kx-\omega t)$ is not a solution.
You should make sure you know how to confirm whether a particular function is a solution or not as this regularly comes up in the exam.
ψ represents the probability of finding a particle in a point of space at a certain time (although to some extent is a little bit more difficult).
From this wave function we obtain the probability distribution/density function:

$$|\psi(x,t)|^2 = \psi(x,t)\psi^*(x,t)$$

Which again is a measure of the likelihood of finding a particle in all given locations within the space we are considering and set this equal to 1 (as we can't have a total probability more than 1).
This leads us to

$$\int_{allspace} |\psi(x,t)|^2 dx = 1$$

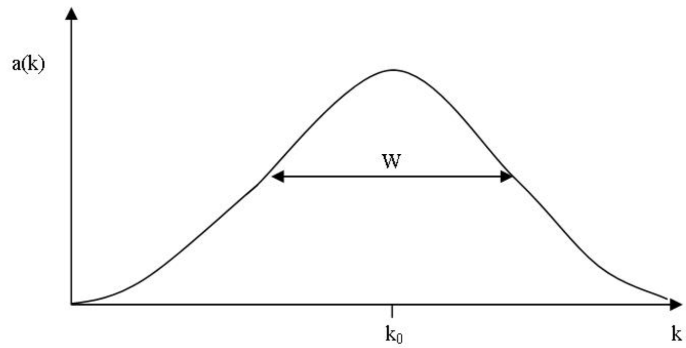
This process is called normalisation.
This leads to the property that wave functions cannot be infinite over finite regions of space. Here the reader should also note that all examples of solutions to the TDSE are not normalisable along an infinite line but are along a finite line.
For a particle travelling through space we would expect a probability density function of the form:



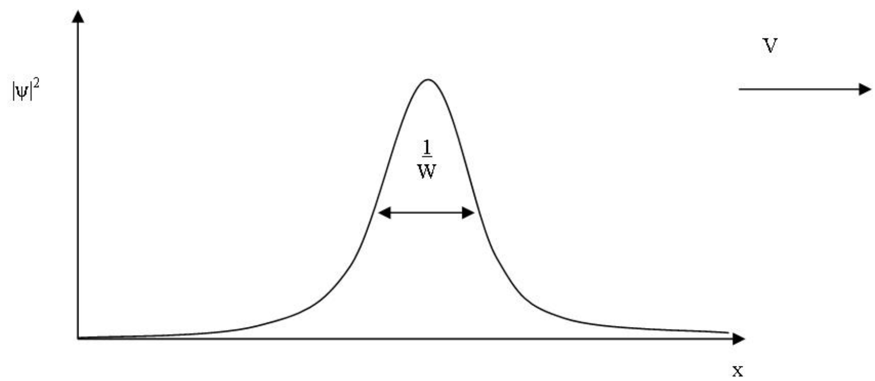
To obtain this we combine waves of similar k value to form a "wave packet". This gives us a wave function:

$$\psi = \int dk a(k) e^{i(kx-\omega t)}$$

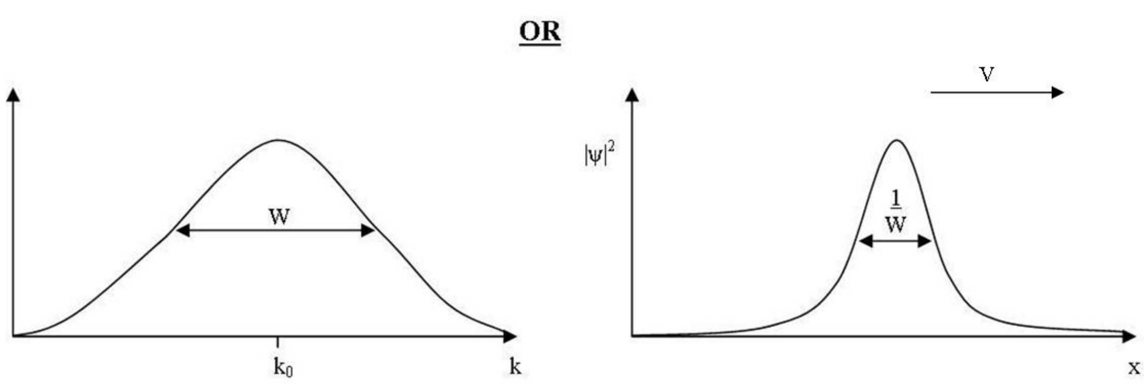
where $a(k)$ is a continuous distribution looking something like:



