Time dependent perturbation
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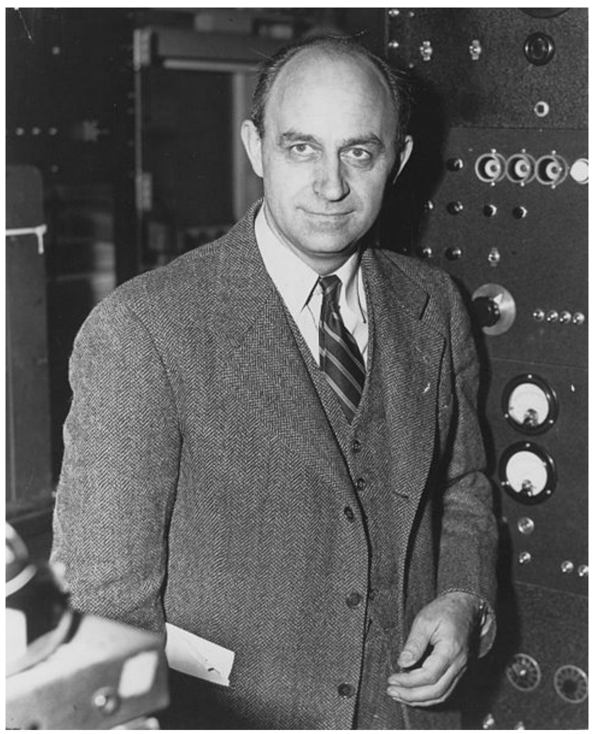
Dirac picture
Fermi's golden rule
Heisenberg's uncertainty of principle

Enrico Fermi (29 September 1901 – 28 November 1954) was an Italian physicist particularly known for his work on the development of the first nuclear reactor, Chicago Pile-1, and for his contributions to the development of quantum theory, nuclear and particle physics, and statistical mechanics. He was awarded the 1938 Nobel Prize in Physics for his work on induced radioactivity.



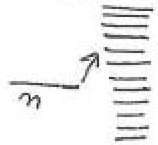
http://en.wikipedia.org/wiki/Enrico_Fermi

Important special case. At $t=0$ system in state n. Then $a_n(0)=1$, all other a's are zeros.

$$(10)\quad \underset{(s\neq n)}{} \quad a_s(t) = -\frac{i}{\hbar}\int_0^t \mathcal{H}_{sn}(t)\, e^{\frac{i}{\hbar}\left(E_0^{(s)}-E_0^{(n)}\right)t}\, dt$$

Matrix element $\mathcal{H}_{sn}(t)$ causes transitions $n \to s$.

Transitions from n to a continuum of states



(11) Assume $\mathcal{H}_{sn}$ indep. of time, then

$$a_s(t) = -\mathcal{H}_{sn}\,\frac{e^{\frac{i}{\hbar}(E_0^s-E_0^n)t}-1}{E_0^s-E_0^n}$$

$$|a_s(t)|^2 = 4|\mathcal{H}_{sn}|^2\,\frac{\sin^2\frac{t}{2\hbar}\left(E_0^{(s)}-E_0^{(n)}\right)}{\left(E_0^{(s)}-E_0^{(n)}\right)^2}$$

Prob of transition to one state s

(12)
$$P(t) = \sum_s |a_s(t)|^2 = 4\overline{|\mathcal{H}_{sn}|^2}\sum\frac{\sin^2\frac{t}{2\hbar}(E^s-E^n)}{(E^s-E^n)^2} =$$

$$= 4\overline{|\mathcal{H}_{sn}|^2}\,\rho(E_n)\underbrace{\int\frac{\sin^2\frac{t}{2\hbar}(E^s-E^n)\; d(E^s-E^n)}{(E^s-E^n)^2}}_{\frac{\pi t}{2\hbar}}$$

$$= t\,\frac{2\pi}{\hbar}|\mathcal{H}_{sn}|^2\rho(E_n)$$

$$\int\frac{\sin^2\alpha x}{x^2}dx = \pi\alpha$$

(13) & $\rho(E_n)$ = no of states s, close to E_n per unit energy interval.

$$\boxed{\text{Rate of transition} = \frac{2\pi}{\hbar}\overline{|\mathcal{H}_{sn}|^2}\,\rho(E_n)}$$

Discuss: distribution of final states as function of t & relation with uncertainty principle

from E, Fermi "Lecture Notes on Quantum Mechanics (Dover).

((Fermi golden rule))

Although named after Enrico Fermi, most of the work leading to the Golden Rule is due to Paul Dirac who formulated 20 years earlier a virtually identical equation, including the three components of a constant, the matrix element of the perturbation and an energy difference. It was given this name because, on account of its importance, Fermi dubbed it "Golden Rule No. 2.
https://en.wikipedia.org/wiki/Fermi's_golden_rule

((**Golden rule No.2**))
From p.142 of the book by E. Fermi, E. Fermi Nuclear Physics, revised edition (University of Chicago, 1940).

"From quantum mechanics, the probability per unit time of transition = number of transitions per unit time = w is given by "Golden Rule No.2":

$$w = \frac{2\pi}{\hbar}\left|H\right|^2 \frac{dn}{dE},$$

where H is the matrix element of the perturbation causing the transition, and $\frac{dn}{dE}$ = energy density of final states, counting each degenerate state separately."

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1. Time-dependent perturbation (Dirac picture, or interaction picture)

The Hamiltonian is given by

$$\hat{H} = \hat{H}_0 + \lambda \hat{V}(t),$$

where $\hat{H}_0$ is independent of t. The state vector in the Schrödinger picture is related to that in the Dirac picture (the interaction picture) by

$$\left|\psi_s(t)\right\rangle = e^{-\frac{i}{\hbar}\hat{H}_0 t}\left|\psi_I(t)\right\rangle,$$

or

$$\left|\psi_I(t)\right\rangle = e^{\frac{i}{\hbar}\hat{H}_0 t}\left|\psi_s(t)\right\rangle.$$

The state vector $\left|\psi_s(t)\right\rangle$ satisfies the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\left|\psi_s(t)\right\rangle = \hat{H}\left|\psi_s(t)\right\rangle = [\hat{H}_0 + \lambda\hat{V}(t)]\left|\psi_s(t)\right\rangle. \qquad \text{(Schrödinger picture)}$$

In the Dirac picture, the state vector $|\psi_I(t)\rangle$ satisfies the following equation of motion, based on the Schrödinger equation for $|\psi_s(t)\rangle$,

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}|\psi_I(t)\rangle &= i\hbar\frac{\partial}{\partial t}e^{\frac{i}{\hbar}\hat{H}_0 t}|\psi_s(t)\rangle \\
&= -\hat{H}_0 e^{\frac{i}{\hbar}\hat{H}_0 t}|\psi_s(t)\rangle + e^{\frac{i}{\hbar}\hat{H}_0 t} i\hbar\frac{\partial}{\partial t}|\psi_s(t)\rangle \\
&= -\hat{H}_0 e^{\frac{i}{\hbar}\hat{H}_0 t}|\psi_s(t)\rangle + e^{\frac{i}{\hbar}\hat{H}_0 t}[\hat{H}_0 + \lambda\hat{V}(t)]|\psi_s(t)\rangle . \\
&= \lambda e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{V}(t)e^{-\frac{i}{\hbar}\hat{H}_0 t}|\psi_I(t)\rangle \\
&= \lambda\hat{V}_I(t)|\psi_I(t)\rangle
\end{aligned}$$

or

$$i\hbar\frac{\partial}{\partial t}|\psi_I(t)\rangle = \lambda\hat{V}_I(t)|\psi_I(t)\rangle . \qquad \text{(the Dirac picture)}$$

where the new interaction operator is given by

$$\hat{V}_I(t) = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{V}(t)e^{-\frac{i}{\hbar}\hat{H}_0 t}$$

This definition is true even if the perturbation depends on time.

Now we introduce the time evolution operator $\hat{U}_I(t,t_0)$ in the interaction picture, such that

$$|\psi_I(t)\rangle = \hat{U}_I(t,t_0)|\psi_I(t_0)\rangle .$$

Since

$$i\hbar\frac{\partial}{\partial t}|\psi_I(t)\rangle = \lambda\hat{V}_I(t)|\psi_I(t)\rangle .$$

the time evolution operator $\hat{U}_I(t,t_0)$ satisfies the differential equation given by

$$i\hbar\frac{\partial}{\partial t}\hat{U}_I(t,t_0) = \lambda\hat{V}_I(t)\hat{U}_I(t,t_0) .$$

Using the initial condition that $\hat{U}_I(t_0,t_0) = \hat{1}$, we get the integral equation

$$\hat{U}_I(t,t_0) = \hat{1} - \frac{i}{\hbar}\lambda\int_{t_0}^{t}\hat{V}_I(t')\hat{U}_I(t',t_0)dt'.$$

By successive iteration, we get an approximate solution to this integral equation [Dyson series] as

$$\hat{U}_I(t,t_0) = \hat{1} - \frac{i}{\hbar}\lambda\int_{t_0}^{t}\hat{V}_I(t')[\hat{1} - \frac{i}{\hbar}\lambda\int_{t_0}^{t'}\hat{V}_I(t'')\hat{U}_I(t'',t_0)dt'']dt'$$

$$= \hat{1} + (-\frac{i}{\hbar})\lambda\int_{t_0}^{t}\hat{V}_I(t')dt' + (-\frac{i}{\hbar})^2\lambda^2\int_{t_0}^{t}\hat{V}_I(t')dt'\int_{t_0}^{t'}dt''\hat{V}_I(t'') + ...$$

It is sometimes convenient to write this series expansion in more symmetric form by using the time-ordered product T (or time ordering operator). We define time ordered product of two operators as

$$T[\hat{V}_I(t')\hat{V}_I(t'')] = \begin{cases} \hat{V}_I(t')\hat{V}_I(t'') & (t'' \leq t') \\ \hat{V}_I(t'')\hat{V}_I(t') & (t' \leq t'') \end{cases}.$$

or

$$T[\hat{V}_I(t')\hat{V}_I(t'')] = \Theta(t'-t'')\hat{V}_I(t')\hat{V}_I(t'') + \Theta(t''-t')\hat{V}_I(t'')\hat{V}_I(t').$$

where $\Theta(x)$ is a step function, $\Theta(x) = 1$ for $x \geq 0$ and 0 for $x<0$. This convention is easily generalized to products of any number of time-dependent operators. With it we can prove that if $t>t_0$, the time evolution operator may be written in the form

$$\hat{U}_I(t,t_0) = \hat{1} + \sum_{n=1}^{\infty}\frac{1}{n!}(-\frac{i}{\hbar})^n\lambda^n\int_{t_0}^{t}\int_{t_0}^{t}\int_{t_0}^{t}\cdots\int_{t_0}^{t}dt_1'dt_2'\cdots dt_n'T[\hat{V}_I(t_1')\hat{V}_I(t_1')\hat{V}_I(t_1')\cdots\hat{V}_I(t_n')],$$

or formally and compactly as

$$\hat{U}_I(t,t_0) = T\exp[-\frac{i}{\hbar}\int_{t_0}^{t}\hat{V}_I(t')dt'],$$

Although this is just a compact way of writing the original series, but nevertheless it represents a very important advance of the formalism because many formal manipulations are facilitated much by this notation. Such a series are called Dyson series, named after Freeman J. Dyson.

