Adiabatic and sudden change for the perturbation

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((**Adiabatic approximation**))

If the Hamiltonian changes very slowly with the time, one can expect to be able to approximate solutions of the Schrödinger equation by means of the stationary energy eigenfunction of the instantaneous Hamiltonian. So that a particular eigenfunctions at one time goes over continuously into the corresponding eigenfunction at a later time.

((**Sudden approximation**))

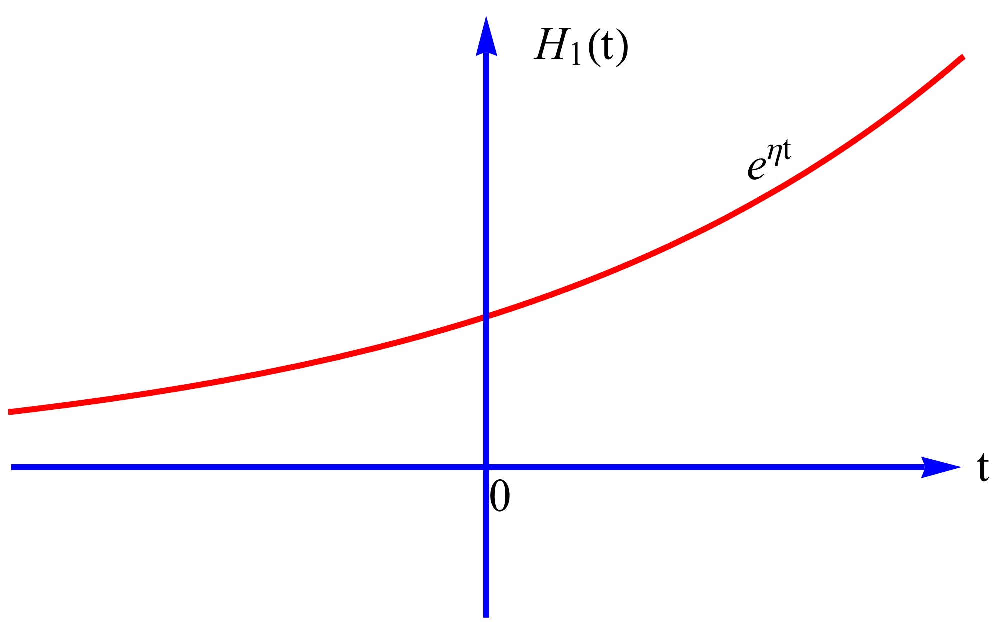
If the Hamiltonian changes from one steady form to another over very short time interval, one expect that the wavefunction does not change much, although the expansion of this function in eigenfunctions of the initial and final Hamiltonian may be quite different.

1. Adiabatic and sudden change

Suppose that the Hamiltonian has the form

$$\left(\hat{H}_1\right) = e^{\eta t}\hat{V} \qquad (V = \text{constant})$$

where η is a small positive value.



The time evolution operator in the Dirac picture is given by

$$\hat{U}_I(t,-\infty) = \hat{1} + \left(\frac{-i}{\hbar}\right)\int_{-\infty}^{t} e^{i\hat{H}_0 t'/\hbar}\hat{V}e^{\eta t'}e^{-i\hat{H}_0 t'/\hbar}dt'$$
$$+\left(\frac{-i}{\hbar}\right)^2 \int_{-\infty}^{t} dt' \int_{-\infty}^{t'} dt'' e^{i\hat{H}_0 t'/\hbar}\hat{V}e^{\eta t'}e^{-i\hat{H}_0 t'/\hbar}e^{i\hat{H}_0 t''/\hbar}\hat{V}e^{\eta t''}e^{-i\hat{H}_0 t''/\hbar} + \cdots$$

