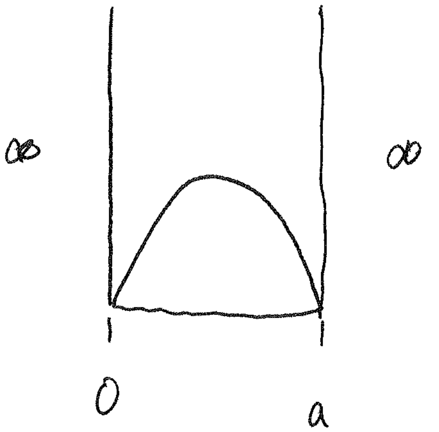
Time Dependent Potentials

So far we have only considered systems for which the potential energy is independent of time. Of course this is rather limiting - in the real world every time we do something to a system we are introducing time dependence, either in the potential or in the boundary conditions. It's useful to start by considering two extreme cases

1) A very sudden change which happens much faster than the time scale on which the system can react
2) A very slow change (adiabatic) which happens much slower than the time scale on which the system can react.

A. The Sudden Approximation

This is best illustrated by a simple example:

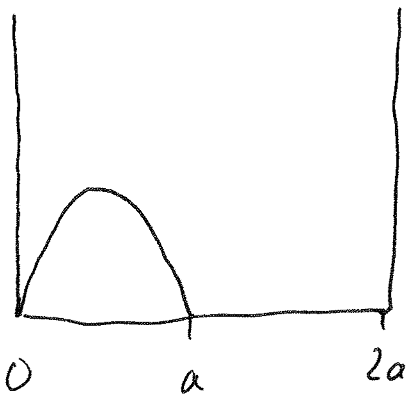


particle in the ground state of square well potential

$$\phi = \sqrt{\frac{2}{a}} \sin \frac{\pi x}{a}$$

energy $E = \dfrac{\hbar^2 \pi^2}{2ma^2}$

Now let's suddenly move the right hand wall to $2a$. This happens so fast that the wavefunction does not initially change



However of course this wavefn ϕ is <u>not</u> an eigenstate of the new Hamiltonian; these are

$$\chi_n = \sqrt{\frac{2}{2a}} \sin \frac{n\pi x}{2a} \quad \text{with } E_n = \frac{\hbar^2 n^2 \pi^2}{8ma^2}$$

and

$$\phi = \sum_n a_n \chi_n$$

$$a_n = \int_0^{2a} dx \, \phi \, \chi_n$$

$$= \int_0^a dx \sqrt{\frac{2}{a}} \sin\frac{\pi x}{a} \sqrt{\frac{1}{a}} \sin\frac{n\pi x}{2a}$$

$$\theta = \frac{\pi x}{2a}$$

$$= \frac{\sqrt{2}}{a} \int_0^{\pi/2} \frac{2a}{\pi} d\theta \sin 2\theta \sin n\theta$$

$$= \frac{\sqrt{2}}{\pi} \int_0^{\pi/2} \cos(n-2)\theta - \cos(n+2)\theta \quad d\theta$$

$$= \frac{1}{\sqrt{2}} \quad \text{if} \quad n = 2$$

$$= \frac{\sqrt{2}}{\pi} \left\{ + \left[\frac{\sin(n-2)\theta}{n-2} - \frac{\sin(n+2)\theta}{n+2} \right]_0^{\pi/2} \right\} \text{ otherwise}$$

$$= \frac{\sqrt{2}}{\pi} \left(-\sin\frac{n\pi}{2} \right) \frac{1}{n-2} - \frac{1}{n+2}$$

$$= -\frac{\sqrt{2}}{\pi} \sin\frac{n\pi}{2} \frac{4}{n^2-4}$$

So we see that:

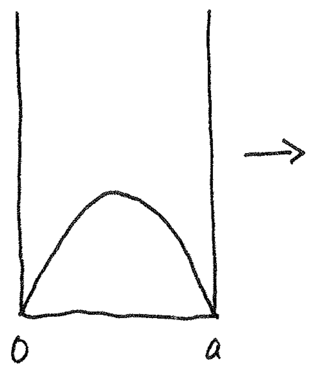
1. with probability $|a_2|^2 = \frac{1}{2}$ the particle is in the $n=2$ state which has energy $\frac{\hbar^2\pi^2}{2ma^2}$ – ie it's energy has not changed.