((**Note**)) **G. Baym, Lectures on Quantum Mechanics (Westview, 1990).**

$$
\begin{aligned}
\int_{t_0}^{t} dt' \int_{t_0}^{t} dt'' T[\hat{V}_I(t')\hat{V}_I(t'')] &= \int_{t_0}^{t} dt' \int_{t_0}^{t} dt'' \Theta(t'-t'')\hat{V}_I(t')\hat{V}_I(t'') + \int_{t_0}^{t} dt'' \int_{t_0}^{t} dt' \Theta(t''-t')\hat{V}_I(t'')\hat{V}_I(t') \\
&= \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \hat{V}_I(t')\hat{V}_I(t'') + \int_{t_0}^{t} dt'' \int_{t_0}^{t''} dt' \hat{V}_I(t'')\hat{V}_I(t') \\
&= 2! \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \hat{V}_I(t')\hat{V}_I(t'')
\end{aligned}
$$

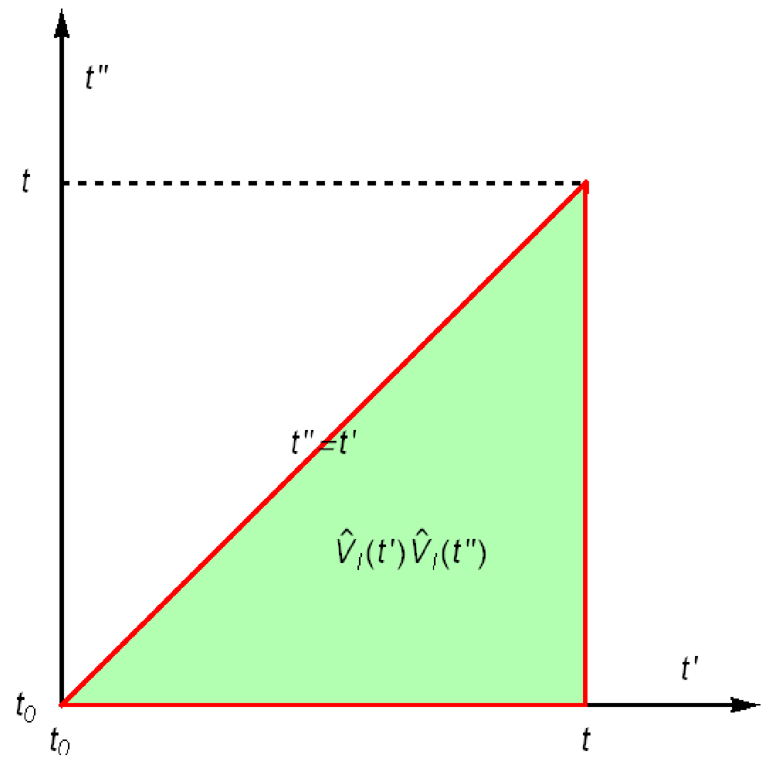


Fig. The integral region for $\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \hat{V}_I(t')\hat{V}_I(t'')$ (green region)

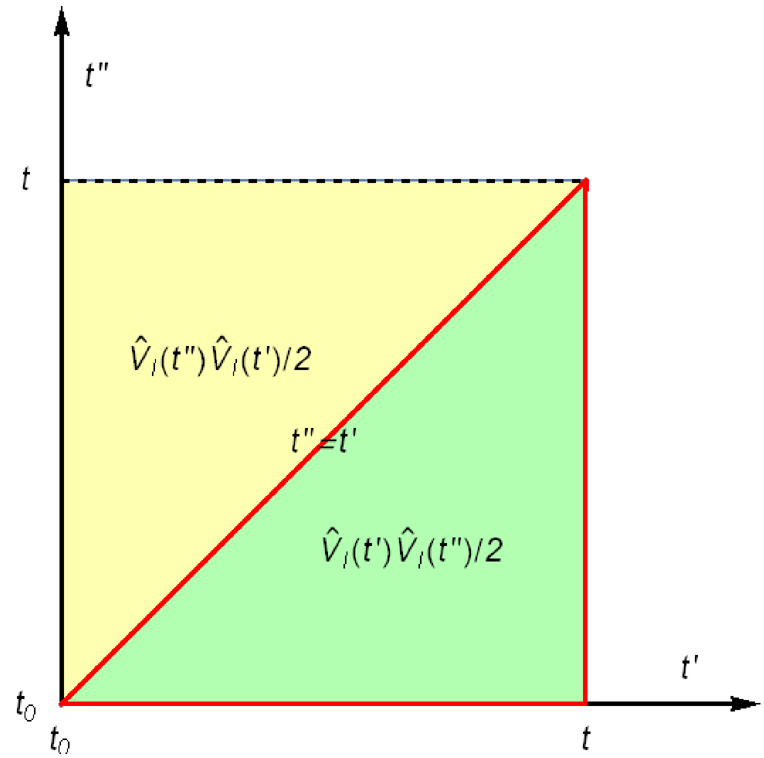


Fig. The integral regions for $\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \hat{V}_I(t')\hat{V}_I(t'')/2$ (green region) and $\int_{t_0}^{t} dt'' \int_{t_0}^{t''} dt' \hat{V}_I(t'')\hat{V}_I(t')/2$ (yellow region). Note that mathematically, $\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \hat{V}_I(t')\hat{V}_I(t'')/2 = \int_{t_0}^{t} dt'' \int_{t_0}^{t''} dt' \hat{V}_I(t'')\hat{V}_I(t')/2$. The later time to the left of the earlier time.

(**J.M. Ziman, *Elements of Advanced Quantum Theory* (Cambridge, 1959))**

Similarly, we have

$$\int_{t_0}^{t} dt_1' \int_{t_0}^{t} dt_2' \int_{t_0}^{t} dt_3' \cdots \int_{t_0}^{t} dt_n' T[\hat{V}_I(t_1')\hat{V}_I(t_2')\cdots\hat{V}_I(t_n')] = n! \int_{t_0}^{t} dt_1' \hat{V}_I(t_1') \int_{t_0}^{t_1'} dt_2' \hat{V}_I(t_2') \cdots \int_{t_0}^{t_{n-1}'} dt_n' \hat{V}_I(t_n'),$$

because there are *n*! possible orderings of *n* times t_1', t_2',…., t_n'.

The time evolution operator in the Schrödinger picture $\hat{U}_s(t,t_0)$ is related to that in the Dirac picture as

$$\hat{U}_I(t,t_0) = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{U}_s(t,t_0)e^{-\frac{i}{\hbar}\hat{H}_0 t_0},$$

since

$$\begin{aligned}
\left|\psi_I(t)\right\rangle &= \hat{U}_I(t,t_0)\left|\psi_I(t_0)\right\rangle \\
&= e^{\frac{i}{\hbar}\hat{H}_0 t}\left|\psi_s(t)\right\rangle \\
&= e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{U}_s(t,t_0)\left|\psi_s(t_0)\right\rangle \\
&= e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{U}_s(t,t_0)e^{-\frac{i}{\hbar}\hat{H}_0 t_0}\left|\psi_I(t_0)\right\rangle
\end{aligned}$$

where

$$\left|\psi_s(t)\right\rangle = \hat{U}_s(t,t_0)\left|\psi_s(t_0)\right\rangle .$$

Let us now look at the matrix element of $\hat{U}_I(t,t_0)$,

$$\hat{H}_0\left|n\right\rangle = E_n^{(0)}\left|n\right\rangle ,$$

$$\left\langle n\right|\hat{U}_I(t,t_0)\left|m\right\rangle = e^{\frac{i}{\hbar}(E_n^{(0)}t - E_m^{(0)}t_0)}\left\langle n\right|\hat{U}_s(t,t_0)\left|m\right\rangle ,$$

$$\left|\left\langle n\right|\hat{U}_I(t,t_0)\left|m\right\rangle\right|^2 = \left|\left\langle n\right|\hat{U}_s(t,t_0)\left|m\right\rangle\right|^2 .$$

((**Note**))
Suppose that

$$[\hat{H}_0, \hat{A}] \neq 0 \qquad \text{and} \qquad [\hat{H}_0, \hat{B}] \neq 0 ,$$

$$\hat{A}\left|a'\right\rangle = a'\left|a'\right\rangle \quad \text{and} \qquad \hat{B}\left|b'\right\rangle = b'\left|b'\right\rangle .$$

In this case,

$$\left|\left\langle b'\right|\hat{U}_I(t,t_0)\left|a'\right\rangle\right|^2 \neq \left|\left\langle b'\right|\hat{U}_s(t,t_0)\left|a'\right\rangle\right|^2 .$$

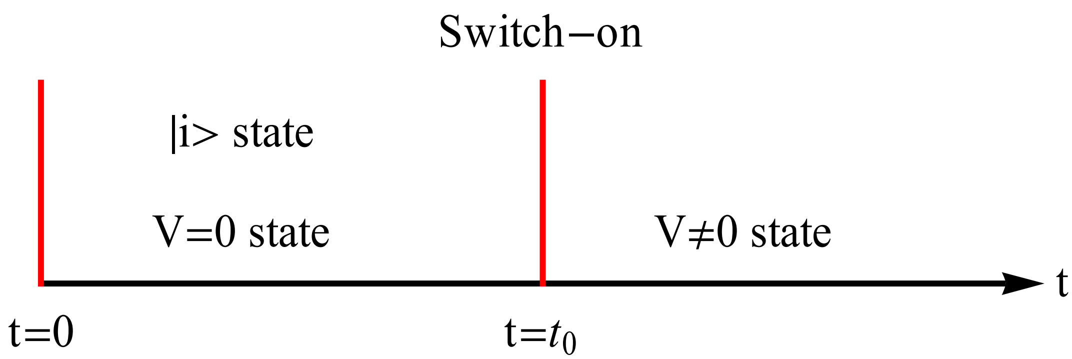
since

$$\langle b'|\hat{U}_I(t,t_0)|a'\rangle = \sum_{n,m}\langle b'|e^{\frac{i}{\hbar}\hat{H}_0 t}|n\rangle\langle n|\hat{U}_s(t,t_0)|m\rangle\langle m|e^{-\frac{i}{\hbar}\hat{H}_0 t_0}|a'\rangle$$

$$= \sum_{n,m} e^{\frac{i}{\hbar}(E_n^{(0)}t - E_m^{(0)}t_0)}\langle b'|n\rangle\langle n|\hat{U}_s(t,t_0)|m\rangle\langle m|a'\rangle$$

2. Transition probability (Dirac picture)

We now consider the case as shown below.



At $t = 0$,

$$|\psi_s(t=0)\rangle = |i\rangle$$

At $t = t_0$,

$$|\psi_s(t_0)\rangle = \hat{U}_s(t_0,0)|\psi_s(0)\rangle = e^{-\frac{i}{\hbar}\hat{H}_0 t_0}|i\rangle .$$

Since

$$|\psi_s(t_0)\rangle = e^{-\frac{i}{\hbar}\hat{H}_0 t_0}|\psi_I(t_0)\rangle ,$$

from the definition, we have

$$|\psi_I(t_0)\rangle = e^{\frac{i}{\hbar}\hat{H}_0 t_0}|\psi_s(t_0)\rangle = e^{\frac{i}{\hbar}\hat{H}_0 t_0}e^{-\frac{i}{\hbar}\hat{H}_0 t_0}|i\rangle = |i\rangle .$$

((**Note**))

The state vector in the Dirac picture does not evolve in the absence of the perturbation, while it does in its presence.

$$i\hbar\frac{\partial}{\partial t}|\psi_I(t)\rangle = \lambda\hat{V}_I(t)|\psi_I(t)\rangle ,$$

$$i\hbar\frac{\partial}{\partial t}\left|\psi_I(t)\right\rangle = 0\,,$$

for $0 < t < t_0$, since $\hat{V}_I(t) = 0$. Then we have

$$\left|\psi_I(t)\right\rangle = \left|i\right\rangle,$$

in this time region.

At a later time ($t>t_0$), we have

$$\left|\psi_I(t)\right\rangle = \hat{U}_I(t,t_0)\left|\psi_I(t_0)\right\rangle = \hat{U}_I(t,t_0)\left|i\right\rangle,$$

We assume that

$$\left|\psi_I(t)\right\rangle = \sum_n c_n(t)\left|n\right\rangle, \qquad \text{(Dirac picture)}$$

or

$$\left|\psi_I(t)\right\rangle = \sum_n \left|n\right\rangle\left\langle n\right|\hat{U}_I(t,t_0)\left|i\right\rangle,$$

or

$$c_n(t) = \left\langle n\middle|\psi_I(t)\right\rangle = \left\langle n\right|\hat{U}_I(t,t_0)\left|i\right\rangle.$$

Note we use $c_n(t)$ for the Dirac picture and $a_n(t)$ for the Schrődinger picture.

Now we go back to the perturbation expansion ($V \rightarrow \lambda V$)

$$\begin{aligned}
c_n(t) &= \left\langle n\right|\hat{U}_I(t,t_0)\left|i\right\rangle \\
&= c_n^{(0)}(t) + \lambda c_n^{(1)}(t) + \lambda^2 c_n^{(2)}(t) + \ldots \\
&= \left\langle n\right|\hat{1} + \lambda(-\frac{i}{\hbar})\int_{t_0}^{t}\hat{V}_I(t')dt' + \lambda^2(-\frac{i}{\hbar})^2\int_{t_0}^{t}dt'\int_{t_0}^{t'}dt''\hat{V}_I(t')\hat{V}_I(t'') + \ldots\left|i\right\rangle
\end{aligned}$$

Thus we have

$$c_n^{(0)}(t) = \left\langle n\middle|i\right\rangle = \delta_{n,i}\,,$$

$$c_n^{(1)} = (-\frac{i}{\hbar})\int_{t_0}^{t} dt' \langle n|\hat{V}_I(t')|i\rangle .$$

$$c_n^{(2)}(t) = (-\frac{i}{\hbar})^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \langle n|\hat{V}_I(t')\hat{V}_I(t'')|i\rangle$$

....