and

$$c_n(t) = \langle n|\hat{U}_I(t,-\infty)|i\rangle$$
$$= \delta_{ni} + \left(\frac{-i}{\hbar}\right)\langle n|\hat{V}|i\rangle \int_{-\infty}^{t} e^{\eta t'}e^{i\omega_{ni}t'}dt'$$
$$+\left(\frac{-i}{\hbar}\right)^2 \sum_k \int_{-\infty}^{t} dt' \int_{-\infty}^{t'} dt'' e^{iE_n t'/\hbar}\langle n|\hat{V}|k\rangle e^{\eta t'}e^{-iE_k t'/\hbar}e^{iE_k t''/\hbar}\langle k|\hat{V}|i\rangle e^{\eta t''}e^{-iE_i t''/\hbar} + \cdots$$
$$= \delta_{ni} + \left(\frac{-i}{\hbar}\right)\langle n|\hat{V}|i\rangle \frac{e^{\eta t + i\omega_{ni}t}}{\eta + i\omega_{ni}}$$
$$+\left(\frac{-i}{\hbar}\right)^2 \sum_k \langle n|\hat{V}|k\rangle\langle k|\hat{V}|i\rangle \int_{-\infty}^{t} dt' \int_{-\infty}^{t'} dt'' e^{i\omega_{nk}t'}e^{i\omega_{ki}t''}e^{\eta t'}e^{\eta t''} + \cdots$$

where $\langle k|\hat{V}|i\rangle$ is the matrix of the perturbation in the Schrödinger picture. Here we note that

$$\int_{-\infty}^{t} e^{\eta t'}e^{i\omega_{ni}t'}dt' = \frac{e^{(i\omega_{ki}+\eta)t'}}{i\omega_{ki}+\eta}$$

$$\int_{-\infty}^{t} dt' \int_{-\infty}^{t'} dt'' e^{(i\omega_{nk}+\eta)t'}e^{(i\omega_{ki}+\eta)t''} = \int_{-\infty}^{t} dt' e^{(i\omega_{nk}+\eta)t'}\frac{e^{(i\omega_{ki}+\eta)t'}}{(i\omega_{ki}+\eta)}$$
$$= \frac{1}{(i\omega_{ki}+\eta)}\frac{e^{(i\omega_{nk}+i\omega_{ki}+2\eta)t}}{(i\omega_{nk}+i\omega_{ki}+2\eta)}$$

where the Bohr angular frequency is defined by

$$\omega_{ni} = \frac{1}{\hbar}(E_n^{(0)} - E_n^{(i)}).$$

We now consider the second term

$$c_n^{(1)}(t) = -\frac{i}{\hbar}\langle n|\hat{V}|i\rangle \frac{e^{\eta t + i\omega_{ni}t}}{\eta + i\omega_{ni}},$$

$$\left|c_n^{(1)}(t)\right|^2 = \frac{1}{\hbar^2}\left|\langle n|\hat{V}|i\rangle\right|^2 \frac{e^{2\eta t}}{\eta^2+\omega_{ni}^2}.$$

((**Note**))

When $t = 0$,

$$c_n^{(1)}(t=0) = -\frac{i}{\hbar}\langle n|\hat{V}|i\rangle \frac{1}{\eta + i\omega_{ni}}.$$

In the limit of $\eta \to 0$, we have

$$\lim_{\eta\to 0} c_n^{(1)}(t=0) = -\frac{i}{\hbar}\langle n|\hat{V}|i\rangle \frac{1}{i\omega_{ni}} = -\frac{\langle n|\hat{V}|i\rangle}{\hbar\omega_{ni}} = \frac{\langle n|\hat{V}|i\rangle}{E_i^{(0)} - E_n^{(0)}}.$$

On the other hand, this is the same as the co-efficient of the expansion in the time-independent perturbation such that

$$|\psi_n\rangle = |i\rangle + \sum_{n\neq i} |n\rangle \frac{\langle n|\hat{H}_1|i\rangle}{E_i^{(0)} - E_n^{(0)}}.$$

The derivative of $\left|c_n^{(1)}(t)\right|^2$ with respect to t is given by

$$\frac{d}{dt}\left|c_n^{(1)}(t)\right|^2 = \frac{2}{\hbar^2}\left|\langle n|\hat{V}|i\rangle\right|^2 \frac{\eta e^{2\eta t}}{\eta^2+\omega_{ni}^2}.$$

Using the formula,

$$\lim_{\eta\to 0} \frac{\eta}{\eta^2+\omega_{ni}^2} = \pi\delta(\omega_{ni}) = \pi\hbar\delta(E_n - E_i)$$

we get

$$\frac{d}{dt}\left|c_n^{(1)}(t)\right|^2 = \frac{2\pi}{\hbar}\left|\langle n|\hat{V}|i\rangle\right|^2 \delta(E_n - E_i)$$

which coincides with the Fermi's golden rule.