which is characterised by W, the full width at half maximum.
After some calculations, which you should have in your notes (and I would advise reading for a fuller understanding), we get a probability distribution as required with full width at half maximum of $\frac{1}{\omega}$ travelling with velocity v through space.



So what does this all mean? Well effectively it gives us 2 ways to view wave packets, as a distribution $a(k)$ with width W or as a function of real space with width $\frac{1}{w}$



ie. a wavepacket with width w can represent a particle with width $\frac{1}{w}$ in a localised region.
This relates very closely to the Heisenberg Uncertainty principle we have seen that:

1. a wide distribution of k values leads to a narrow probability density and therefore a narrow distribution in x

2. a narrow distribution of a k values leads to a wide probability density and therefore a wide distribution in x

Combining this with De Broglie's hypothesis in the form $p = \hbar k$, we see that a well defined k value and thus momentum (i.e a narrow distribution of our wave packet $a(k)$ leading to a wide distribution in x, $|\psi(x,t)|^2$, implies an ill defined position. Therefore a wave desciption is probably more suitable. An ill defined k value and thus momentum (a wide distribution of our wavepacket $a(k)$ leading to a narrow distribution in x, $|\psi(x,t)|^2$) implies a well defined position. Therefore a particle description is probably more suitable.
This leads to the Heisenberg Uncertainty Principle

$$\Delta x \Delta p \geq \frac{\hbar}{2} \text{ where } \Delta a = \sqrt{< a^2 > - < a >^2}$$

6 Non-Free Particle

Note the TDSE given is for a free particle, but we can adapt this for a non-free particle (for example, one in a potential such as an electric or magnetic field) by the addition of a potential term to the right hand side of the TDSE.

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial^2 x} + V(x,t)\psi(x,t)$$

Note now that the simple plane wave $\psi = e^{i(kx-\omega t)}$ is no longer (generally) a solution.
We can further simplify this by assuming V is just a function of x i.e $V(x)$.

7 Time Independant Schrödinger Equation (TISE)

From the above assumptions and an extra one in that $\psi(x,t)$ can be written as $\phi(x)\rho(t)$ we obtain the time independent schrodinger equation, namely:

$$-\frac{\hbar^2}{2m} \frac{d^2\phi}{dx^2} + V(x)\phi = E\phi$$

Where E is energy of the wave packet/particle. I would heavily recommend looking at your notes and the handout and make sure you can follow the derivation through, this will also help you to understand why the above assumptions are necessary.
Also note that $|\psi(x,t)|^2$ is independent of time and so becomes $|\psi(x)|^2$ i.e it varies with position, but not with time, although ψ may still vary with time. (Think about it).
Solutions of this type, where $|\psi(x,t)|^2 = |\psi(x)|^2$, are called stationary states.
There are 3 important things to know about stationary states:

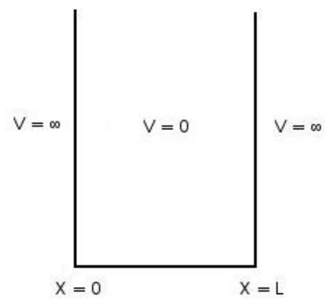
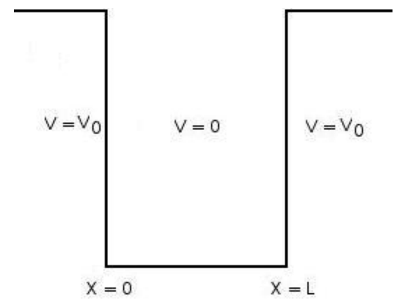
1. Probability doesn't change with time (although ψ will) meaning the likelihood of finding a particle in a particular position is constant.