Since

$$\hat{V}_I(t) = ^{\frac{i}{\hbar}\hat{H}_0 t}\ \hat{V}(t) e^{-\frac{i}{\hbar}\hat{H}_0 t} ,$$

the matrix element in the Schrödinger picture is related to that in the Dirac picture such that

$$\begin{aligned}\langle n|\hat{V}_I(t')|i\rangle &= \langle n|e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{V}(t)e^{-\frac{i}{\hbar}\hat{H}_0 t}|i\rangle \\ &= e^{\frac{i}{\hbar}(E_n - E_i)t'}\langle n|\hat{V}(t')|i\rangle = e^{i\omega_{ni}t'}V_{ni}(t')\end{aligned}$$

where

$$V_{ni}(t) = \langle n|\hat{V}(t)|i\rangle ,$$

and

$$\omega_{ni} = \frac{E_n - E_i}{\hbar} .$$ (the transition angular frequency, Bohr frequency)

Then we hve

$$c_n^{(1)} = (-\frac{i}{\hbar})\int_{t_0}^{t} dt' \langle n|\hat{V}_I(t')|i\rangle = (-\frac{i}{\hbar})\int_{t_0}^{t} dt' e^{i\omega_{ni}t'}V_{ni}(t') .$$

Similarly, we get

$$c_n^{(2)} = (-\frac{i}{\hbar})^2 \sum_m \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \langle n|\hat{V}_I(t')|m\rangle\langle m|\hat{V}_I(t'')|i\rangle ,$$

or

$$c_n^{(2)} = (-\frac{i}{\hbar})^2 \sum_m \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' e^{i\omega_{nm}t'} V_{nm}(t') e^{i\omega_{mi}t''} V_{mi}(t'').$$

The transition probability for $|i\rangle \rightarrow |f\rangle$ is given by

$$P(i \rightarrow f) = |c_f(t)|^2 = |c_f^{(0)}(t) + \lambda c_f^{(1)}(t) + ...|^2 .$$

When $c_f^{(0)}(t) = 0$, $P(i \rightarrow f)$ can be approximated as

$$P(i \rightarrow f) = \lambda^2 |c_f^{(1)}(t)|^2 = \frac{\lambda^2}{\hbar^2} \left| \int_{t_0}^{t} e^{i\omega_{fi}t'} \langle f|\hat{V}(t')|i\rangle dt' \right|^2 .$$

Note that this probability is clearly only valid provided

$$P(i \rightarrow f) << 1 .$$

3. Exact solution in the Dirac picture

In the Dirac picture, we have the following equations without any approximation,

$$i\hbar \frac{\partial}{\partial t} \langle n|\psi_I(t)\rangle = \lambda \sum_k \langle n|\hat{V}_I(t)|k\rangle \langle k|\psi_I(t)\rangle ,$$

$$\langle n|\hat{V}_I(t)|k\rangle = e^{\frac{i}{\hbar}(E_n^{(0)} - E_k^{(0)})t} \langle n|\hat{V}(t)|k\rangle = e^{i\omega_{nk}t} V_{nk} ,$$

where

$$V_{nk} = \langle n|\hat{V}(t)|k\rangle ,$$

and

$$\omega_{nk} = \frac{E_n^{(0)} - E_k^{(0)}}{\hbar} . \qquad \text{(Bohr frequency)}$$

Then we have

$$i\hbar \frac{\partial}{\partial t} c_n(t) = \lambda \sum_k e^{i\omega_{nk}t} V_{nk} c_k(t).$$

Using the matrix notation we get

$$
i\hbar\frac{\partial}{\partial t}\begin{pmatrix} c_1(t) \\ c_2(t) \\ c_3(t) \\ . \\ . \\ . \end{pmatrix} = \begin{pmatrix} V_{11} & V_{12}e^{i\omega_{12}t} & V_{13}e^{i\omega_{13}t} & . & . & . \\ V_{21}e^{i\omega_{21}t} & V_{22} & V_{23}e^{i\omega_{23}t} & . & . & . \\ V_{31}e^{i\omega_{31}t} & V_{32}e^{i\omega_{32}t} & V_{33} & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \end{pmatrix}\begin{pmatrix} c_1(t) \\ c_2(t) \\ c_3(t) \\ . \\ . \\ . \end{pmatrix}
$$

((**Two-level system**))

For the two-level system (exact solution), we have

$$
i\hbar\frac{\partial}{\partial t}c_1(t) = V_{11}c_1(t) + V_{12}e^{i\omega_{12}t}c_2(t) ,
$$

$$
i\hbar\frac{\partial}{\partial t}c_2(t) = V_{21}e^{i\omega_{21}t}c_1(t) + V_{22}c_2(t) .
$$

where

$$
\omega_{21} = -\omega_{12} .
$$

((**Sakurai Problem 5-30**))

Consider a two-level system with $E_1 < E_2$. There is a time-dependent potential that connects the two levels as follows:

$$
V_{11} = V_{22} = 0 , \qquad V_{12} = \gamma e^{i\omega t} , \qquad V_{21} = \gamma e^{-i\omega t} \qquad (\gamma \text{ real})
$$

At t = 0, it is known that only the lower level is populated- that is

$$
c_1(0) = 1, \qquad c_2(0) = 0 .
$$

Find $|c_1(t)|^2$ and $|c_2(t)|^2$ for t>0 by exactly solving the coupled differential equation.

((**Solution**))

Interaction picture

$$
i\hbar\frac{\partial}{\partial t}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 & \gamma e^{i\omega' t} \\ \gamma e^{-i\omega' t} & 0 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}
$$

with initial condition;

$$c_1(0) = 1, \qquad c_2(0) = 0$$

where

$$\omega' = \omega - \omega_{2,1}$$

The probability:

$$|c_1(t)|^2 = (1 - \frac{\gamma^2}{\hbar^2\Omega^2}) + \frac{\gamma^2}{\hbar^2\Omega^2}\cos^2(\Omega t)$$

$$|c_2(t)|^2 = \frac{\gamma^2}{\hbar^2\Omega^2}\sin^2(\Omega t)$$

(Rabi formula)

with

$$\Omega = \sqrt{\frac{\omega'^2}{4} + \frac{\gamma^2}{\hbar^2}}$$

4. Exact solution in the Schrödinger picture

Here we discuss the time-dependent perturbation using the Schrödinger picture and compare the results with those derived from the Dirac picture as described above.

We consider $\hat{H}_0$ to be discrete and non-degenerate.

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

$\hat{H}_0$ is not explicitly time-dependent. So that eigenstates are stationary. At $t = 0$, a perturbation is applied to the system

$$\hat{H}(t) = \hat{H}_0 + \lambda\hat{V}(t) \qquad (0\leq\lambda<1),$$

The Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi_s(t)\rangle = [\hat{H}_0 + \lambda\hat{V}(t)]|\psi_s(t)\rangle ,$$

with the initial condition:

$$\left|\psi_s(t=0)\right\rangle = \left|i\right\rangle.$$

We assume that

$$\left|\psi_s(t)\right\rangle = \sum_n a_n(t)\left|n\right\rangle, \qquad \text{(Schrödinger picture)}$$

with

$$a_n(t) = \left\langle n\middle|\psi_s(t)\right\rangle = e^{-\frac{i}{\hbar}E_n^{(0)}t}\left\langle n\middle|\psi_I(t)\right\rangle = e^{-\frac{i}{\hbar}E_n^{(0)}t}c_n(t),$$

where $c_n(t)$ is the co-efficient for the Dirac picture, while $a_n(t)$ is the co-efficient for the Schrödinger equation.

$$a_n(t=0) = \left\langle n\middle|\psi_s(t=0)\right\rangle = \delta_{ni}.$$

For simplicity, we introduce

$$V_{nk}(t) = \left\langle n\middle|\hat{V}(t)\middle|k\right\rangle.$$

Recalling that

$$\left\langle n\middle|\hat{H}_0\middle|k\right\rangle = E_n^{(0)}\delta_{n,k},$$

we get

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}\left|\psi_s(t)\right\rangle &= i\hbar\sum_n\frac{d}{dt}a_n(t)\left|n\right\rangle \\
&= [\hat{H}_0 + \lambda\hat{V}(t)]\left|\psi_s(t)\right\rangle \\
&= [H_0 + \lambda\hat{V}(t)]\sum_n a_n(t)\left|n\right\rangle \\
&= \sum_n a_n(t)E_n^{(0)}\left|n\right\rangle + \sum_k \lambda a_k(t)\hat{V}(t)\left|k\right\rangle
\end{aligned}$$

or

$$i\hbar\frac{d}{dt}a_n(t) = E_n^{(0)}a_n(t) + \sum_n \lambda V_{nk}(t)a_k(t) \qquad \text{(Schrödinger picture)} \qquad (1)$$

with

$$a_n(0) = \delta_{ni}\,.$$

We note that $c_n(t)$ for the Dirac picture is related to $a_n(t)$ for the Schrödinger picture by

$$a_n(t) = c_n(t) e^{-iE_n^{(0)}t/\hbar}. \tag{2}$$

Substituting Eq.(2) into Eq.(1), we obtain

$$i\hbar\left\{\dot{c}_n(t)e^{-iE_n t/\hbar} + c_n(t)\left(-\frac{i}{\hbar}E_n^{(0)}\right)e^{-iE_n t/\hbar}\right\} = E_n^{(0)}c_n(t)e^{-iE_n t/\hbar} + \sum_k \lambda V_{nk}(t)c_k(t)e^{-iE_k t/\hbar}\,.$$

Then

$$i\hbar\frac{d}{dt}c_n(t) = \lambda\sum_k e^{i\omega_{nk}t}V_{nk}(t)c_k(t),$$

which is exactly the same result derived directly from the approach of Dirac picture.

5. Constant perturbation

We discuss the case of the constant perturbation using the Dirac picture. Here we assume that $t_0 = 0$ for simplicity and $\hat{V}(t)$ is given by

$$\hat{V}(t) = \hat{V}\Theta(t) = \begin{cases} 0 & \text{for} \quad t < 0 \\ \hat{V} & \text{for} \quad t \geq 0 \end{cases}$$

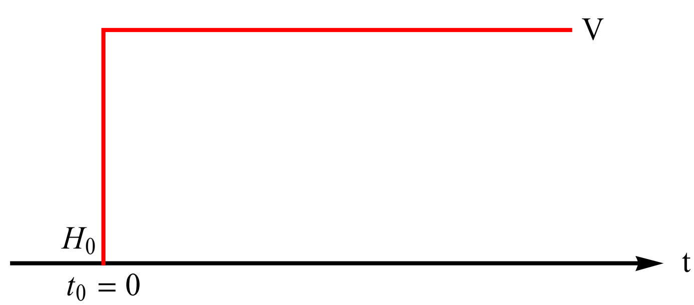


Fig. Constant perturbation.