Note that

$$\lim_{\varepsilon \to +0} \frac{1}{x \pm i\varepsilon} = P\left(\frac{1}{x}\right) \mp i\pi\delta(x),$$

$$\int_{-\infty}^{\infty} \frac{f(x)}{x+i\varepsilon} dx = P\int \frac{f(x)}{x} dx + \int_{C_1} \frac{f(z)}{z} dz,$$

$$\int_{C_1} \frac{f(z)}{z} dz = \int_{\pi}^{0} \frac{f(\varepsilon e^{i\theta})}{\varepsilon e^{i\theta}} \varepsilon e^{i\theta} i d\theta$$

$$= -f(0)\int_{0}^{\pi} i d\theta = -\pi i f(0) = -\pi i \int f(x)\delta(x) dx$$

Similarly,

$$\int_{C_2} \frac{f(z)}{z} dz = \pi i f(0) = \pi i \int f(x)\delta(x) dx$$

$$\Rightarrow \begin{cases} \dfrac{1}{x+i\varepsilon} = P\left(\dfrac{1}{x}\right) - \pi i\delta(x) \\ \dfrac{1}{x-i\varepsilon} = P\left(\dfrac{1}{x}\right) + \pi i\delta(x) \end{cases}$$

$$-\frac{1}{x-i\varepsilon} + \frac{1}{x+i\varepsilon} = \frac{x - i\varepsilon - x - i\varepsilon}{x^2+\varepsilon^2} = -2\pi i\delta(x)$$

or

$$\frac{-2i\varepsilon}{x^2+\varepsilon^2} = -2\pi i\delta(x)$$

$$\frac{\varepsilon}{x^2+\varepsilon^2} = \pi\delta(x) \qquad (\varepsilon \to 0)$$

The third term is given by

$$c_n^{(2)}(t) = \left(-\frac{i}{\hbar}\right)^2 \sum_k \langle n|\hat{V}|k\rangle\langle k|\hat{V}|i\rangle \frac{e^{2\eta t + i\omega_{ni} t}}{(2\eta + i\omega_{ni})(\eta + i\omega_{ki})}$$

2. Relaxation

We now consider the case for *n* = *i* (*i* denotes the initial state, but not imaginary); in other words, the final state *n* is the same as the initial state.

$$c_i^{(1)}(t) = -\frac{i}{\hbar}\langle i|\hat{V}|i\rangle \frac{e^{\eta t}}{\eta}$$

$$c_i^{(2)}(t) = \left(-\frac{i}{\hbar}\right)^2 \sum_k \left|\langle i|\hat{V}|k\rangle\right|^2 \frac{e^{2\eta t}}{2\eta(\eta + i\omega_{ki})}$$

Thus

$$c_i(t) \approx c_i^{(1)}(t) + c_i^{(2)}(t) = 1 - \frac{i}{\hbar\eta}\langle i|\hat{V}|i\rangle e^{\eta t} - \frac{1}{\hbar^2}\left|\langle i|\hat{V}|i\rangle\right|^2 \frac{e^{2\eta t}}{2\eta^2} + \left(-\frac{i}{\hbar}\right)^2 \sum_{k\neq i} \left|\langle i|\hat{V}|k\rangle\right|^2 \frac{e^{2\eta t}}{2\eta(\eta + i\omega_{ki})}$$

$$\dot{c}_i(t) \approx \dot{c}_i^{(1)}(t) + \dot{c}_i^{(2)}(t) = -\frac{i}{\hbar}\langle i|\hat{V}|i\rangle e^{\eta t} - \frac{1}{\hbar^2\eta}\left|\langle i|\hat{V}|i\rangle\right|^2 e^{2\eta t} + \left(-\frac{i}{\hbar}\right)^2 \sum_{k\neq i} \left|\langle i|\hat{V}|k\rangle\right|^2 \frac{e^{2\eta t}}{\eta + i\omega_{ki}}$$