2. Stationary states have a definitive constant energy, E.

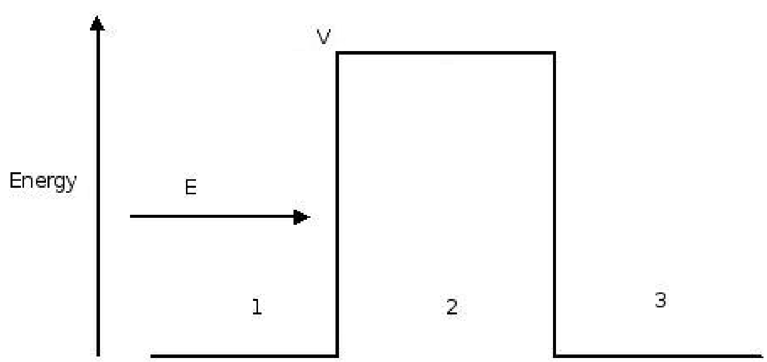
3. All other states are combinations of these stationary states.

7.1 Potential Wells

Here I will sum up what I believe to be the important bits of the 3 potentials you should be aware of, and continually come up on the exam. Note these solutions are of the form $\psi(x,t) = \phi(x)\rho(t)$.

	Infinite Potential Well	Finite Potential Well
Diagrams:		
Boundary Conditions:	$\phi(0) = \phi(L) = 0$	$\phi(x) \to 0$ as $\|x\| \to \infty$ otherwise we would have a wave function with infinite energy.
Solution:	$\phi = \left(\frac{2}{L}\right)^{\frac{1}{2}} sin\left(\frac{n\pi x}{L}\right)$ You should know what the wave functions and probability densities for those look like.	There is no analytical solution but you should still be aware of the general shape and how this differs from the infinite potential well, in that it can escape into the classically forbidden region where $(V_0 - E) < 0$. This would seem to imply a negative kinetic energy as $E = KE + V$ but we cannot measure the KE this precisely enough to say so, due to the uncertainty principle. The energies of the states are dependent on V_0 but they still share the same n^2 dependence

7.2 Finite Potential Barrier



Boundary conditions:

$$\text{where at } x = 0 \quad \phi_1 = \phi_2 \qquad \text{and at } x = L \quad \phi_2 = \phi_3$$

$$\frac{\partial \phi_1}{\partial x} = \frac{\partial \phi_2}{\partial x} \qquad\qquad \frac{\partial \phi_2}{\partial x} = \frac{\partial \phi_3}{\partial x}$$

Classically for a particle with energy E and $V = \sqrt{\frac{2E}{m}}$, the solution would be:

- If $E > V_0$: the particle continues with constant velocity.
- $E < V_0$ particle deflected.

However in QM:

- if $E > V_0$ it has a high probability of passing through the barrier but there is also a probability it will be reflected.
- if $E < V_0$ the wave function does not go to zero at $x = 0$ but it penetrates the step and decays until $x = L$, meaning that there is a probability that the particle will continue with the same velocity although this probability decreases with barrier length. Although it is more probable it won't.

Note that there is no probability of finding the particle in region 2 even though the wave function exists inside the barrier, this is because the wave function does not oscillate inside the barrier.

8 Conclusion

Well that's that. I reiterate that now you should really attempt some exam papers to apply the knowledge that you hopefully have gleaned from this guide. Learn the formulas and definitions and make sure you understand the main concepts involved. Finally I would just like to thank myself, my mum, my dad, all the editors and people who have helped to make this guide and you the (hopefully enlightened) reader. I leave you with the words of Voltaire

"They can conquer who believe they can."

Good Luck!