Then the probability is given by

$$P_{if}(t) = \left|c_f(t)\right|^2,$$

where

$$c_f(t) = c_f^{(0)}(t) + \lambda c_f^{(1)}(t) + \lambda^2 c_f^{(2)}(t) + \cdots.$$

From now on, we shall assume that the sate $|i\rangle$ and $|f\rangle$ are different.

$$c_f^{(0)}(t) = \delta_{f,i} = 0 .$$

Thus we get

$$\begin{aligned} P_{if}(t) &= \lambda^2 \left| c_f^{(1)}(t) \right|^2 \\ &= \frac{\lambda^2}{\hbar^2} \left| \int_0^t e^{i\omega_{fi}t'} V_{fi}(t') dt' \right|^2 \end{aligned}$$

What happens to the higher order term: $c_n^{(2)}$?

$$c_n^{(2)}(t) = (-\frac{i}{\hbar})^2 \sum_m V_{nm} V_{mi} \int_0^t e^{i\omega_{nm}t'} dt' \int_0^{t'} dt'' e^{i\omega_{mi}t''} .$$

We note

$$\begin{aligned} I &= \int_0^t e^{i\omega_{nm}t'} dt' \int_0^{t'} dt'' e^{i\omega_{mi}t''} = \int_0^t dt' e^{i\omega_{nm}t'} (\frac{e^{i\omega_{mi}t'} - 1}{i\omega_{mi}}) \\ &= \frac{1}{i\omega_{mi}} \int_0^t dt' (e^{i(\omega_{nm}+\omega_{mi})t'} - e^{i\omega_{nm}t'}) \\ &= \frac{1}{i\omega_{mi}} \int_0^t dt' (e^{i\omega_{ni}t'} - e^{i\omega_{nm}t'}) \\ &= \frac{1}{i\omega_{mi}} [\left(\frac{e^{i\omega_{ni}t} - 1}{i\omega_{ni}} \right) - \left(\frac{e^{i\omega_{nm}t} - 1}{i\omega_{nm}} \right)] \end{aligned}$$

The second term gives rise to a rapid oscillation when $t \to \infty$. The first term is dominant when $E_n \approx E_i$.

$$c_n^{(2)}(t) = -\frac{1}{\hbar^2 \omega_{ni}} \sum_m \frac{V_{nm} V_{mi}}{\omega_{mi}} (1 - e^{i\omega_{ni}t}) = \sum_m (\frac{V_{nm} V_{mi}}{E_i - E_m})(\frac{1 - e^{i\omega_{ni}t}}{E_n - E_i}) .$$

6. The transition probability for constant perturbation

Here we discuss the probability (to the first order of λ) which is given by

$$P_{if} = \lambda^2 \left| c_f^{(1)}(t) \right|^2 = \frac{\lambda^2}{\hbar^2} \left| \int_0^t dt' e^{i\omega_{fi} t'} V_{fi}(t') \right|^2 .$$

Since

$$c_f^{(1)}(t) = -\frac{i}{\hbar} \int_0^t dt' e^{i\omega_{fi} t'} V_{fi} = -\frac{V_{fi}}{\hbar \omega_{fi}} (e^{i\omega_{fi} t} - 1),$$

we get

$$\begin{aligned} \left| c_f^{(1)}(t) \right|^2 &= \frac{\left| V_{fi} \right|^2}{\hbar^2 \omega_{fi}^2} \left[2 - 2\cos(\omega_{fi} t) \right] \\ &= \frac{1}{\hbar^2} \left[\frac{\sin(\omega_{fi} t/2)}{\omega_{fi}/2} \right]^2 \left| V_{fi} \right|^2 \end{aligned}$$

or

$$P_{if} = \frac{\lambda^2 t^2}{\hbar^2} \left[\frac{\sin(\omega_{fi} t/2)}{\omega_{fi} t/2} \right]^2 \left| V_{fi} \right|^2 .$$

We now consider the probability normalized by $\frac{\lambda^2 t^2 \left| V_{fi} \right|^2}{\hbar^2}$ as

$$\frac{P_{if}}{\frac{\lambda^2 t^2 \left| V_{fi} \right|^2}{\hbar^2}} = \frac{\sin^2\left(\frac{x}{2}\right)}{\left(\frac{x}{2}\right)^2} .$$

where $x = \omega_{fi} t$. This function has a maximum (= 1) at = 0. Since $P_{if} < 1$, the above perturbation theory is valid only if

$$\frac{\lambda^2 t^2 \left| V_{fi} \right|^2}{\hbar^2} << 1.$$

Here we make a plot of the function $\left[\frac{\sin(\omega_{fi}t/2)}{\omega_{fi}t/2}\right]^2$ as a function of $x=\omega_{fi}t$. As t becomes large, $\left|c_f^{(1)}(t)\right|^2$ is appreciable only for those final states satisfy the condition

$$x=\left|\omega_{fi}\right|t\approx 2\pi \; .$$

Note that

$$\int_{-\infty}^{\infty}\frac{\sin^2\left(\frac{x}{2}\right)}{(\frac{x}{2})^2}dx=2\pi \; , \qquad \text{or} \qquad \int_{-\infty}^{\infty}\frac{\sin^2 x}{x^2}dx=\pi \; ,$$

and

$$\lim_{x\to 0}\frac{\sin^2\left(\frac{x}{2}\right)}{(\frac{x}{2})^2}=1 \; .$$

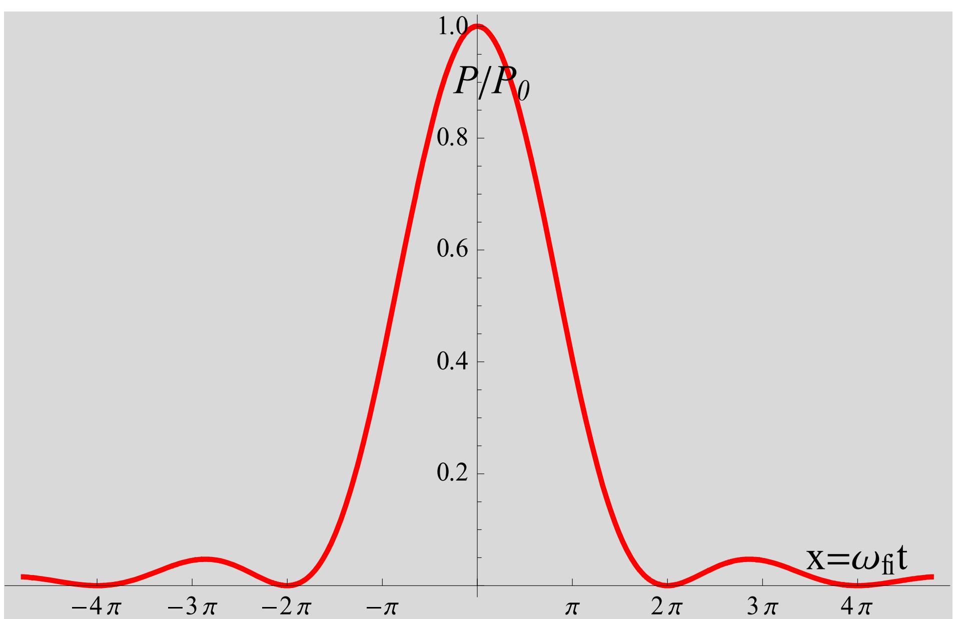


Fig. Normalized transition probability P/P_0 as a function of $x=\omega_{fi}t$. $P_0=\frac{\lambda^2 t^2\left|V_{fi}\right|^2}{\hbar^2}$.
Note that this function becomes zero at $x=\omega_{fi}t=\pm 2\pi, \pm 4\pi.$

((**Note**)) The Dirac delta function
The Dirac delta function $\delta(x)$ has a very sharp peak at $x = 0$ and

$$\int_{-\infty}^{\infty} \delta(x) dx = 1$$

We consider the probability given by

$$P_{if} = \frac{\lambda^2 t^2}{\hbar^2} \left[\frac{\sin(\omega_{fi} t/2)}{\omega_{fi} t/2} \right]^2 |V_{fi}|^2 .$$

We note that

$$\int_{-\infty}^{\infty} \frac{\sin^2(\omega_{fi} t/2)}{(\omega_{fi} t/2)^2} d\omega_{fi} = \frac{2}{t} \int_{-\infty}^{\infty} \frac{\sin^2 x}{x^2} dx = \frac{2\pi}{t} ,$$

where t is sufficiently large and

$$x = \frac{\omega_{fi} t}{2}$$

Since

$$\lim_{t\to\infty} \frac{t}{2\pi} \int_{-\infty}^{\infty} \frac{\sin^2(\omega_{fi} t/2)}{(\omega_{fi} t/2)^2} d\omega_{fi} = 1$$

and

$$\lim_{\omega_{fi}\to 0} \frac{t}{2\pi} \frac{\sin^2(\omega_{fi} t/2)}{(\omega_{fi} t/2)^2} = \frac{t}{2\pi} \qquad \text{(which becomes extremely large as } t \to \infty\text{)}$$

we can define the delta function as

$$\frac{t}{2\pi} \frac{\sin^2(\omega_{fi} t/2)}{(\omega_{fi} t/2)^2} \to \delta(\omega_{fi}) = \delta(\frac{E_f - E_i}{\hbar}) = \hbar\delta(E_f - E_i)$$

Using this definition of the delta function, the probability can be rewritten as

$$P_{if} = \frac{\lambda^2 t^2}{\hbar^2}\left[\frac{\sin(\omega_{fi} t/2)}{\omega_{fi} t/2}\right]^2 |V_{fi}|^2$$

$$= \frac{\lambda^2 t^2}{\hbar^2}\frac{2\pi\hbar}{t}|V_{fi}|^2 \delta(E_f - E_i) \qquad \text{(Fermi's golden rule)}$$

$$= t\frac{2\pi}{\hbar}\lambda^2 |V_{fi}|^2 \delta(E_f - E_i)$$

((Note))

$$P_{if} = t\frac{2\pi}{\hbar}\left|\langle f|\hat{V}|i\rangle + \sum_m \frac{\langle f|\hat{V}|m\rangle\langle m|\hat{V}|i\rangle}{E_f - E_i}\right|^2 \delta(E_f - E_i) \qquad \text{(to the second order of } \lambda\text{)}$$

or

$$w_{if} = \frac{2\pi}{\hbar}\left|\langle f|\hat{V}|i\rangle + \sum_m \frac{\langle f|\hat{V}|m\rangle\langle m|\hat{V}|i\rangle}{E_f - E_i}\right|^2 \delta(E_f - E_i)$$

7. Heisenberg's principle of uncertainty

When we use

$$\omega_{fi} = \frac{\Delta E}{\hbar},$$

we get the transition probability as

$$\frac{P_{if}}{\lambda^2 |V_{fi}|^2} = \frac{t^2}{\hbar^2}\frac{\sin^2\left(\frac{\Delta E}{2\hbar}t\right)}{\left(\frac{\Delta E}{2\hbar}t\right)^2}.$$

Here we make a plot of $P_{if}/\lambda^2|V_{fi}|^2$ as a function of $\Delta E(=\hbar\omega_{fi})$. This function shows a sharp peak at $\Delta E = 0$. The peak height at $\Delta E = 0$ is $t^2/\hbar^2$, while the width of the peak is $\Delta E = 4\pi\hbar/t$. The area of the peak is proportional to

$$A \approx \frac{t^2}{\hbar^2}\frac{4\pi\hbar}{t} = \frac{4\pi t}{\hbar}.$$

When t is long enough, the peak height becomes large. The width becomes narrow. The function becomes a Dirac-type delta function around $\Delta E = 0$. Such a behavior corresponds to the Heisenberg's principle of uncertainty;

$$t\Delta E \approx \hbar.$$

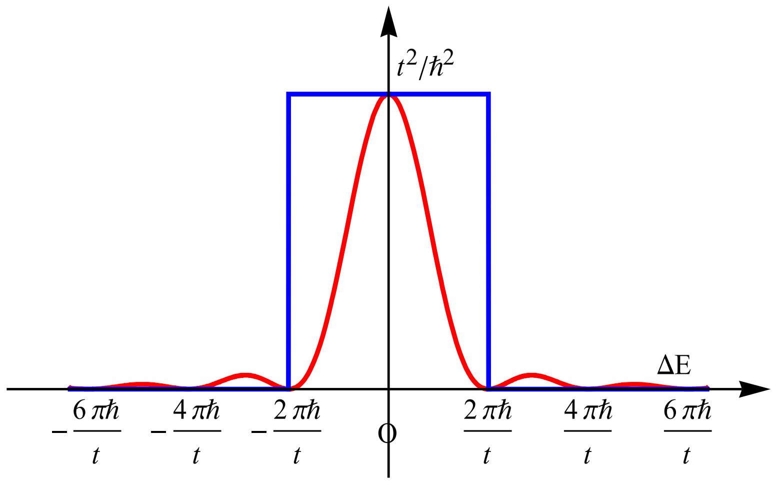


Fig. Plot of $P_{if} / \lambda^2 |V_{fi}|^2$ as a function of $\Delta E = \hbar\omega_{fi}$.