When $e^{\eta t} \to 1$, $e^{2\eta t} \to 1$,

$$\frac{\dot{c}_i(t)}{c_i(t)} = \frac{-\frac{i}{\hbar}\langle i|\hat{V}|i\rangle - \frac{1}{\hbar^2\eta}\left|\langle i|\hat{V}|i\rangle\right|^2 + \left(-\frac{i}{\hbar}\right)^2 \sum_{k\neq i}\left|\langle i|\hat{V}|k\rangle\right|^2 \frac{1}{\eta + i\omega_{ki}}}{1 - \frac{i}{\hbar\eta}\langle i|\hat{V}|i\rangle}$$

$$= -\frac{i}{\hbar}\langle i|\hat{V}|i\rangle - \frac{1}{\hbar^2\eta}\left|\langle i|\hat{V}|i\rangle\right|^2 + \left(-\frac{i}{\hbar}\right)^2 \sum_{k\neq i}\left|\langle i|\hat{V}|k\rangle\right|^2 \frac{1}{\eta + i\omega_{ki}} + \frac{1}{\hbar^2\eta}\left|\langle i|\hat{V}|i\rangle\right|^2$$

$$= -\frac{i}{\hbar}\langle i|\hat{V}|i\rangle - \frac{i}{\hbar}\sum_{k\neq i}\frac{\left|\langle i|\hat{V}|k\rangle\right|^2}{E_i - E_k + i\hbar\eta} = -\frac{i}{\hbar}\Delta_i$$

Then we have

$$c_i(t) = \exp(-\frac{i}{\hbar}\Delta_i t)$$

$$|\psi_s(t)\rangle = c_i(t)\exp(-\frac{i}{\hbar}E_i t)|i\rangle + ... = \exp[-\frac{i}{\hbar}(E_i + \Delta_i)t]|i\rangle$$

We note that

$$\exp[-\frac{i}{\hbar}(E_i + \Delta_i)t] = \exp[-\frac{i}{\hbar}(E_i + \mathrm{Re}(\Delta_i) - i\,\mathrm{Im}(\Delta_i))t]$$

$$= \exp[-\frac{i}{\hbar}(E_i + \mathrm{Re}(\Delta_i)t]\exp[-\mathrm{Im}(\Delta_i)t]$$

Here

$$\Delta_i = \mathrm{Re}(\Delta_i) - i\,\mathrm{Im}(\Delta_i)$$

$$= \langle i|\hat{V}|i\rangle + \sum_{k\neq i}\frac{\left|\langle i|\hat{V}|k\rangle\right|^2}{E_i - E_k + i\hbar\eta}$$

$$= \langle i|\hat{V}|i\rangle + \sum_{k\neq i}\left|\langle i|\hat{V}|k\rangle\right|^2[P\left(\frac{1}{E_i - E_k}\right) - i\pi\delta(E_i - E_k)]$$

The energy shift:

$$\mathrm{Re}(\Delta_i) = \langle i|\hat{V}|i\rangle + \sum_{k\neq i}\left|\langle i|\hat{V}|k\rangle\right|^2\left(\frac{1}{E_i - E_k}\right),$$