2. with probability $\frac{32}{\pi^2(n^2-4)^2} \sin^2\frac{n\pi}{2}$ the particle is in the state n with energy $\frac{\hbar^2 n^2 \pi^2}{8ma^2}$. This probability is clearly non-zero only if n is odd – and in every

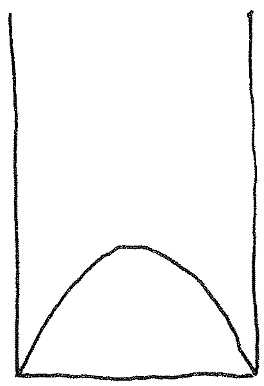
case the energy has changed. The particle has made a <u>transition</u> to a state of different energy; the difference in the two energies is provided, or absorbed, by the "environment" – in this case whatever device is moving the wall.

B. <u>The Adiabatic Approximation</u>

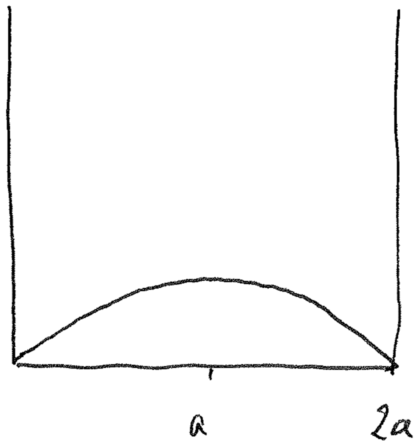
Start with same system as before



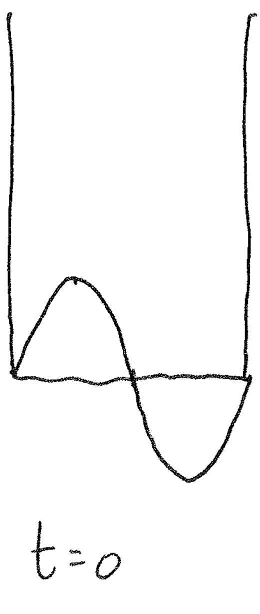
but this time move the wall <u>so slowly</u> that the wavefunction is able to spread out

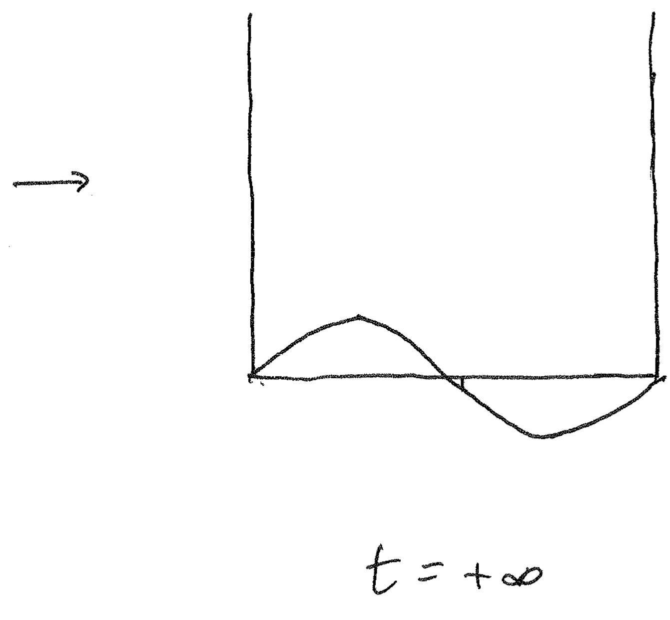


so now the particle always stays in the ground state and makes no transitions; when the wall gets to $2a$



Basically the rule is that for adiabatic changes the wavefunction deforms continuously into the wavefunction for the corresponding state of the new Hamiltonian; so the first excited state morphs into the new first excited state and so on





Now these sudden and adiabatic approximations are a useful way of thinking about things but we really need to know how fast, or how slow, the change has to be for the approximation to be a good one. To establish this more detailed calculation is required.