We note that

$$\int_{-\infty}^{\infty} \frac{\sin^2\left(\frac{\Delta E}{2\hbar}t\right)}{\left(\frac{\Delta E}{2\hbar}t\right)^2} d(\Delta E) = \frac{2\hbar}{t}\int_{-\infty}^{\infty} \frac{\sin^2 x}{x^2} dx = \frac{2\pi\hbar}{t},$$

where $x = \frac{\Delta E}{2\hbar}t$. Then the total area enclosed under the red line is evaluated as

$$A_{exact} = \frac{t^2}{\hbar^2}\frac{2\pi\hbar}{t} = \frac{2\pi t}{\hbar}.$$

8. Multiple final states

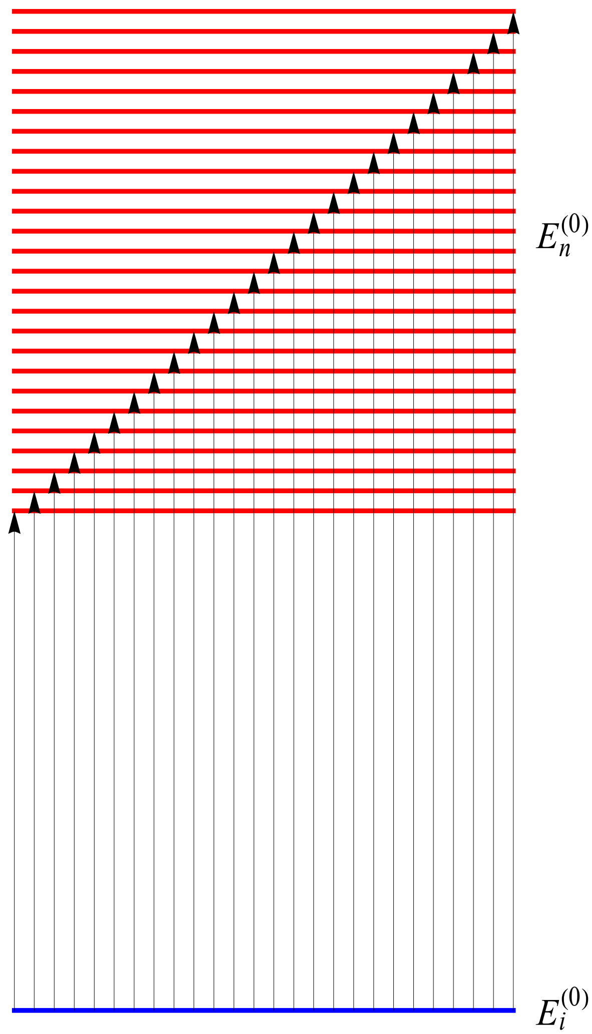


Fig. Energy levels. The discrete energy level ($E_i^{(0)}$) and the continuous energy levels ($E_n^{(0)}$).

A group of final states around the state with $E_i^{(0)}$. $E_i^{(0)}$ is not the state in the continuous region. $E_i^{(0)} \neq E_n^{(0)}$ (or $E_i^{(0)} \cong E_n^{(0)}$). For simplicity hereafter we use E_n instead of $E_n^{(0)}$. Then we have the probability

$$
\begin{aligned}
P &= \lambda^2 \sum_{n, E_n \cong E_i} \left| c_n^{(1)} \right|^2 \\
&= \lambda^2 \int dE_n \rho(E_n) \left| c_n^{(1)} \right|^2 \\
&= \lambda^2 \left| V_{fi} \right|^2 \frac{2\pi t}{\hbar} \int \delta(\Delta E) \rho(E_n) dE_n \\
&= \frac{2\pi}{\hbar} t \lambda^2 \left| V_{fi} \right|^2 \int \delta(E_n - E_i) \rho(E_n) dE_n
\end{aligned}
$$

with

$$\left|c_n^{(1)}\right|^2 = \lambda^2 \left|V_{fi}\right|^2 \frac{t^2}{\hbar^2}\frac{2\pi\hbar}{t}\delta(\Delta E) = \lambda^2 \left|V_{fi}\right|^2 t\frac{2\pi}{\hbar}\delta(E_n - E_i)$$

where t is sufficiently large, $\rho(E)dE$ is the number of states within interval (E ~ E + dE) and $\rho(E)$ is the density of states. Note that $\delta(E_n - E_i)$ (the unit of [energy]$^{-1}$) is the Dirac delta function, which has a sharp peak at $E_n = E_i$,

$$\int_{-\infty}^{\infty}\delta(E_n - E_i)dE_n = 1.$$

Thus the total probability is proportional to t for large value of t. We can define a transition probability per unit time

$$W_{i\to[n]} = \frac{2\pi}{\hbar}\lambda^2\left|V_{ni}\right|^2\delta(E_n - E_i),$$ (Fermi's golden rule)

where $[n]$ stands for a group of final states with energy similar to i. It must be understood that expression is integrated with $\int dE_n \rho(E_n)$

((Note)) Density of states for the 3D system for free electrons

$$\rho(E)dE = \frac{4\pi k^2 dk}{\left(\frac{2\pi}{L}\right)^3}$$

$$E = \frac{\hbar^2}{2m}k^2 \qquad \text{or} \qquad \sqrt{\frac{2m}{\hbar^2}E} = k$$

$$\rho(E)dE = \frac{L^3}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E}dE$$

Thus we have

$$\rho(E) = \frac{L^3}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E}$$ (the density of states for the 3D system)

((**Mathematica**))

```
Clear["Global`*"];
Integrate[Sin[x]^2/x^2, {x, -∞, ∞}]
```

π

```
Integrate[Sin[x]/x, {x, -∞, ∞}]
```

π

9 Harmonic (sinusoidal) perturbation
A. Formulation

We consider a perturbation which oscillates sinusoidally with time. This is usually termed a harmonic perturbation. Now we assume that $\hat{V}(t)$ has one of the simple forms

$$\hat{V}(t) = \hat{V}e^{i\omega t} + \hat{V}^{+}e^{-i\omega t},$$

where $\hat{V}$ is time-independent observable; $t_0 = 0$. For simplicity hereafter we use E_n instead of $E_n^{(0)}$. Then we have

$$\begin{aligned} c_f^{(1)}(t) &= -\frac{i}{\hbar}\int_0^t e^{i\omega_{fi}t'}[\langle f|\hat{V}|i\rangle e^{i\omega t'} + \langle f|\hat{V}^{+}|i\rangle e^{-i\omega t'}]dt' \\ &= -\frac{i}{\hbar}[(\frac{e^{i(\omega+\omega_{fi})t}-1}{\omega+\omega_{fi}})\langle f|\hat{V}|i\rangle + (\frac{e^{i(-\omega+\omega_{fi})t}-1}{-\omega+\omega_{fi}})\langle f|\hat{V}^{+}|i\rangle] \end{aligned}$$

As $t \rightarrow \infty$, $\left|c_f^{(1)}\right|^2$ is appreciable only if

$$\omega + \omega_{fi} = 0 \quad \text{or} \quad E_f = E_i - \hbar\omega, \qquad \text{(stimulated emission)}$$

or

$$-\omega + \omega_{fi} = 0 \quad \text{or} \quad E_f = E_i + \hbar\omega, \qquad \text{(absorption)}$$

where

$$\omega_{fi} = \frac{E_f - E_i}{\hbar}.$$

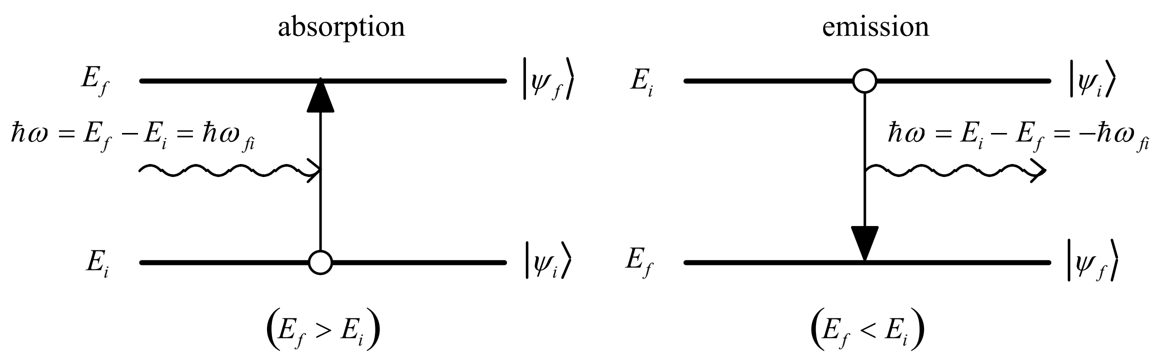
Therefore, we have

$$P_{if}(t;\omega) = \lambda^2 \left| c_f^{(1)}(t) \right|^2$$

$$= \frac{\lambda^2}{\hbar^2} \left| \left(\frac{e^{i(\omega+\omega_{fi})t} - 1}{\omega + \omega_{fi}} \right) \langle f | \hat{V} | i \rangle + \left(\frac{e^{i(-\omega+\omega_{fi})t} - 1}{-\omega + \omega_{fi}} \right) \langle f | \hat{V}^+ | i \rangle \right|^2$$

B. Resonant nature of the transition probability

We consider the following case (two discrete case)



We have

$$A_+ \equiv \frac{e^{i(\omega_{fi}+\omega)t} - 1}{\omega_{fi} + \omega} = ie^{i(\omega_{fi}+\omega)t/2} \frac{\sin[(\omega_{fi} + \omega)t/2]}{(\omega_{fi} + \omega)/2}.$$

for the emission

$$A_- \equiv \frac{e^{i(\omega_{fi}-\omega)t} - 1}{\omega_{fi} - \omega} = ie^{i(\omega_{fi}-\omega)t/2} \frac{\sin[(\omega_{fi} - \omega)t/2]}{(\omega_{fi} - \omega)/2}.$$

for the absorption.

(i) When $E_f > E_i$, $\Rightarrow$ $\omega_{fi} > 0$. Under such conditions, A_- dominates (absorption).

$$P_{if}(t;\omega) = \frac{\lambda^2}{\hbar^2} \left| \langle f | \hat{V}^+ | i \rangle \right|^2 F(t, \omega - \omega_{fi}),$$

with

$$F(t, \omega - \omega_{fi}) = \left[\frac{\sin(\omega_{fi} - \omega)t/2}{(\omega_{fi} - \omega)/2} \right]^2,$$

$$F = 0 \text{ at } \omega_{fi} - \omega = \pm\frac{2\pi}{t}, \pm\frac{4\pi}{t}, \cdots. \ \Delta\omega \cong \frac{4\pi}{t}.$$

The function $F(t,\omega-\omega_{fi})$ is only non-negligible when

$$\left|\omega_{fi}-\omega\right|\leq\frac{2\pi}{t}.$$

For finite *t*,

$$\lim_{\omega\to\omega_{fi}} F(t;\omega-\omega_{fi})=t^2.$$

In the limit of larger *t*, we have

$$\begin{aligned}F(t,\omega-\omega_{fi}) &= \left[\frac{\sin(\omega_{fi}-\omega)t/2}{(\omega_{fi}-\omega)/2}\right]^2 \\ &= 2\pi t\delta(\omega_{fi}-\omega) \\ &= 2\pi\hbar t\delta(E_f-E_i-\hbar\omega)\end{aligned}$$

since

$$\begin{aligned}\int_{-\infty}^{\infty}\left[\frac{\sin(\omega_{fi}-\omega)t/2}{(\omega_{fi}-\omega)/2}\right]^2 d\omega_{fi} &= t^2\int_{-\infty}^{\infty}\left[\frac{\sin(\omega_{fi}-\omega)t/2}{(\omega_{fi}-\omega)t/2}\right]^2 d\omega_{fi} \\ &= 2t\int_{-\infty}^{\infty} dx\frac{\sin^2 x}{x^2}dx \\ &= 2\pi t \\ &= 2\pi t\int_{-\infty}^{\infty} d\omega_{fi}\delta(\omega_{fi}-\omega)\end{aligned}$$

Then we have

$$\begin{aligned}P_{if}(t;\omega) &= \frac{\lambda^2}{\hbar^2}\left|\langle f|\hat{V}^+|i\rangle\right|^2 2\pi\hbar t\delta(E_f-E_i-\hbar\omega) \\ &= t\frac{2\pi}{\hbar}\lambda^2\left|\langle f|\hat{V}^+|i\rangle\right|^2\delta(E_f-E_i-\hbar\omega)\end{aligned}$$

Taking into account of the number of states $\rho(E_f)dE_f$, the total probability is given by

$$P=t\frac{2\pi}{\hbar}\lambda^2\int\rho(E_n)dE_n\left|\langle f|\hat{V}^+|i\rangle\right|^2\delta(E_f-E_i-\hbar\omega) \qquad \text{(absorption)}$$

This is proportional to t. $\delta(E_f - E_i - \hbar\omega)$ indicates the energy conservation. We can define a transition probability per unit time

$$W_{i\to[n]} = \frac{2\pi}{\hbar}\lambda^2 \left|\langle f|\hat{V}^+|i\rangle\right|^2 \delta(E_f - E_i - \hbar\omega), \qquad \text{(Fermi's golden rule)}$$

where $[n]$ stands for a group of final states with energy similar to i. It must be understood that expression is integrated with $\int dE_n \rho(E_n)$

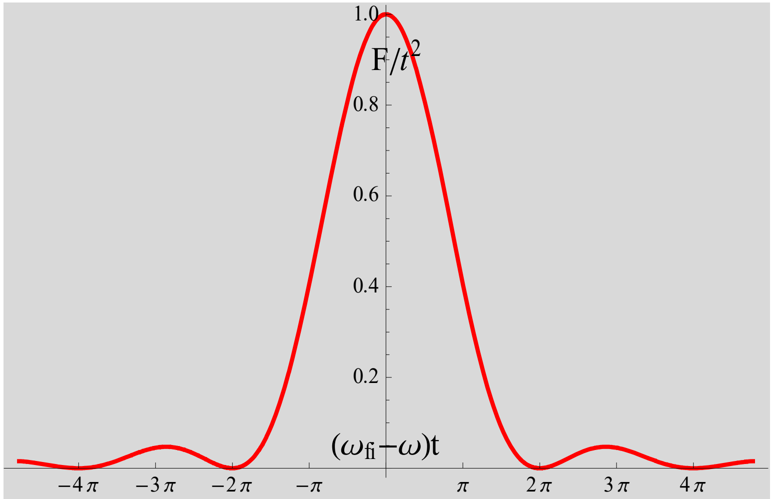


Fig. Transition probability as a function of $(\omega_{fi} - \omega)t$ at a fixed time t.