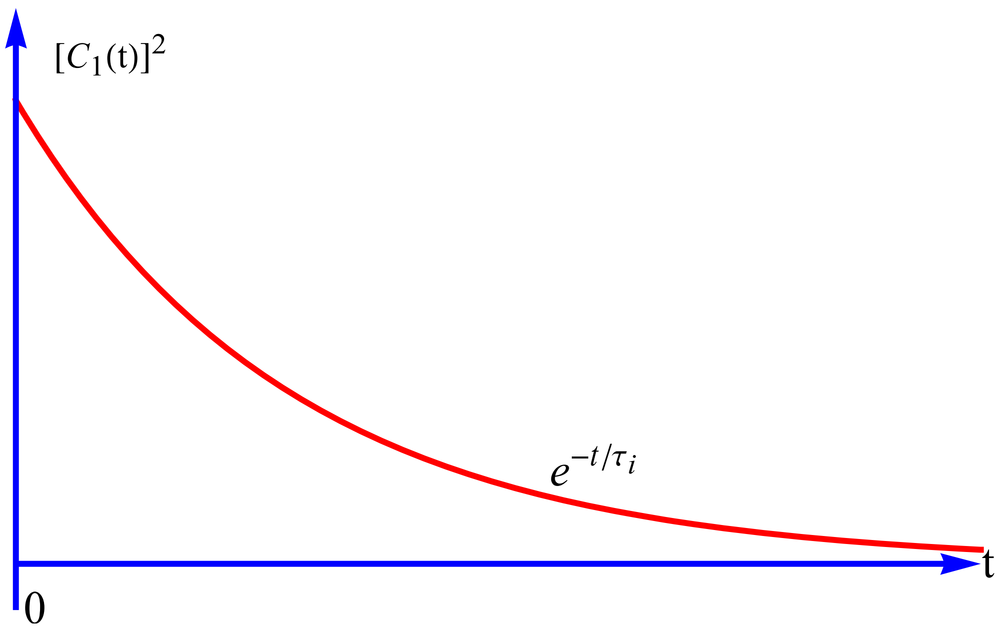
$$\mathrm{Im}(\Delta_i) = \pi\sum_{k\neq i}\left|\langle k|\hat{V}|i\rangle\right|^2\delta(E_i - E_k)].$$

Using the Fermi's golden rule, we have

$$\frac{2\pi}{\hbar}\sum_{k\neq i}\left|\langle k|\hat{V}|i\rangle\right|^2\delta(E_i - E_k)] = \frac{2}{\hbar}\mathrm{Im}(\Delta_i).$$

We define the relaxation time,

$$\frac{\Gamma_i}{\hbar} = \frac{2}{\hbar}\mathrm{Im}(\Delta_i) = \tau_i.$$

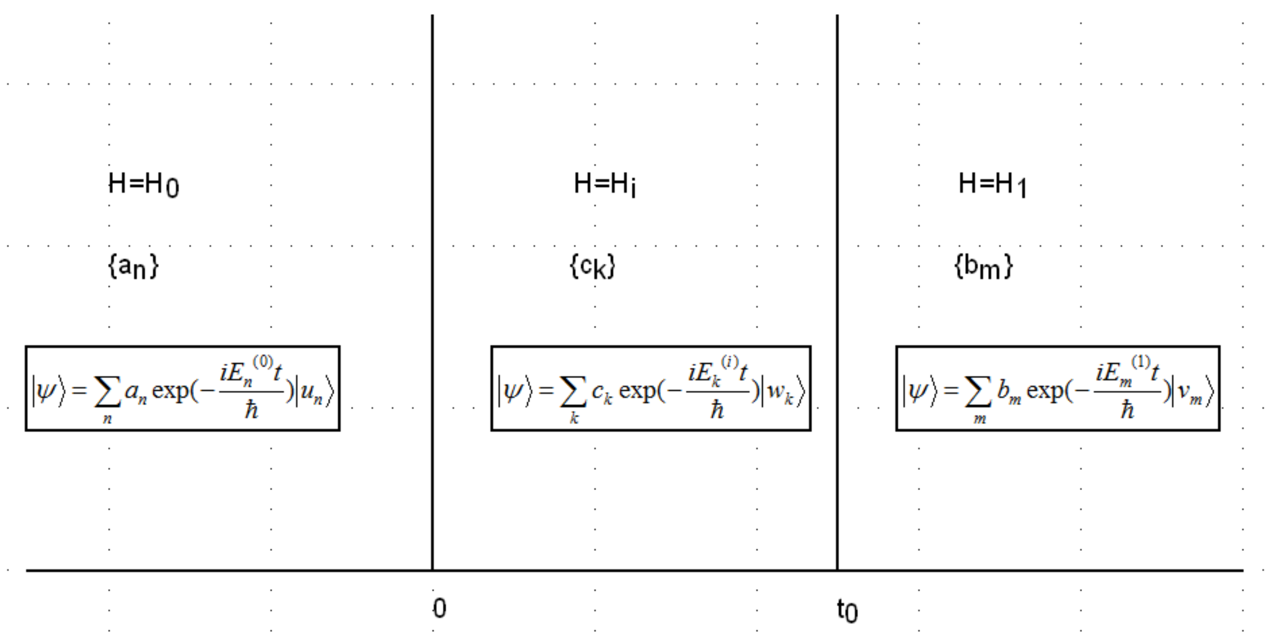


3. Sudden approximation

The wave function in the Schrodinger picture is related to that in the Dirac picture as

$$|\psi_s(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}_0 t}|\psi_I(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}_0 t}\sum_n c_n(t)|n\rangle = \sum_n c_n(t)e^{-\frac{i}{\hbar}\hat{H}_0 t}|n\rangle$$

