4.1   Interpretation of Ψ

The wavefunction describes something about how the particle is distributed in space but the fact that we needed to use complex numbers in our justification for the Schroedinger equation shows immediately that we should not attempt to give wavefunctions a physical existence in the same way as water waves have a physical existance. complex quantities cannot be measured by any actual physical instrument.

so we don't want to ask the questions like what is waving and what is it waving in. its questions like these that led to the aether in electromagnetism! but because our wave function here can be complex we are not tempted to make the same mistake again.

Instead, we should think of the wave function as containing all the information which the uncertainty principle allows us to know.

Going back to the double slit experiment, but turn down the intensity of the electon source so that only one electron comes through at a time. we can see the single hits on the screen where each electron lands (showing that individual electrons really are going through the slits). But after a while, when many 'single' particles have built up a pattern, we get the characteristic pattern of interference. Interference does not occur between electrons, but is a property of a single electron.

One single measurement does not have a predictable result - the electron hit can be anywhere in the pattern. only when we consider many identical systems do we get the full pattern. This suggests that for an individual particle the process is of a statistical nature, so it is telling us something about the *probability* that the particle will hit the screen at a certain point.

Our wavefunction is complex, but probabilities must be real. This suggests that we should associate probability $\propto |\Psi(x,t)|^2 = \Psi^*\Psi$ - this is always real for any complex number! Suppose $\Psi = a + ib$ where a, b are real. Then $\Psi^*\Psi = (a-ib)(a+ib) = a^2 + b^2$. And the square makes is similar to classical waves where the intensity of a wave $I \propto \text{Amplitude}^2$.

Then the probability of finding a particle between x and x+dx at time t is

$\propto |\Psi(x,t)|^2 dx$ and the interpretation of the wavefunction is a statistical one. We talk about the wavefunction of an individual particle but it is more useful to think about it as describing the behaviour expected from an ensemble of identical systems.

4.2   Normalisation

If we are interpreting $|\Psi(x,t)|^2$ as relating to probability of detection of the particle, then this means we have a normalisation condition since there is unity probability that the particle is SOMEWHERE i.e. if we integrate over all space $\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx = 1$

Then we can interpret $|\Psi(x,t)|^2 dx$ as the probability to find the particle within position $x \to x+dx$ at time t. $|\Psi(x,t)|^2$ is NOT in itself the probability - its the probability density function.

lets go into this with our 1D Schrodinger equation for a free particle $\Psi(x,t) = Ae^{i(kx-\omega t)}$. Then

$$\int_{-\infty}^{+\infty} \Psi^*(x,t)\Psi(x,t)dx = A^2 \int_{-\infty}^{+\infty} e^{-i(kx-\omega t)}e^{i(kx-\omega t)}dx = A^2 \int_{-\infty}^{+\infty} dx = \infty$$

Thats not a good start. Its because a plane wave along the x axis is completely delocalised - there is constant probability to find it anywhere along the x-axis. Our plane wave has definite momentum $p = \hbar k$ in the x-direction so $\Delta p = 0$ hence Δx is ∞ because of the Heisenburg uncertainty principle.

In practice we'd confine it by the experiment to a box of length $L >> \lambda$ (e.g. the size of the room!) so

$$A^2 \int_0^L e^{-i(kx-\omega t)}e^{i(kx-\omega t)}dx = A^2 L = 1$$

so then $A^*A = 1/L$ so we are free to choose this to be any (complex) number where $A^2 = 1/L$ eg $A = 1/\sqrt{L}$ or $A = -1/\sqrt{L}$ or $A = i/\sqrt{L}$ or $A = -i/\sqrt{L}$ or.... so pick the one which makes life easy and go for $A = 1/\sqrt{L}$. we know that we don't have a physical meaning for the wavefunction itself, only its square, so this phase doesn't matter.

so our normalised wavefunction is $\Psi(x,t) = 1/\sqrt{L}e^{i(kx-\omega t)}$. The probability of finding it in any section from x to $x + dx$ is $\Psi^*(x,t)\Psi(x,t)dx$ and $\Psi^*(x,t)\Psi(x,t)dx = dx/L$ so there is equal probability of finding a particle with this wavefunction anywhere in the box of size L

The animation linked from the webpage shows what this looks like for a particle travelling from left to right - the top panel shows the potential (black line, $U(x) = 0$) and the particle energy (green). The second panel shows the real (red) and imaginary (blue) part of the wavefunction.

$$\Psi(x,t) \propto e^{i(kx-\omega t)} = \cos(kx - \omega t) + i\sin(kx - \omega t)$$

so the real part (red) is $\propto \cos(kx - \omega t)$ and the imaginary is $\propto \sin(kx - \omega t)$ These are both travelling waves - they depend on time.

but the probability (bottom panel) is constant with time even though the $\Psi(x,t)$ are clearly not as $\Psi(x,t)^*\Psi(x,t) \propto e^{-i(kx-\omega t)}e^{i(kx-\omega t)} = 1$

if instead we had added together multiple waves of different wavelength to localise the electron (a wavepacket) then the different $\lambda \propto 1/p \propto 1/v$ so they have different velocities and the it spreads out (unlike photons which all travel at c)

5 time independent Schroedinger equation

The example above has $U(x,t) = U(x) = 0$, i.e. there is no external potential. More generally, if $U(x,t) = U(x)$ (so the potential is independent of time but is not necessarily zero) then the Schroedinger equation simplifies as the wavefunction is separable $\Psi(x,t) = \psi(x)T(t)$ e.g the free particle solution is $\Psi(x,t) = Ae^{i(kx-\omega t)} = Ae^{ikx}e^{-i\omega t} = \psi(x)e^{-iEt/\hbar}$ This time dependence is the same for ANY constant potential, so we can always write $\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$ and then get an equation for the spatial (time independent) part of the wavefunction for any energy E, separated out from its time dependence, and we can solve for it from the time independent Schroedinger equation which is now in standard not partial derivatives

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

The wave function $\Psi(x,t)$ for a state of definite energy E is the product of a time independent wavefunction $\psi_E(x)$ and its time dependence which is $e^{-iEt/\hbar}$.

