Time-dependent perturbation Theory

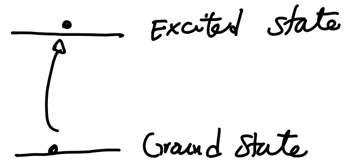
Note Title 3/27/2008

Electron scattering probability?

Fermi's Golden rule?

What causes an electron to transit from one state to another? (i.e. scatter?)

Transition $\equiv$ scattering



The cause is: change in potential V

This change in V can be slowly or abruptly. Let's first consider:

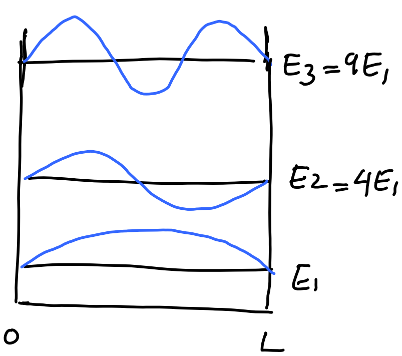
An abrupt change in potential

Consider an electron in a 1D infinity potential well;

$\sqrt{\frac{2}{L}} \sin k_3 x$

$\sqrt{\frac{2}{L}} \sin k_2 x$

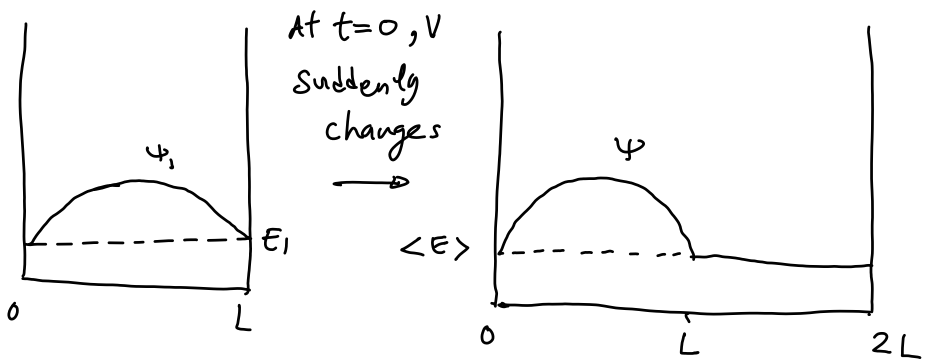
$\sqrt{\frac{2}{L}} \sin k_1 x$



$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin k_n x \quad \text{where } k_n = \frac{n\pi}{L} \quad n = 1, 2, \ldots$$

Suppose that the electron is in the ground state ψ_1. Suddenly at $t=0$ the well width changes from L to $2L$. This happens abruptly.

The question is, what effect this abrupt change in V has on the expectation value of the electron's energy $\langle E \rangle$, and on its state.



Let's look at the Eenergy:

At $t<0$: $\langle E \rangle = E_1$ because e is at ground state.

At $t>0$: the wavefunction is the same and is zero at $L<x<2L$. Thus the energy of electron is still $\langle E \rangle = E_1$

Note 1: $E\psi = \frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi$

$V = 0$ in both wells

Same ψ shape

energy must be similar.

Note 2: Be careful about the kink at $x=L$ (See sec. 3.1.1 of the book)

But for the wider well the eigenstate are different:

$$\psi_n = \sqrt{\frac{2}{2L}} \sin \frac{n\pi}{2L} x$$ ← for the wider well of 2L