We consider the wave function in the three time regions.



where the index i denotes the time region $(0 < t < t_0)$.

$$\hat{H}_0|u_n\rangle = E_n^{(0)}|u_n\rangle, \qquad (t<0)$$

$$\hat{H}_i|w_k\rangle = E_k^{(i)}|w_k\rangle, \qquad (0<t<t_0)$$

$$\hat{H}_1|v_m\rangle = E_m^{(1)}|v_n\rangle \qquad (t_0<t)$$

(a) $t<0$,

$$|\psi_0\rangle = \sum_n a_n \exp(-\frac{iE_n^{(0)}t}{\hbar})|u_n\rangle, \qquad \text{(Schrödinger picture)}$$

with

$$\hat{H}_0|u_n\rangle = E_n^{(0)}|u_n\rangle$$

where the co-efficient a_n is independent of time t. $\hat{H}_0$ is the Hamiltonian of the system.

(b) $0 < t < t_0$

$$|\psi_i\rangle = \sum_k c_k \exp(-\frac{iE_k^{(i)}t}{\hbar})|w_k\rangle.$$

with

$$\hat{H}_i|w_k\rangle = E_k^{(i)}|w_k\rangle.$$

where the co-efficient c_k is independent of time t. $\hat{H}_i$ is the Hamiltonian of the system.

(c) $t > t_0$

$$|\psi_1\rangle = \sum_m b_m \exp(-\frac{iE_m^{(1)}t}{\hbar})|v_m\rangle \qquad (t > t_0)$$

with

$$\hat{H}_1|v_m\rangle = E_m^{(1)}|v_n\rangle \qquad (t > t_0)$$

where the co-efficient b_m is independent of time t. $\hat{H}_1$ is the Hamiltonian of the system.

4. Continuity of the wavefunctions

(i) The continuity of the wave function at at $t = 0$

$$|\psi(t=0)\rangle = \sum_k c_k |w_k\rangle = \sum_n a_n |u_n\rangle,$$

or

$$\langle w_k|\psi(t=0)\rangle = c_k = \sum_n a_n \langle w_k|u_n\rangle. \qquad (1)$$

(ii) The continuity of the wavefunction at $t = t_0$

$$|\psi(t=t_0)\rangle = \sum_m b_m \exp(-\frac{iE_m^{(1)}t_0}{\hbar})|v_m\rangle$$

or

$$\langle v_m|\psi(t=t_0)\rangle = b_m \exp(-\frac{iE_m^{(1)}t_0}{\hbar}) = \sum_k c_k \exp(-\frac{iE_k^{(i)}t_0}{\hbar})\langle v_m|w_k\rangle$$

or

$$b_m = \sum_k c_k \exp\exp[\frac{i(E_m^{(1)} - E_k^{(i)})t_0}{\hbar}]\langle v_m|w_k\rangle,$$

or

$$b_m = \sum_n \sum_k a_n \langle w_k|u_n\rangle\langle v_m|w_k\rangle \exp\exp[\frac{i(E_m^{(1)} - E_k^{(i)})t_0}{\hbar}]. \qquad (2)$$

5. Limit of $t_0 \rightarrow 0$

When $t_0 \rightarrow 0$, we get

$$b_m = \sum_n \sum_k a_n \langle w_k|u_n\rangle\langle v_m|w_k\rangle = \sum_n \sum_k a_n \langle v_m|w_k\rangle\langle w_k|u_n\rangle = \sum_n a_n \langle v_m|u_n\rangle$$

or

$$b_m = \sum_n a_n \langle v_m | u_n \rangle . \qquad (3)$$

Then we have

$$|\psi_0\rangle = \sum_n a_n \exp(-\frac{iE_n^{(0)}t}{\hbar})|u_n\rangle \qquad (t<0)$$

$$|\psi_1\rangle = \sum_m b_m \exp(-\frac{iE_m^{(1)}t}{\hbar})|v_m\rangle \qquad (t>0)$$