States of definite energy are called stationary states because their probability distribution function is NOT dependent on time

$$|\Psi(x,t)|^2 = \Psi^*(x,t)\Psi(x,t) = \psi^*(x)[e^{-iEt/\hbar}]^*\psi(x)e^{-iEt/\hbar}$$

$$= \psi^*(x)e^{iEt/\hbar}\psi(x)e^{-iEt/\hbar} = \psi^*(x)\psi(x) = |\psi(x)|^2$$

5.1   particle in an infinite potential 1-D box

consider a particle trapped in a 1-D box by an infinite potential well at $x = 0$ and $x = L$. so $U(x) = \infty$ for $x < 0$ and $x > L$ while $U(x) = 0$ for $0 \leq x \leq L$.

$\psi(x)$ must be zero where the potential is infinite - there is no probability to find a particle here!

in the region $0 < x < L$ with $U(x) = 0$ then we are back to the free particle equation

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

when we looked at the solution of this for a particle travelling from left to right we had $\psi(x) = e^{ikx}$ but this is not zero for $x < 0$ (the free particle wave went over all space).

but a wave travelling from right to left is also a solution to the free particle Schroedinger equation $\psi(x) = e^{-ikx}$. And so a more general solution is the combination of the two:

$\psi(x) = Ae^{ikx} + Be^{-ikx}$. And physically this is what we actually expect from REFLECTION OF A WAVE FROM A BOUNDAY! (see linked animation!)

so then we have $\psi(x) = A[\cos(kx) + i\sin(kx)] + B[\cos(-kx) + i\sin(-kx)]$

$= A[\cos(kx)+i\sin(kx)]+B(\cos(kx)-i\sin(kx)] = (A+B)\cos(kx)+i(A-B)\sin(kx)$

we need $\psi(0) = 0$ so this means $A + B = 0$ i.e. $B = -A$ which is what we expect for complete reflection. so then $\psi(x) = 2iA\sin(kx) = C\sin(kx)$ where we simplify by setting $C = 2iA_1$.

but we also need $\psi(L) = 0$ so this means that $0 = C\sin(kL)$ which is satisfied for $kL = n\pi$ or $k = n\pi/L = 2\pi/\lambda$ so $\lambda = 2L/n$ for $n = 1, 2, 3\ldots$

The wavelength is QUANTISED into units which fit a (half) integer number of times into the box.

5.1.1 Normalisation

the probability to find the electron if we look over all space must be unity (its somewhere!)

$$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = \int_{-\infty}^{0} |\psi(x)|^2 dx + \int_{0}^{L} |\psi(x)|^2 dx + \int_{L}^{+\infty} |\psi(x)|^2 dx$$

$$= \int_{0}^{L} |\psi(x)|^2 dx = C^2 \int_{0}^{L} \sin^2 n\pi x/L dx$$

$\sin^2\theta = 1/2[1 - \cos(2\theta)]$ so we can evaluate - set $y = 2n\pi x/L$ so $dy = 2n\pi dx/L$

$$= C^2 \int_{0}^{L} 1/2[1 - \cos 2n\pi x/L]dx = C^2 \int_{0}^{L} 1/2 dx - C^2 \int_{0}^{2n\pi} \cos y(L/(2n\pi))dy$$

$$= C^2 L/2 - C^2(L/(2n\pi)[\sin y]_{0}^{2n\pi} = C^2 L/2$$

hence $C^2 = L/2 = C^*C$. We can choose $C = \sqrt{L/2}$ for simplicity.

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L} \quad E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \quad n = 1, 2, 3\ldots$$

5.1.2 Examples

what is the probability to find the electron within $0 \leq x \leq L/4$ in the $n = 1$ state? compare this to the classically expected probability?

$$2/L \int_0^{L/4} \sin^2(\pi x/L)dx = 2/L \int_0^{L/4} \frac{1}{2}[1 - \cos(2\pi x/L)]dx$$

$$= 1/L \int_0^{L/4} dx - 2/L \int_0^{L/4} \cos(2\pi x/L)dx$$

let $y = 2\pi x/L$ so $dy = 2\pi dx/L$ (remember to change the limits on the integral)

$$(1/L)(L/4) - 2/L1/2 \int_0^{2\pi L/(4L)} \cos y L dy/(2\pi) = 1/4 - 1/L(L/2\pi)[\sin y]_0^{\pi/2}$$

$$= 1/4 - 1/(2\pi) = 0.0908$$

challenge: sketch the probability distribution for the $n = 1$ state used above. Now sketch the one for the $n = 10$ state and the classical expectation. which one of $n = 1$ and $n = 10$ is closer to the classical case?