Time Dependent Perturbation Theory

We start with a time-independent Hamiltonian H_0 whose properties are known ie we know states $|n\rangle$

$$H_0 |n\rangle = E_n |n\rangle$$

(of course here n could stand for ~~more~~ a list of several quantum numbers; we will assume that $n=0$ labels the ground state). It's perfectly possible that we only know $|n\rangle$ and E_n up to some order of accuracy - eg from perturbation theory; this doesn't make any difference to what follows.

Now we add some time dependent perturbation $h(\underline{r}, t)$ to the Hamiltonian to get

$$H = H_0 + h$$

We want to find states $|\chi(t)\rangle$ such that

$$H |\chi\rangle = i\hbar \frac{\partial |\chi\rangle}{\partial t}$$

The full time-dependent states for H_0 are

$$|n, t\rangle = e^{-iE_n t/\hbar} |n\rangle$$

and we will exploit the fact that these form a complete set ~~to~~ so we can write

$$|\chi(t)\rangle = \sum_n a_n(t)\, |n,t\rangle$$

time dependent coefficients

substituting this in the Schrodinger equation

$$H|\chi(t)\rangle = \sum_n a_n(t)\,(H_0 + h)\,|n,t\rangle$$

$$= i\hbar \frac{\partial}{\partial t} \sum_n a_n(t)\,|n,t\rangle$$

$$= i\hbar \sum_n \dot{a}_n(t)\,|n,t\rangle + a_n(t) \frac{\partial}{\partial t}|n,t\rangle$$

so

$$\sum_n a_n(t)\, h\, |n,t\rangle = i\hbar \sum_n \dot{a}_n(t)\,|n,t\rangle$$

Taking matrix elements with $\langle m|$ gives

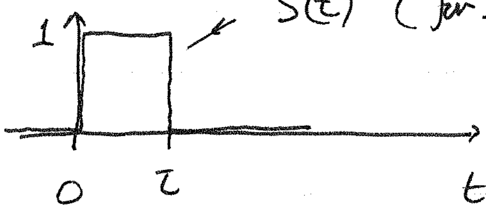
$$\sum_n a_n(t)\, \langle m|h|n\rangle\, e^{-iE_n t/\hbar} = i\hbar\, \dot{a}_m(t)\, e^{-iE_m t/\hbar}$$

or

$$\dot{a}_m(t) = \sum_n a_n(t)\, e^{i(E_m - E_n)t/\hbar} \langle m|h|n\rangle$$

This set of equations is exact; given a set of initial conditions $a_n(t=0)$ which specify $|\chi(0)\rangle$ they can always be solved but of course it's hard in general to write down the explicit solution

B. <u>Let's consider a simple example:</u>

$$h(\underline{r}, t) = V(\underline{r}) \times$$ 

$S(t)$ (for square fn)

and a two state system, $n = 0, 1$ starting in the ground state so

$$\left.\begin{array}{l} a_0(0) = 1 \\ a_1(0) = 0 \end{array}\right\} \; |\chi(0)\rangle = |0\rangle$$

Then

$$i\hbar \frac{d a_0}{dt} = a_0(t)\, S(t)\, h_{00} + a_1(t)\, e^{i(E_0 - E_1)t/\hbar}\, S(t)\, h_{01}$$

$$i\hbar \frac{d a_1}{dt} = a_0(t)\, e^{i(E_1 - E_0)t/\hbar}\, S(t)\, h_{10} + a_1(t)\, S(t)\, h_{11}$$

Note that if $h_{10} = 0$ (and so $h_{01} = 0$ too)

then $$i\hbar \frac{d a_1}{dt} = a_1(t)\, S(t)\, h_{11}$$

and since $a_1(0) = 0$, we find $a_1(t) = 0$ for $t > 0$

ie the probability of finding the system in state $|1\rangle$ at subsequent times is zero.