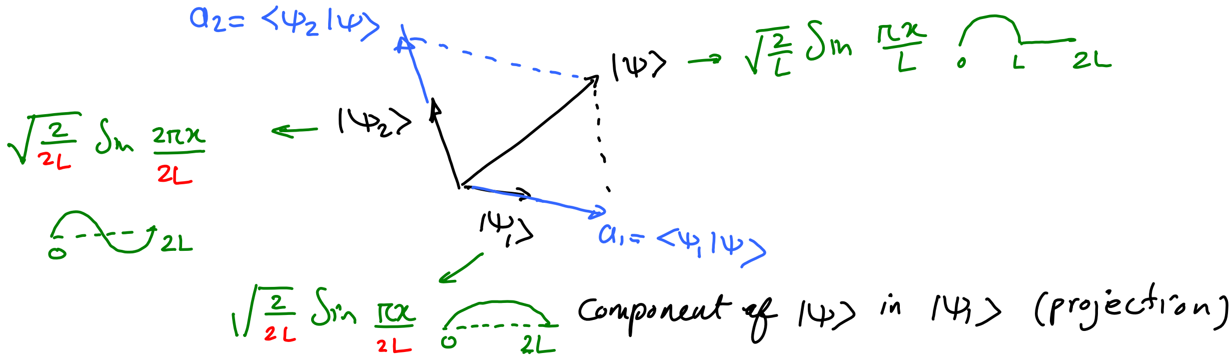
Obviously $\psi =$ 

is not an eigenstate. But we can expand it versus the eigenstates:

$$\psi = \sum_n a_n \psi_n \qquad \text{or:} \quad |\psi\rangle = \sum a_n |\psi_n\rangle$$

To find a_n: $\quad \langle \psi_m | \psi \rangle = \sum a_n \underbrace{\langle \psi_m | \psi_n \rangle}_{\delta_{nm}} = a_m$

So $\quad a_n = \langle \psi_n | \psi \rangle = \int \psi_n^*(x)\, \psi(x)\, dx \quad \leftarrow$ overlap integral



So for the electron in state $|\psi\rangle$, $|a_n|^2$ is the probability of finding the electron in the state ψ_n.

Let for example find the probability that the electron is in the ground state of the wide well $2L$:

$$a_1 = \langle \psi_1 | \psi \rangle = \int_{-\infty}^{\infty} \psi_1^*(x)\, \psi(x)\, dx$$

wide well

$$= \int_0^L \underbrace{\sqrt{\frac{1}{L}} \sin \frac{\pi x}{2L}} \; \underbrace{\sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}} \, dx$$

$$= \frac{\sqrt{2}}{L}\frac{1}{2}\int_0^L \left(\cos\frac{\pi x}{2L} - \cos\frac{3\pi x}{2L}\right)dx$$

$$= \frac{\sqrt{2}}{L}\frac{1}{2}\left(\frac{2L}{\pi}\sin\frac{\pi x}{2L}\Big|_0^L - \frac{2L}{3\pi}\sin\frac{3\pi x}{2L}\Big|_0^L\right)$$

$$= \frac{\sqrt{2}}{L}\frac{1}{2}\left(\frac{2L}{\pi} + \frac{2L}{3\pi}\right) = \frac{4\sqrt{2}}{3\pi} \rightarrow a_1^2 = \frac{(16)(2)}{9\pi^2} \simeq 0.36$$

So the electron in the wide well will be in the ground state of the wide well with the probability of 36%. We can calculate the probability that the electron will be in other states in the same way.

Now that we looked at an abrupt change in V, let's look for the more general case the V changes over the time.

Time-dependent change in potential

In general consider a system with Hamiltonian H_0. We know the solution to the time-independent Schrödinger equation:

$$\hat{H}_0 |n\rangle = E_n |n\rangle \qquad E_n = \hbar\omega_n$$

we know that $|n\rangle$ evolves in time according to:

$$|n,t\rangle = |n\rangle e^{-i\omega_n t}$$ so the Schrodinger equ. is:

$$H_0 \underbrace{|n\rangle e^{-i\omega_n t}}_{|n,t\rangle = \Phi_n(x,t)} = i\hbar\frac{\partial}{\partial t}\underbrace{|n\rangle e^{-i\omega_n t}}$$

Suppose at time $t=0$, we apply a time-dependent potential

$\hat{W}(t)$. So the new Hamiltonian is:

$$\hat{H} = \hat{H}_0 + \hat{W}(t)$$

Hence the wavefunction evolves as:

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = (\hat{H}_0 + \hat{W}(t))\,\psi(x,t)$$

We want to know how $\psi(x,t)$ is described versus the known eigenfunctions of the unperturbed system. or in other word, what are a_n's in the expansion of ψ by $|n\rangle$'s:

$$\psi(x,t) = \sum_n \underbrace{a_n(t)}_{?} |n\rangle e^{-i\omega_n t}$$

? (Now a_n is time dependent)

Substitute ψ in Schr. equ:

$$\underbrace{(H_0 + \hat{W}(t))}_{H} \underbrace{\sum a_n(t)|n\rangle e^{-i\omega_n t}}_{\psi} = i\hbar \frac{d}{dt} \underbrace{\sum_n a_n(t)\,|n\rangle e^{-i\omega_n t}}_{\psi}$$

$$= i\hbar \sum_n \left[\frac{\partial a_n}{\partial t}|n\rangle e^{-i\omega_n t} + a_n \underbrace{\frac{\partial}{\partial t}\left(|n\rangle e^{-i\omega_n t}\right)}_{\frac{1}{i\hbar}\hat{H}_0 |n\rangle e^{-i\omega_n t}} \right]$$

$$= i\hbar \sum_n \frac{\partial a_n}{\partial t}|n\rangle e^{-i\omega_n t} + \underbrace{\sum a_n \hat{H}_0 |n\rangle e^{-i\omega_n t}}_{=\sum \hat{H}_0 a_n |n\rangle e^{-i\omega_n t}}$$

As a_n is only a function of time and $\hat{H}_0$ is a spatial operator.

$$\left(\cancel{H_0} + \hat{W}(t)\right) \sum a_n |n\rangle e^{-i\omega_n t} = i\hbar \sum_n \frac{\partial a_n}{\partial t} |n\rangle e^{-i\omega_n t} + \cancel{H_0 \sum a_n |n\rangle e^{-i\omega_n t}}$$

$$\sum a_n(t)\, \hat{W}(t)\, |n\rangle e^{-i\omega_n t} = i\hbar \sum_n |n\rangle e^{-i\omega_n t} \frac{\partial a_n}{\partial t}$$

$\downarrow$

change in H (there is no derivative)

$$\sum_n \langle m| a_n \hat{W} |n\rangle e^{-i\omega_n t} = i\hbar \sum_n \underbrace{\langle m | n\rangle}_{\delta_{mn}} e^{-i\omega_n t} \frac{\partial a_n}{\partial t}$$

$$\sum_n a_n(t) \langle m | \hat{W}(t) | n\rangle e^{-i\omega_n t} = i\hbar\, e^{-i\omega_m t} \frac{da_m}{dt}$$

$$i\hbar \frac{da_m}{dt} = \sum_n a_n(t) \underbrace{\langle m | \hat{W} | n\rangle}_{W_{mn} = \int \varphi_m^*(x)\, \varphi_n(x)\, dx} e^{i\underbrace{(\omega_m - \omega_n)}_{\omega_{mn}} t}$$

$$\boxed{i\hbar \frac{da_m}{dt} = \sum_n^N a_n(t)\, W_{mn}\, e^{i\omega_{mn} t}}$$

Recall that we are looking for $a_n(t)$'s. The above relation gives N coupled differential equations that we need to solve to find a_n's.

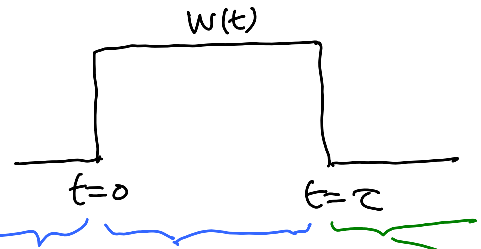
Example

Consider a system in its ground state. So:

$$\begin{cases} a_0 = 1 \\ a_n = 0 \quad n = 0, 1, \ldots \end{cases} \qquad \text{or } a_n = \delta_{n0}$$

At $t=0$ there is step change in potential that last for τ

time and then becomes zero.