(ii) When $E_f > E_i$, $\Rightarrow$ $\omega_{fi} < 0$. A_+ dominant (emission).

$$P_{if}(t;\omega) = \frac{\lambda^2}{\hbar^2}\left|\langle f|\hat{V}|i\rangle\right|^2 F(t,\omega+\omega_{fi}),$$

$$F(t,\omega+\omega_{fi}) = \left[\frac{\sin(\omega_{fi}+\omega)t/2}{(\omega_{fi}+\omega)/2}\right]^2,$$

$$F = 0 \text{ at } \omega_{fi} + \omega = \pm\frac{2\pi}{t}, \pm\frac{4\pi}{t}, \cdots. \ \Delta\omega \cong \frac{4\pi}{t}.$$

In the limit of larger t, we have

$$
\begin{aligned}
F(t,\omega+\omega_{fi}) &= \left[\frac{\sin(\omega_{fi}+\omega)t/2}{(\omega_{fi}+\omega)/2}\right]^2 \\
&= 2\pi t\delta(\omega_{fi}+\omega) \\
&= 2\pi\hbar t\delta(E_f - E_i + \hbar\omega)
\end{aligned}
$$

since

$$
\begin{aligned}
\int_{-\infty}^{\infty}\left[\frac{\sin(\omega_{fi}+\omega)t/2}{(\omega_{fi}+\omega)/2}\right]^2 d\omega_{fi} &= t^2\int_{-\infty}^{\infty}\left[\frac{\sin(\omega_{fi}+\omega)t/2}{(\omega_{fi}+\omega)t/2}\right]^2 d\omega_{fi} \\
&= 2t\int_{-\infty}^{\infty} dx\frac{\sin^2 x}{x^2}dx \\
&= 2\pi t \\
&= 2\pi t\int_{-\infty}^{\infty} d\omega_{fi}\delta(\omega_{fi}+\omega)
\end{aligned}
$$

or

$$
\frac{2\pi}{t}\delta(\omega) = \lim_{t\to\infty}\frac{\sin^2\left(\frac{\omega t}{2}\right)}{\left(\frac{\omega t}{2}\right)^2} \qquad \text{(formula)}
$$

or

$$
2\pi t\delta(\omega) = \lim_{t\to\infty}\frac{\sin^2\left(\frac{\omega t}{2}\right)}{\left(\frac{\omega}{2}\right)^2} \qquad \text{(formula)}
$$

Then we have

$$
\begin{aligned}
P_{if}(t;\omega) &= \frac{\lambda^2}{\hbar^2}\left|\langle f|\hat{V}|i\rangle\right|^2 2\pi\hbar t\delta(E_f - E_i + \hbar\omega) \\
&= t\frac{2\pi}{\hbar}\lambda^2\left|\langle f|\hat{V}|i\rangle\right|^2 \delta(E_f - E_i + \hbar\omega)
\end{aligned}
$$

Taking into account of the number of states $\rho(E_f)dE_f$, the total probability is given by

$$P = t\frac{2\pi}{\hbar}\lambda^2 \int \rho(E_n)dE_n \left|\langle f|\hat{V}|i\rangle\right|^2 \delta(E_f - E_i + \hbar\omega)$$ (emission)

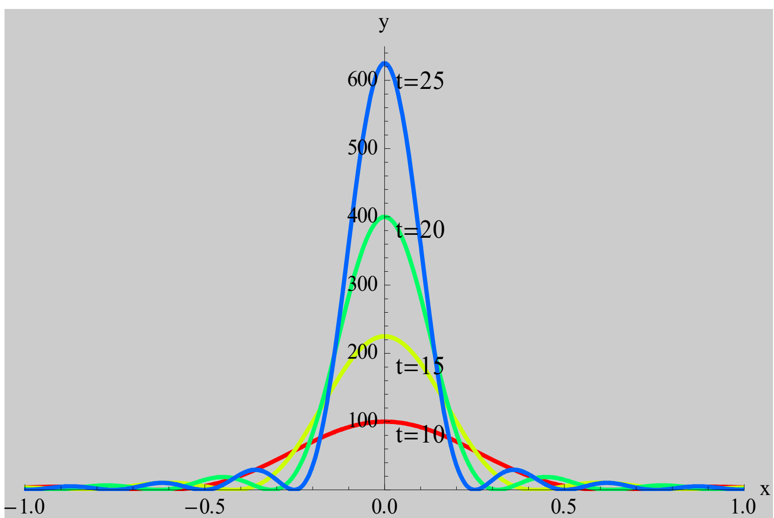
This is proportional to *t*. $\delta(E_f - E_i + \hbar\omega)$ indicates the energy conservation. We can define a transition probability per unit time

$$W_{i\to[n]} = \frac{2\pi}{\hbar}\lambda^2 \left|\langle f|\hat{V}|i\rangle\right|^2 \delta(E_f - E_i + \hbar\omega),$$ (Fermi's golden rule)

where $[n]$ stands for a group of final states with energy similar to *i*. It must be understood that expression is integrated with $\int dE_n \rho(E_n)$

((**Note**))

The plot of the function $y = \dfrac{\sin^2\left(\dfrac{tx}{2}\right)}{\left(\dfrac{x}{2}\right)^2}$ as a function of *x*, where *t* is changed as a parameter.



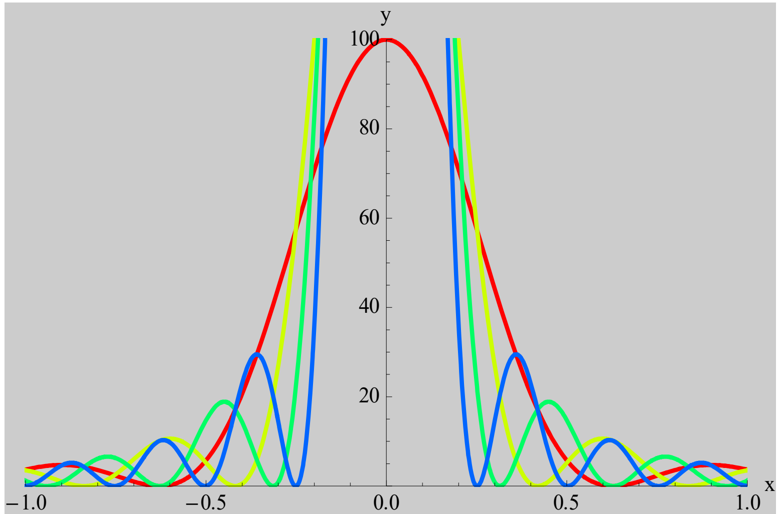


Fig. Plot of $y = \dfrac{\sin^2\left(\dfrac{tx}{2}\right)}{\left(\dfrac{x}{2}\right)^2}$ as a function of x, where $t = 5$, 10, 15, 20, and 25.

C. Discussion of the resonant approximation

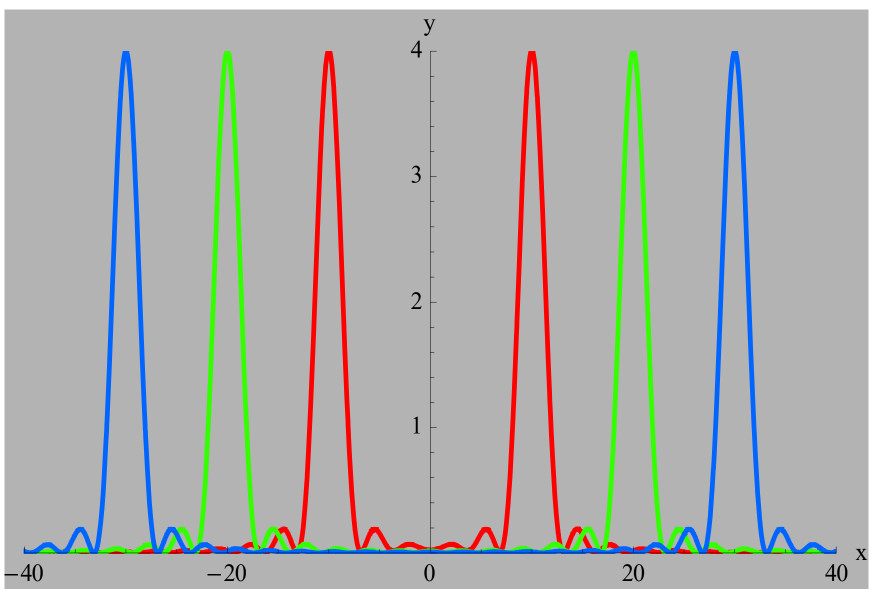


Fig. Plot of $y = \dfrac{\sin^2\left(\dfrac{t(x-a)}{2}\right)}{\left(\dfrac{x}{2}\right)^2} + \dfrac{\sin^2\left(\dfrac{t(x+a)}{2}\right)}{\left(\dfrac{x}{2}\right)^2}$ as a function of x, where $t = 2$. $a = 10$ (red), 20 (green), and 30 (blue). As a is decreased, the position of two peaks approaches to zero.

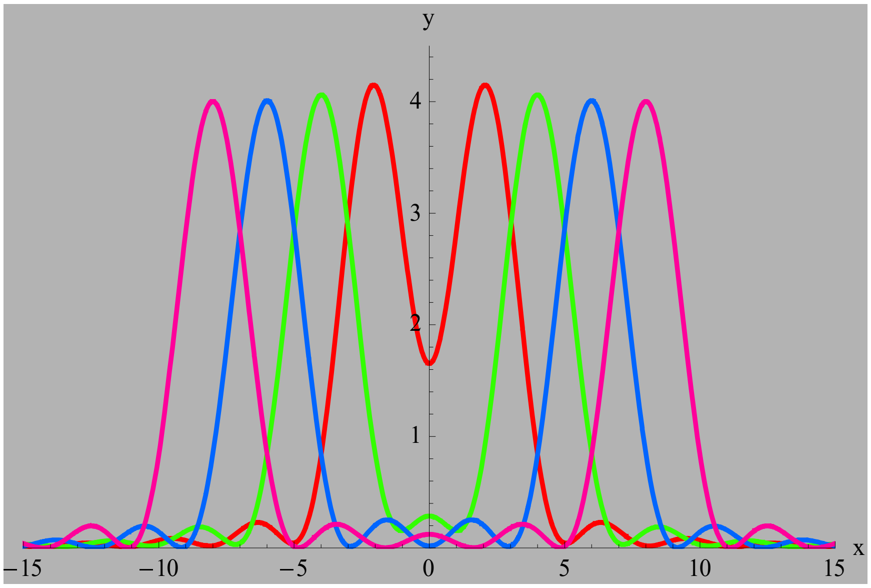
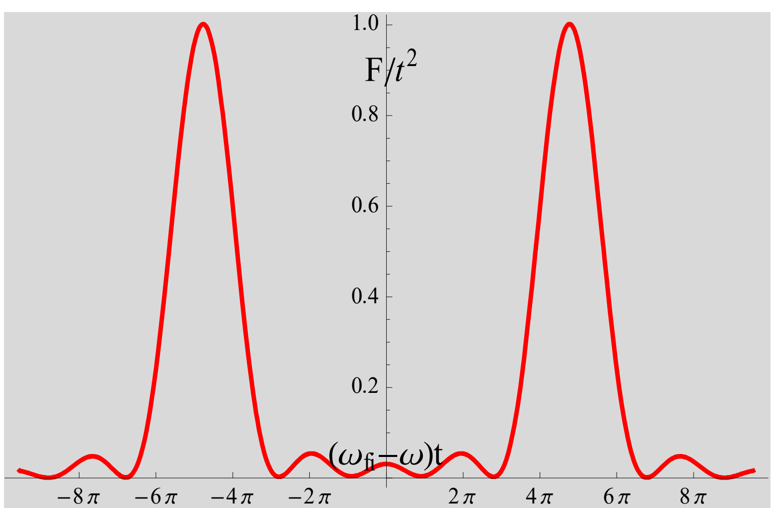


Fig. Plot of $y = \dfrac{\sin^2\left(\dfrac{t(x-a)}{2}\right)}{\left(\dfrac{x}{2}\right)^2} + \dfrac{\sin^2\left(\dfrac{t(x+a)}{2}\right)}{\left(\dfrac{x}{2}\right)^2}$ as a function of x, where $t = 2$. $a = 2$ (red), 4 (green), 6 (blue), and 8 (pink). When a is close to zero, two peaks are overlapped to each other.



