

Now we can solve this by adding some constraints - first,  $\psi^*\psi$  is going to be a probability density function so it'd better be normalisable i.e. FINITE so  $\psi$  should be finite.

**Region 1:**  $x < 0$

$\psi(x) = C_1e^{\rho x} + D_1e^{-\rho x}$ . As  $x \rightarrow -\infty$  then the term  $D_1e^{-\rho x} \rightarrow \infty!$  which is unphysical! Hence  $D_1 = 0$  in region 1, so the wavefunction here is  $\psi(x) = C_1e^{\rho x}$

**Region 3:**  $x > L$

$\psi(x) = C_3e^{\rho x} + D_3e^{-\rho x}$ . now we need to think about what happens as  $x \rightarrow \infty$  and now its the term  $C_3e^{\rho x} \rightarrow \infty$  so  $C_3 = 0$  and  $\psi(x) = D_3e^{-\rho x}$

Solving this in full generality is really nasty, so here we are just going to build physical intuition from the remaining constraints we know we must have - continuity of the wavefunction and its derivative.

when the potential  $U$  is large we must have something like the infinite potential well. But it has to have an exponential tail of  $\psi$  which extends into the classically forbidden region! We have to match the different wavefunction solutions (sines/cosines onto the exponential tail) smoothly across the boundary, and we have to match their derivatives smoothly across the boundary.

### comparison of infinite and finite square well potentials

its clear that with the finite potential  $U_0$  we have something like the infinite well for bound states with  $E < U_0$  for  $0 < x < L$  but with exponential tails which can extend into the classically forbidden regime ( $E < U_0$  for  $x < 0$  and  $x > L$ ). In the region  $x < 0$  we found  $\propto e^{\rho x}$  (as  $x$  is -ve! so the probability of finding the electron within a distance  $dx$  of  $x$  in this forbidden region is  $\propto \psi^*\psi dx = e^{\rho x}e^{\rho x} \propto e^{2\rho x}$ . For  $x > L$  the distance into the barrier is  $l = (x - L)$  rather than just  $x$ . so for  $x > L$  we see the probability  $\propto e^{-2l/l_0}$  where  $l_0 = 1/\rho$  is the characteristic length over which the particle extends into the forbidden region.

This makes a lot of sense as  $l_0 = 1/\rho = \hbar/\sqrt{2m(U_0 - E)}$ . The bigger  $U_0$  is compared to  $E$  i.e. the bigger the energy gap, the smaller the extent to

which the particle can penetrate into the forbidden region.

The fact that the wavefunction extends outside of the well means that the wavefunction in the well doesn't have to be so highly curved i.e. its wavelength is bigger for any given  $n$ , so its energy is lower than the same  $n$  in the infinite well.  $E_{n,finite} < E_{n,\infty}$ .

For any  $n$ , we have to join the exponential tails smoothly onto the bound oscillatory solution. so for odd  $n$  both tails are  $\propto +e^{-\rho l}$  whereas for even  $n$  they have +ve sign on one side, and -ve sign on the other. but remember probability doesn't care about the sign in front of the wavefunction (or whether its real or complex!). for a single energy state, probability  $\propto |\psi_n(x)|^2$

The finite well depth also means that there are only a finite number of bound states, instead of the infinite number in the infinite well.

so the link shows a finite well with otherwise the same properties as the infinite well. Now there are only 4 bound states, and the 4th one is ONLY JUST bound - the probability is peaking at the barrier at  $x = 0, L$  but there are still 4 maxima which are contained within the well.

## 7 Recepte to sketch a general bound wavefunction shape

1) find the regions the particle can exist i.e. where  $E > U$ . the time independent schroedinger equation here will be of the form  $d^2\psi/dx^2 = -k^2\psi$  where  $k^2 = 2m(E - U)/\hbar^2$  and  $E - U > 0$ . solutions are oscillatory  $\psi \propto A \cos kx + B \sin kx$

the lowest energy state will have a wavefunction with one maximum, the next will have 1 max and 1 min, then next will have 2 max, 1 min etc...

THESE WILL NOT GO TO ZERO at 0 and L due to the exponential tails leaking probability to the classically forbidden regions.

2) find the regions where the particle cannot exist i.e.  $E < U$ . The the

Schrodinger equation changes sign and we get  $d^2\psi/dx^2 = \rho^2\psi$   $\rho^2 = 2m(U - E)/\hbar^2$  and the solutions are exponential decaying.

higher energy states see less of a potential barrier, so they extend further into the forbidden region.

This leakage shifts the positions of the peaks in the allowed region towards the forbidden region. its like the wavefunction relaxes a little into the classically forbidden region. In the limit when  $E_n = U$  then the max/min in the allowed regions are at  $x=0$ , L!! in effect, when  $E \rightarrow U$  then all the particle energy is potential rather than kinetic so its going VERY slowly and there is a high probability to find the particle at this point.

## 8 1D finite well with unbound particles?

**example** we have a particle with energy  $E = 2U_0$  on the 1D finite well with potential  $U_0$  for  $x < 0$  and  $x > L$ , and  $U = 0$  for  $0 < x < L$

we split up the region into the three sections

region 1 is  $x < 0$  where  $U = U_0$  and  $E = 2U_0$

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

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

$$\frac{d^2\psi}{dx^2} = -k_1^2\psi$$

and we will have the sine/cosine oscillating wave solutions  $\psi \propto \sin k_1x$  where  $k_1^2 = 2m(E - U_0)/\hbar^2 = 2mU_0/\hbar^2$

in region 2  $0 < x < L$   $U = 0$ . the particle is still free so

$$\frac{d^2\psi}{dx^2} = -\frac{2m(E - U_0)}{\hbar^2}\psi$$

$$\frac{d^2\psi}{dx^2} = -k_2^2\psi$$

but now  $k_2^2 = 2m(E - U_0)/\hbar^2 = 2m2U_0/\hbar^2$

so  $k_2 = \sqrt{2}k_1$  so the wavelength changes at the well by  $\lambda_2 = 1/\sqrt{2}\lambda_1$  which makes sense as the particle has more kinetic energy in the well as it has less potential energy so its moving faster, has more momentum so shorter wavelength. Its its moving faster, then we have less chance to find it at any given point, so the amplitude will be lower.