Wavefunction

$\hat{H}_0|n\rangle = E_n|n\rangle$

$E_n = \hbar\omega_n$

$\psi(t) = |0\rangle$

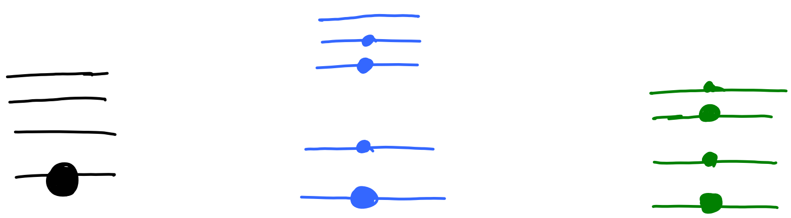
$\psi(t) = \sum \underbrace{a_n(t)}_{?} |n\rangle e^{-i\omega_n t}$

$\hat{H}_0|n\rangle = E_n|n\rangle$

$\psi(t) = \sum a_n(t) |n\rangle e^{-i\omega_n t}$

Energy

Ground state



First Order time-dependent perturbation

We derived a set of ODE's that can result in exact solution.

But now, we like to find some easier to calculate approach based on first order approximation.

Assume at $t<0$, the system is in state $|n\rangle \Rightarrow a_n=1,\ a_{m\neq n}=0$

Recall our final result:

$$i\hbar \frac{da_m}{dt} = \sum_n^N a_n(t) W_{mn} e^{i\omega_{mn} t}$$

Assume at $t=0$: $a_n(0)=1$, $a_{m\neq n}(0)=0$. So:

$$i\hbar \frac{da_m}{dt} = W_{mn} e^{i\omega_{mn} t} \qquad \text{at } t=0$$

$\hookrightarrow$ Matrix element couples $|m\rangle$ and $|n\rangle$ and generates $\underset{m\neq n}{a}(t)$'s for $t>0$.

$$\Rightarrow \qquad \boxed{a_m(t) = \frac{1}{i\hbar} \int_{t'=0}^{t'=t} W_{mn} e^{i\omega_{mn} t'} dt'}$$

Asume that the state $|n\rangle$ is not degenerate. We can write then:

$$|\psi\rangle = \sum_m a_m(t) e^{-i\omega_m t} |m\rangle$$

Perturbed $\qquad\qquad$ unperturbed

If the perturbation is small $|a_m|^2 \ll 1$ for $m\neq n$

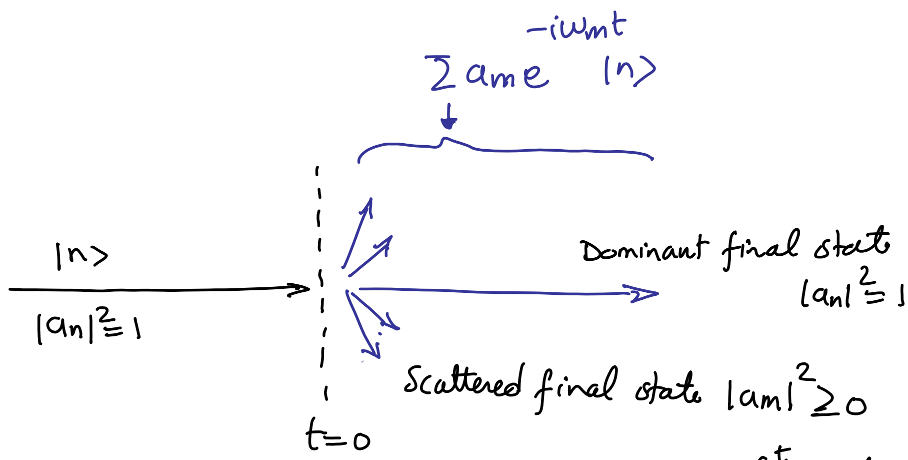
And we can assume $a_n \simeq 1 \Rightarrow$