If $\Delta\omega << 2|\omega_{fi}|$, in the neighborhood of $\omega = \omega_{fi}$, the modulus of A_+ is negligible compare to that of A_-. Since $\Delta\omega = \dfrac{4\pi}{t}$, we have

$$t >> \frac{1}{|\omega_{fi}|} \cong \frac{1}{\omega}$$ (resonance condition).

The condition $\Delta\omega << 2|\omega_{fi}|$ implies that the line width of each peak is much smaller than that the separation between two peaks due to absorption and emission.

D. Limit of first-order calculation

$$P_{if}(t, \omega = \omega_{fi}) = \frac{\lambda^2}{\hbar^2} \left| \langle f | \hat{V}^+ | i \rangle \right|^2 \lim_{\omega \to \omega_{fi}} F(t; \omega - \omega_{fi}) = \frac{\lambda^2}{\hbar^2} \left| \langle f | \hat{V}^+ | i \rangle \right|^2 t^2 . \quad (1)$$

$$P_{if}(t, \omega = -\omega_{fi}) = \frac{\lambda^2}{\hbar^2} \left| \langle f | \hat{V} | i \rangle \right|^2 \lim_{\omega \to -\omega_{fi}} F(t; \omega + \omega_{fi}) = \frac{\lambda^2}{\hbar^2} \left| \langle f | \hat{V} | i \rangle \right|^2 t^2$$

This becomes infinite when $t \to \infty$, which is absurd, since a probability can never be greater than 1. In practice, for the first-order approximation to be valid at resonance, the probability (1) must be much smaller than 1.

$$\frac{\lambda^2}{\hbar^2} \left| \langle f | \hat{V}^+ | i \rangle \right|^2 t^2 << 1, \text{ or } \qquad t << \frac{\hbar}{\lambda \left| \langle f | \hat{V}^+ | i \rangle \right|} .$$

Therefore t should be

$$\frac{1}{\omega} = \frac{1}{|\omega_{fi}|} << t << \frac{\hbar}{\lambda \left| \langle f | \hat{V}^+ | i \rangle \right|} ,$$

or

$$\frac{1}{|\omega_{fi}|} << \frac{\hbar}{\lambda \left| \langle f | \hat{V}^+ | i \rangle \right|} ,$$

or

$$\hbar |\omega_{fi}| >> \lambda \left| \langle f | \hat{V}^+ | i \rangle \right| .$$ (the condition for the validity of perturbation theory)

10. Harmonic perturbation at resonance (exact solution))

If the perturbation acts for a long time at resonance, the above perturbation scheme breaks down. In this case we need to solve the problem exactly. Here we assume that

$$\omega \approx \omega_{fi}.$$

We consider the two states $|i\rangle$ and $|f\rangle$.

$$i\hbar \frac{d}{dt} c_i(t) = V_{ii}(t) c_i(t) + e^{-i\omega_{fi}t} V_{if}(t) c_f(t),$$

$$i\hbar \frac{d}{dt} c_f(t) = V_{ff}(t) c_f(t) + e^{i\omega_{fi}t} V_{fi}(t) c_i(t).$$

We choose the harmonic perturbation as

$$\hat{V}(t) = 2\hat{H}'\sin(\omega t) = -i(e^{i\omega t} - e^{-i\omega t})\hat{H}'.$$

Then we have

$$i\hbar \frac{d}{dt} c_i(t) = -i(e^{i\omega t} - e^{-i\omega t})\langle i|\hat{H}'|i\rangle c_i(t) - i(e^{-i(\omega_{fi}-\omega)t} - e^{-i(\omega+\omega_{fi})t})\langle i|\hat{H}'|f\rangle c_f(t),$$

$$i\hbar \frac{d}{dt} c_f(t) = -i(e^{i\omega t} - e^{-i\omega t})\langle f|\hat{H}'|f\rangle c_f(t) - i(e^{i(\omega_{fi}+\omega)t} - e^{i(\omega_{fi}-\omega)t})\langle f|\hat{H}'|i\rangle c_i(t).$$

In the approximation of $\omega \approx \omega_{fi}$, we can approximate and write

$$i\hbar \frac{d}{dt} c_i(t) = -ie^{-i(\omega_{fi}-\omega)t}\langle i|\hat{H}'|f\rangle c_f(t) = -ie^{-i(\omega_{fi}-\omega)t}\langle f|\hat{H}'|i\rangle^* c_f(t),$$

$$i\hbar \frac{d}{dt} c_f(t) = ie^{i(\omega_{fi}-\omega)t}\langle f|\hat{H}'|i\rangle c_i(t).$$

((**Rotating wave approximation**))

We assume that the system is initially in the *i*-state.

$$c_i(0) = 1, \qquad c_f(0) = 0.$$

The solutions of this differential equations are as follows.

$$c_i(t) = e^{-i\omega_0 t/2}[\cos(\frac{1}{2}\omega_c t) + \frac{i\omega_0}{2\omega_c}\sin(\frac{1}{2}\omega_c t)],$$

$$c_f(t) = \frac{2\langle f|\hat{H}'|i\rangle}{\hbar\omega_c} e^{i\omega_0 t/2}\sin(\frac{1}{2}\omega_c t).$$

where

$$\omega_0 = \omega_{fi} - \omega ,$$

$$\omega_c = \frac{1}{\hbar}\sqrt{\hbar^2 \omega_0{}^2 + 4\,|\langle f|\hat{H}'|i\rangle|^2} \qquad \text{(Rabbi frequency)}$$

The transition probability is given by

$$\begin{aligned} P_{i\to f} &= |c_f(t)|^2 \\ &= 4\frac{|\langle f|\hat{H}'|i\rangle|^2}{\hbar^2 \omega_c{}^2}\sin^2(\frac{1}{2}\omega_c t) \qquad \text{(Breit-Wigner formula)} \\ &= \frac{4|\langle f|\hat{H}'|i\rangle|^2}{\hbar^2 \omega_0{}^2 + 4|\langle f|\hat{H}'|i\rangle|^2}\sin^2(\frac{1}{2}\omega_c t) \end{aligned}$$

This probability is between 0 and 1, no matther how long the perturbation acts. When the transition probability is zero, the system has oscillated back to the initial state. At the resonance ($\omega_0 = 0$), we have

$$P_{i\to f} = \sin^2(\frac{1}{2}\omega_c t) = \sin^2(\frac{1}{\hbar}|\langle f|\hat{H}'|i\rangle| t) .$$

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

$$P_{i\to f} = \frac{1}{\hbar^2}|\langle f|\hat{H}'|i\rangle|^2 t^2 .$$

((**Mathematica**))

```
Clear["Global`*"];
eq1 = ℏ C1'[t] + Exp[-ⅈ ω0 t] A C2[t] == 0;
eq2 = ℏ C2'[t] - Exp[ⅈ ω0 t] A1 C1[t] == 0;
eq3 = C1[0] == 1; eq4 = C2[0] == 0;
f1 = DSolve[{eq1, eq2, eq3, eq4},
    {C1[t], C2[t]}, t] //
   FullSimplify[#,
     {A > 0, A1 > 0, ω0 > 0, ℏ > 0}] &;
```

$$\text{rule1} = \left\{ \frac{\sqrt{4\,A\,A1 + \omega 0^2\,\hbar^2}}{\hbar} \to \omega c,\ \frac{1}{\sqrt{4\,A1\,A + \omega 0^2\,\hbar^2}} \to \frac{1}{\hbar\,\omega c} \right\};$$

```
f1 //. rule1 // Simplify
```

$$\left\{\left\{C1[t] \to e^{-\frac{1}{2}\,i\,t\,\omega 0}\left(\mathrm{Cos}\left[\frac{t\,\omega c}{2}\right] + \frac{i\,\omega 0\,\mathrm{Sin}\left[\frac{t\,\omega c}{2}\right]}{\omega c}\right),\right.\right.$$
$$\left.\left. C2[t] \to \frac{2\,A1\,e^{\frac{i\,t\,\omega 0}{2}}\,\mathrm{Sin}\left[\frac{t\,\omega c}{2}\right]}{\omega c\,\hbar}\right\}\right\}$$

11. Fermi's golden rule

From the above discussion we have

$$P_{i\to f} = \frac{4\left|\langle f|\hat{H}'|i\rangle\right|^2}{\hbar^2\omega_0{}^2 + 4\left|\langle f|\hat{H}'|i\rangle\right|^2}\sin^2(\frac{1}{2}\omega_c t)$$
$$\approx \frac{4\left|\langle f|\hat{H}'|i\rangle\right|^2}{\hbar^2(\omega-\omega_{fi})^2}\sin^2\frac{(\omega-\omega_{fi})t}{2}$$

We assume that the final state is a state of the continuum, labeled by the wave number k_f (energy E_f).

$$\omega_{fi} - \omega = \frac{1}{\hbar}(E_f - E_i - \hbar\omega).$$

Note that $E_f \approx (E_i + \hbar\omega) \pm \Delta E$. So the resultant transition probability is

$$P_{i\to f} = \int_{-\Delta E}^{\Delta E} \frac{4\left|\langle f|\hat{H}'|i\rangle\right|^2}{\hbar^2} \frac{\sin^2\frac{(\omega_{fi}-\omega)t}{2}}{(\omega_{fi}-\omega)^2} \rho_f(E_f)dE_f \ .$$

The function $\dfrac{\sin^2\frac{(\omega_{fi}-\omega)t}{2}}{(\omega_{fi}-\omega)^2}$ behaves like a Dirac delta function. This funcntion shows a shapr peak at $\omega_{fi}-\omega=0$. We put $x=\dfrac{(\omega_{fi}-\omega)t}{2}$

$$\begin{aligned}
P_{i\to f} &= \frac{4\left|\langle f|\hat{H}'|i\rangle\right|^2}{\hbar^2} \rho(E_f)\frac{t^2}{4}\frac{2\hbar}{t}\int_{-\infty}^{\infty}\frac{\sin^2 x}{x^2}dx \\
&= \frac{4\left|\langle f|\hat{H}'|i\rangle\right|^2}{\hbar} \frac{\rho(E_f)t}{2}\int_{-\infty}^{\infty}\frac{\sin^2 x}{x^2}dx \\
&= \frac{2\pi}{\hbar}\left|\langle f|\hat{H}'|i\rangle\right|^2 \rho(E_f)t
\end{aligned}$$

where

$$dE_f = \frac{2\hbar}{t}dx\,, \qquad \int_{-\infty}^{\infty}\frac{\sin^2 x}{x^2}dx = \pi\,.$$

Thus, the rate of transition to such a group of states is

$$\boxed{R_{i\to f} = \frac{P_{i\to f}}{t} = \frac{2\pi}{\hbar}\left|\langle f|H'|i\rangle\right|^2 \rho(E_f)}$$

12. Summary on Femi's golden rule (Wikipedia)

http://en.wikipedia.org/wiki/Fermi%27s_golden_rule

In quantum physics, **Fermi's golden rule** is a way to calculate the transition rate (probability of transition per unit time) from one energy eigenstate of a quantum system into a continuum of energy eigenstates, due to a perturbation.