The inner product of the two wavefunctions is given by

$$\langle\psi_0|\psi_1\rangle = \sum_n \sum_m a_n^* b_m \exp[\frac{i(E_n^{(0)} - E_m^{(1)})t}{\hbar}]\langle u_n | v_m\rangle$$

or

$$\langle\psi_0|\psi_1\rangle = \sum_n \sum_m \sum_{n'} a_n^* a_{n'} \exp[\frac{i(E_n^{(0)} - E_m^{(1)})t}{\hbar}]\langle v_m | u_{n'}\rangle\langle u_n | v_m\rangle$$

We now consider the special case (a pure state)

$$|\psi_0\rangle = a_n \exp(-\frac{iE_n^{(0)}t}{\hbar})|u_n\rangle \qquad \text{(pure state)}$$

Then we have

$$b_m = \sum_n a_n \langle v_m | u_n \rangle = a_n \langle v_m | u_n \rangle$$

leading to

$$|\psi_1\rangle = \sum_m b_m \exp(-\frac{iE_m^{(1)}t}{\hbar})|v_m\rangle = a_n \sum_m \exp(-\frac{iE_m^{(1)}t}{\hbar})|v_m\rangle\langle v_m | u_n\rangle$$

and

$$\langle\psi_0|\psi_1\rangle = \sum_m |a_n|^2 \exp[\frac{i(E_n^{(0)} - E_m^{(1)})t}{\hbar}]|\langle v_m | u_n\rangle|^2$$

6. Example

A particle of mass m is in lowest energy (ground) state of the infinite potential energy well

$V(x) = 0$ for $0<x<L$ and ∞ elsewhere.

At time $t = 0$, the wall located at $x = L$ is suddenly pulled back to a position at $x = 2L$. This change occurs so rapidly that instantaneously the wave function does not change.

(a) Calculate the probability that a measurement of the energy will yield the ground-state energy of the new well. What is the probability that a measurement of the energy will yield the first excited energy of the new well?

(b) Describe the procedure you would use to determine the time development of the system. Is the system in a stationary state?

((**Solution**))

The old wave function of the ground state is given by

$$\varphi_1(x) = \sqrt{\frac{2}{a}}\sin(\frac{\pi x}{a}) \qquad \text{only for } 0<x<a \qquad \text{(0 otherwise).}$$

The new wave function is given by

$$\psi_{new}^{(n)}(x) = \sqrt{\frac{2}{2a}}\sin(\frac{n\pi x}{2a}) = \sqrt{\frac{1}{a}}\sin(\frac{n\pi x}{2a})$$

with the energy of

$$E_{new}^{(n)} = \frac{\hbar^2}{2m}\left(\frac{\pi n}{2a}\right)^2$$

(a) From the continuity of the wave function at $t = 0$, we have

$$\varphi_1(x) = \sum_n c_n \psi_{new}^{(n)}(x)$$

Then we have

$$
\begin{aligned}
c_n &= \int_0^{2a} \psi_{new}{}^{(n)*}(x)\varphi_1(x)dx \\
&= \frac{\sqrt{2}}{a}\int_0^{a} \sin(\frac{n\pi x}{2a})\sin\left(\frac{\pi x}{a}\right)dx \\
&= \frac{4\sqrt{2}}{\pi(4-n^2)}\sin(\frac{n\pi}{2})
\end{aligned}
$$

Note that

$$
|c_1|^2 = \frac{32}{9\pi^2} = 0.360253, \qquad |c_2|^2 = \frac{1}{2} = 0.5
$$

(b)

The system is not stationary since $|\psi(t=0)\rangle$ is not an eigenstate of the new Hamiltonian $\hat{H}_{new}$, but is a superposition of the eigenstates $|\psi_{new}{}^{(n)}\rangle$ with various kinds of *n*.