$$|\psi\rangle = e^{-i\omega_n t} |n\rangle + \sum_{m\neq n} \underbrace{a_m(t)} e^{-i\omega_m t} |n\rangle$$

$$\boxed{\psi(x,t) = e^{-i\omega_n t} \varphi_n(x) + \sum_{m\neq n} \frac{1}{i\hbar} \int_{t'=0}^{t'=t} W_{mn} e^{i\omega_{mn} t'} dt' \, e^{-i\omega_m t} \varphi_n(x)}$$

First order perturbation theory

Note: This has a normalization problem that has to be considered



$$a_m = \frac{1}{i\hbar}\int^t W_{mn} e^{i\omega_{mn} t} dt$$

Fermi's Golden rule

What is the transition probability for the particle to scatter from state $|n\rangle$ to $|m\rangle$ due to a perturbation $\hat{W}(t)$?

Recall:

$$a_m(t) = \frac{1}{i\hbar}\int_0^t W_{mn} e^{i\omega_{mn} t} dt$$

If $\hat{W}(t)$ doesn't change with time:

$$P_n(t) = |a_m(t)|^2 = \frac{1}{\hbar^2}\left|\int_0^t W_{mn} e^{i\omega_{mn} t} dt\right|^2 = \frac{|W_{mn}|^2}{\hbar^2}\left|\int_0^t e^{i\omega_{mn} t} dt\right|^2$$

$$= \frac{|W_{mn}|^2}{\hbar^2}\frac{1}{\omega_{mn}^2}\left|e^{i\omega_{mn} t} - 1\right|^2$$

$$e^{ix} - 1 = e^{ix/2}\left(e^{ix/2} - e^{-ix/2}\right) = e^{ix/2}\, 2i \sin\frac{x}{2} \Rightarrow$$

$$|e^{ix} - 1| = 2 \sin\frac{x}{2}$$

$$|a_m(t)|^2 = \frac{|W_{mn}|^2}{\hbar^2} \frac{\sin^2 \frac{\omega_{mn} t}{2}}{\left(\frac{\omega_{mn}}{2}\right)^2}$$

Now take the long time limit and the relation;

$$\left. \frac{\sin^2(xt)}{\pi t x^2} \right|_{t \to \infty} = \delta(x)$$

$$\Rightarrow \quad P_n(t) = \frac{|W_{mn}|^2}{\hbar^2} \pi t \, \delta\left(\frac{\omega_{mn}}{2}\right)$$

Using the fact that $\delta(ax) = \frac{\delta(x)}{|a|} \Rightarrow$

$$\delta\left(2\hbar \times \frac{\omega_{mn}}{2}\right) = \frac{\delta(\omega_{mn}/2)}{2\hbar} \Rightarrow \delta\left(\frac{\omega_{mn}}{2}\right) = 2\hbar \, \delta(\hbar \omega_{mn}) \Rightarrow$$

$$P_n(t) = \frac{2\pi t}{\hbar} |W_{mn}|^2 \delta(\hbar \omega_{mn})$$

$$P_n(t) = \frac{2\pi t}{\hbar} |W_{mn}|^2 \delta(E_m - E_n)$$

If there are continous states with density of $D(E)$:

$$P_n(t) = \frac{2\pi t}{\hbar} \int |W_{mn}|^2 D(E_m) \, \delta(E_m - E_n) \, dE_m$$

The transition rate is the time derivative:

$$\frac{dP_n}{dt} = \frac{2\pi}{\hbar} |W_{mn}|^2 D(E_m) \, \delta(E_m - E_n)$$

This is the probability life time $1/\tau_n$

Fermi's Golden rule

$$\boxed{\frac{1}{\tau_n} = \frac{2\pi}{\hbar} |W_{mn}|^2 D(E_m) \delta(E_m - E_n)}$$