1st order approximation

if $h_{10} \neq 0$ then at small times  can be written

$$i\hbar \frac{da_1}{dt} = e^{i(E_1-E_0)t/\hbar}\, S(t)\, h_{10}$$

we've put $a_0(t) = 1$

which we can integrate

$$i\hbar\, a_1(t) = h_{10} \int_0^t e^{i(E_1-E_0)t/\hbar}\, S(t)\, dt$$

if $t < \tau$

$$i\hbar\, a_1(t) = h_{10} \int_0^t e^{i(E_1-E_0)t/\hbar}\, dt$$

$$= h_{10} \frac{\hbar}{i(E_1-E_0)} \left(e^{i(E_1-E_0)t/\hbar} - 1 \right)$$

$$a_1(t) = \frac{2i\, h_{10}}{E_0-E_1}\, e^{i(E_1-E_0)t/2\hbar} \sin \frac{(E_1-E_0)t}{2\hbar}$$

and if $t > \tau$

$$a_1(t) = \frac{2i\, h_{10}}{E_0-E_1}\, e^{i(E_1-E_0)\tau/2\hbar} \sin \frac{(E_1-E_0)\tau}{2\hbar}$$

at small $t \ll \tau$:

We see that for small t, the amplitude to find that the system has made a transition to the excited state grows linearly with time:

$$a_1(t) \simeq -i \frac{h_{10}\, t}{\hbar} \times \text{phase}$$

Of course it follows that

$$|a_0(t)|^2 = 1 - |a_1(t)|^2 = 1 - \left(\frac{h_{10}}{\hbar}\right)^2 t^2$$

Provided $(E_1 - E_0)\dfrac{\tau}{2\hbar} \ll 1$

it also follows that the entire effect of the perturbation (which is a pulse of duration τ) is to induce a transition from $|0\rangle$ to $|1\rangle$ with probability $\left(\dfrac{h_{10}\tau}{\hbar}\right)^2$

<u>at $t > \tau$</u>:

Let's suppose that the perturbation is small enough that it is always a good approximation that

$a_0(t) \simeq 1$.

This means that the $a_1(t)$ we compute must satisfy $a_1(t) \ll 1$ for all t ie that

$$\left|\frac{h_{10}}{E_0 - E_1}\right| \ll 1$$

Then the expression

$$a_1(t > \tau) = 2i\,\frac{h_{10}}{E_0 - E_1}\, e^{i(E_1 - E_0)\tau/2\hbar} \sin\frac{(E_1 - E_0)\tau}{2\hbar}$$

is accurate whatever the value of τ. We see that the probability to find the system in the excited state after a pulse of duration τ is

$$P(1) = \frac{4\,|h_{10}|^2}{(E_0-E_1)^2} \sin^2 \frac{(E_1-E_0)\tau}{2\hbar}$$

Note that it oscillates! There are values of τ for which it is zero. What's happening is that the effect of the perturbation is to induce transitions from the ground state to the excited state <u>and</u> from the excited state to the ground state. You'll learn in due course that this has massive implications – for example it is the basic process by which lasers work.

Of course this example shows us that there is a characteristic time scale for the system τ_0 given by

$$(E_1-E_0)\frac{\tau_0}{\hbar} = 1$$

if $\tau \ll \tau_0$ then $P(1) = |h_{10}|^2 \frac{\tau^2}{\hbar^2}$

if $\tau \gtrsim \tau_0$ then we get oscillatory behaviour