$$
|\psi(t=0)\rangle = |\varphi_1\rangle = \sum_n c_n |\psi_{new}{}^{(n)}\rangle
$$

$$
\begin{aligned}
|\psi(t)\rangle &= \exp(-\frac{i}{\hbar}\hat{H}_{new}t)|\psi(t=0)\rangle \\
&= \sum_n c_n \exp(-\frac{i}{\hbar}\hat{H}_{new}t)|\psi_{new}{}^{(n)}\rangle \\
&= \sum_n c_n \exp(-\frac{i}{\hbar}E_{new}{}^{(n)}t)|\psi_{new}{}^{(n)}\rangle
\end{aligned}
$$

or

$$
\psi(x,t) = \langle x|\psi(t)\rangle = \sum_n c_n \exp(-\frac{i}{\hbar}E_{new}{}^{(n)}t)\psi_{new}{}^{(n)}(x)
$$

where c_n are determined as in (a)

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

and

$$
E_{new}{}^{(n)} = \frac{\hbar^2}{2m}\left(\frac{\pi n}{2a}\right)^2,
$$

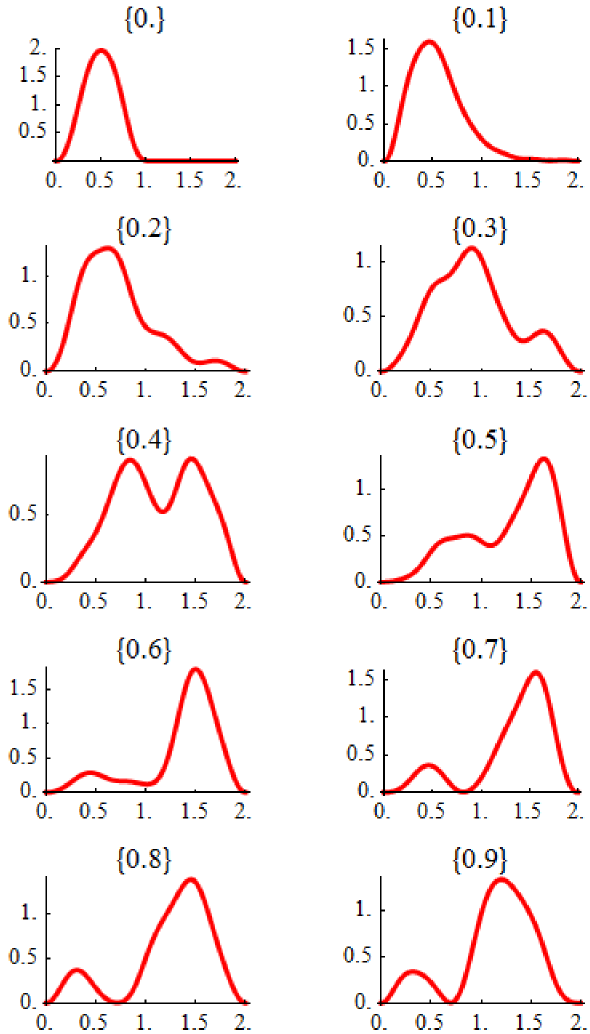
$$\psi_{new}{}^{(n)}(x) = \sqrt{\frac{2}{2a}} \sin(\frac{n\pi x}{2a}) = \sqrt{\frac{1}{a}} \sin(\frac{n\pi x}{2a})$$

Then we get

$$\begin{aligned}
|\psi(x,t)|^2 &= \sum_m c_m{}^* \exp(\frac{i}{\hbar} E_{new}{}^{(m)} t) \psi_{new}{}^{(m)*}(x) \sum_n c_n \exp(-\frac{i}{\hbar} E_{new}{}^{(n)} t) \psi_{new}{}^{(n)}(x) \\
&= \sum_{n,m} c_m{}^* c_n \psi_{new}{}^{(m)*}(x) \psi_{new}{}^{(n)}(x) \exp[-\frac{i}{\hbar}(E_{new}{}^{(n)} - E_{new}{}^{(n)})t]
\end{aligned}$$

((**Mathematica**))

We use $m = \hbar = 1$. $a = 1$. Red (At $t = 0$). The Plot of $|\psi(x,t)|^2$ as a function of x ($0<x<2a$), where t is changed as parameter; $t = 0$ - 3 with $\Delta t = 0.1$. The summation over n (n = 1 – 10).



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