We consider the system to begin in an eigenstate, $|i\rangle$, of a given Hamiltonian, $\hat{H}_0$. We consider the effect of a (possibly time-dependent) perturbing Hamiltonian, $\hat{H}'$. If $\hat{H}'$is time-independent, the system goes only into those states in the continuum that have the same energy as the initial state. If $\hat{H}'$ is oscillating as a function of time with an angular frequency ω, the transition is into states with energies that differ by $\hbar\omega$ from the energy of the initial state. In both cases, the one-to-many transition probability per unit of time from the state $|i\rangle$ to a set of final states $|f\rangle$ is given, to first order in the perturbation, by

$$R_{i\to f} = \frac{P_{i\to f}}{t} = \frac{2\pi}{\hbar}\left|\langle f|H'|i\rangle\right|^2 \rho_f ,$$

where ρ is the density of final states (number of states per unit of energy) and $\langle f|H'|i\rangle$ is the matrix element of the perturbation $\hat{H}'$ between the final and initial states. This transition probability is also called decay probability and is related to mean lifetime. Fermi's golden rule is valid when the initial state has not been significantly depleted by scattering into the final states.

Although named after Fermi, most of the work leading to the Golden Rule was done by Dirac who formulated an almost identical equation, including the three components of a constant, the matrix element of the perturbation and an energy difference. It is given its name because, being such a useful relation, Fermi himself called it "Golden Rule No. 2."

13. Free electron gas in three dimensions

We consider the Schrödinger equation of an electron confined to a cube of edge L.

$$H\psi_{\boldsymbol{k}} = \frac{\boldsymbol{p}^2}{2m}\psi_{\boldsymbol{k}} = -\frac{\hbar^2}{2m}\nabla^2\psi_{\boldsymbol{k}} = \varepsilon_{\boldsymbol{k}}\psi_{\boldsymbol{k}} . \tag{3}$$

It is convenient to introduce wavefunctions that satisfy periodic boundary conditions.

Boundary condition (Born-von Karman boundary conditions).

$$\psi_{\boldsymbol{k}}(x+L,y,z) = \psi_{\boldsymbol{k}}(x,y,z) ,$$
$$\psi_{\boldsymbol{k}}(x,y+L,z) = \psi_{\boldsymbol{k}}(x,y,z) ,$$
$$\psi_{\boldsymbol{k}}(x,y,z+L) = \psi_{\boldsymbol{k}}(x,y,z) .$$

The wavefunctions are of the form of a traveling plane wave.

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} , \tag{4}$$

with

$k_x = (2\pi/L)\, n_x$, ($n_x = 0, \pm1, \pm2, \pm3,\ldots..$),

$k_y = (2\pi/L)\, n_y$, ($n_y = 0, \pm1, \pm2, \pm3,\ldots..$),

$k_z = (2\pi/L)\, n_z$, ($n_z = 0, \pm1, \pm2, \pm3,\ldots..$).

The components of the wavevector $\boldsymbol{k}$ are the quantum numbers, along with the quantum number m_s of the spin direction. The energy eigenvalue is

$$\varepsilon(\boldsymbol{k}) = \frac{\hbar^2}{2m}(k_x{}^2 + k_y{}^2 + k_z{}^2) = \frac{\hbar^2}{2m}\boldsymbol{k}^2 . \tag{5}$$

Here

$$\boldsymbol{p}\psi_k(\boldsymbol{r}) = \frac{\hbar}{i}\nabla_{\boldsymbol{k}}\psi_k(\boldsymbol{r}) = \hbar\boldsymbol{k}\psi_k(\boldsymbol{r}) . \tag{6}$$

So that the plane wave function $\psi_{\boldsymbol{k}}(\boldsymbol{r})$ is an eigenfunction of $\boldsymbol{p}$ with the eigenvalue $\hbar\boldsymbol{k}$. The ground state of a system of N electrons, the occupied orbitals are represented as a point inside a sphere in $\boldsymbol{k}$-space.

Because we assume that the electrons are noninteracting, we can build up the N-electron ground state by placing electrons into the allowed one-electron levels we have just found.

14. The Pauli's exclusion principle

The one-electron levels are specified by the wavevectors $\boldsymbol{k}$ and by the projection of the electron's spin along an arbitrary axis, which can take either of the two values $\pm\hbar/2$. Therefore associated with each allowed wave vector k are two levels:

$$\left|\boldsymbol{k},\uparrow\right\rangle,\ \left|\boldsymbol{k},\downarrow\right\rangle .$$

In building up the N-electron ground state, we begin by placing two electrons in the one-electron level $k = 0$, which has the lowest possible one-electron energy $\varepsilon = 0$. We have

$$N = 2\frac{L^3}{(2\pi)^3}\frac{4\pi}{3}k_F{}^3 = \frac{V}{3\pi^2}k_F{}^3 .$$

Density of states

There is one state per volume of $\boldsymbol{k}$-space $(2\pi/L)^3$. We consider the number of one-electron levels in the energy range from ε to ε+dε; $D(\varepsilon)$dε

$$D(\varepsilon)d\varepsilon = 2\frac{L^3}{(2\pi)^3}4\pi k^2 dk ,$$

where $D(\varepsilon)$ is called a density of states. Since $k = (2m/\hbar^2)^{1/2}\sqrt{\varepsilon}$, we have $dk = (2m/\hbar^2)^{1/2}d\varepsilon/(2\sqrt{\varepsilon})$. Then we get the density of states

$$D(\varepsilon) = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\varepsilon} .$$

where the spin factor (2) is included.

15. Time dependent perturbation: selected examples

$$|\psi_I(t)\rangle = \sum_n c_n(t)|n\rangle$$

where

$$c_n(t) = c_n^{(0)}(t) + \lambda c_n^{(1)}(t) + \lambda^2 c_n^{(2)}(t) + ...$$

Using the following formula, we solve several problems.

$$c_n^{(0)}(t) = \delta_{n,i}$$

$$c_n^{(1)} = (-\frac{i}{\hbar})\int_{t_0}^{t} dt' e^{i\omega_{ni}t'} V_{ni}(t')$$

$$c_n^{(2)} = (-\frac{i}{\hbar})^2 \sum_m \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' e^{i\omega_{nm}t'} V_{nm}(t') e^{i\omega_{mi}t''} V_{mi}(t'')$$

$$P(i \to f) = \lambda^2 \left|c_f^{(1)}(t)\right|^2 = \frac{\lambda^2}{\hbar^2}\left|\int_{t_0}^{t} e^{i\omega_{fi}t'}\langle f|\hat{V}(t')|i\rangle dt'\right|^2$$

15.1 A linear harmonic oscillator is acted upon a uniform electric field which is considered to be a perturbation and which depends as follows on the time:

$$\varepsilon(t) = A\frac{1}{\sqrt{\pi}\tau}e^{-(t/\tau)^2},$$

where A is a constant. (Since the action of a uniform field is equivalent to a shift of the point of suspension, this problem can be solved not only by perturbation theory, but also exactly). Assuming that when the field is switched on (that is, at $t = -\infty$) the oscillator is in its ground state, evaluate to a first approximation the probability that it is excited at the end of the action of the field (that is, at $t = +\infty$).

((**Solution**))
The total pulse P_0 is defined by

$$P_0 = \int_{-\infty}^{\infty} e\varepsilon(t)dt = \frac{eA}{\sqrt{\pi}\tau}\int_{-\infty}^{\infty}\exp[-(\frac{t}{\tau})^2]dt = eA = const.$$

P_0 is classically transferred to the system by the electric field. $A = P_0/e$.

$$\hat{H}_0 = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega_0{}^2\hat{x}^2, \qquad \hat{H}_1 = -e\varepsilon\hat{x} \ (e<0),$$

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

with

$$E_n{}^{(0)} = (n+\frac{1}{2})\hbar\omega_0,$$

$$\hat{H}_1|n\rangle = -e\varepsilon\hat{x}|n\rangle = (-e\varepsilon)\sqrt{\frac{\hbar}{2m\omega_0}}(\sqrt{n}|n-1\rangle + \sqrt{n+1}|n+1\rangle).$$

The probability for a transition from the state $|n\rangle$ to the state $|k\rangle$ is equal to

$$P(n \to k) = \lambda^2 \left|c_f{}^{(1)}(t)\right|^2 = \frac{1}{\hbar^2}\left|\int_{-0}^{t}\exp(i\omega_{kn}t')\langle k|\hat{H}_1|n\rangle dt'\right|^2,$$

where

$$\hbar\omega_{kn} = E_k{}^{(0)} - E_n{}^{(0)}.$$

For $|n\rangle = |0\rangle$,

$$\langle k|\hat{H}_1|0\rangle = -e\varepsilon\langle k|\hat{x}|0\rangle = (-e\varepsilon)\sqrt{\frac{\hbar}{2m\omega_0}}\langle k|1\rangle = (-e\varepsilon)\sqrt{\frac{\hbar}{2m\omega_0}}\delta_{k,1}.$$

So the matrix element is not zero only if $k = 1$.

$$P(0 \to 1) = \left|c_f{}^{(1)}(t)\right|^2 = \frac{1}{\hbar^2}\left|\int_{-\infty}^{t}\exp(i\omega_{10}t')\langle 1|\hat{H}_1|0\rangle dt'\right|^2,$$

or

$$P(0 \to 1) = \left|c_f{}^{(1)}(t)\right|^2 = \frac{1}{\hbar^2}\frac{e^2\hbar}{2m\omega_0}\left|\int_{-\infty}^{t}\exp(i\omega_{10}t')\varepsilon(t')dt'\right|^2,$$

or

$$P(0\to 1)=\left|c_f{}^{(1)}(t)\right|^2=\frac{P_0^{\;2}}{2\pi\tau^2 m\hbar\omega_0}\left|\int_{-\infty}^{t}\exp[i\omega_{10}t'-(t'/\tau)^2]dt'\right|^2,$$

or

$$P(0\to 1)=\left|c_f{}^{(1)}(t)\right|^2=\frac{P_0^{\;2}}{8m\hbar\omega_0}\exp[-\frac{(\omega_{10}\tau)^2}{2}]\left|1+erf[\frac{t}{\tau}-\frac{i\omega_{10}\tau}{2})\right|^2.$$

When $t\to\infty$,

$$P(0\to 1)=\left|c_f{}^{(1)}(t)\right|^2=\frac{P_0^{\;2}}{2m\hbar\omega_0}\exp[-\frac{(\omega_{10}\tau)^2}{2}].$$

For a given P_0, the probability for excitation decreases steeply with increasing effective duration of the perturbation τ. If $\omega_{10}\tau>>1$, this probability is very small and we are dealing with a so-called adiabatic perturbation.

(b)

$$\lim_{\tau\to 0}\varepsilon(t)=\lim_{\tau\to 0}[A\frac{1}{\sqrt{\pi}\tau}e^{-(t/\tau)^2}]=A\delta(t)=\frac{P_0}{e}\delta(t).$$

Then we have

$$P(0\to 1)=\left|c_f{}^{(1)}(t)\right|^2=\frac{1}{\hbar^2}\frac{P_0^{\;2}\hbar}{2m\omega_0}\left|\int_{-\infty}^{t}\exp(i\omega_{10}t')\delta(t')dt'\right|^2=\frac{P_0^{\;2}}{2m\hbar\omega_0}.$$

The criterion of applicability of perturbation theory is that the probability for excitation should be much smaller than 1.

$$P(0\to 1)=\frac{P_0^{\;2}}{2m\hbar\omega_0}<<1,$$

or

$$\frac{P_0^{\;2}}{2m}<<\hbar\omega_0.$$

15.2 Solve the preceding problem for a field which varies as follows,

$$\varepsilon(t) = \frac{A}{t^2 + \tau^2},$$

and which corresponds to a given total classical imparted impulse P.

((**Solution**))

$$\varepsilon(t) = \frac{A}{t^2 + \tau^2},$$

$$P_0 = \int_{-\infty}^{\infty} e\varepsilon(t)dt = eA\int_{-\infty}^{\infty} \frac{1}{t^2 + \tau^2}dt = eA\frac{\pi}{\tau},$$

or

$$A = \frac{P_0\tau}{e\pi},$$

$$P(0 \to 1, t) = \left|c_f^{(1)}(t)\right|^2 = \frac{1}{\hbar^2}\frac{e^2\hbar}{2m\omega_0}\left|\int_{-\infty}^{t} \exp(i\omega_{10}t')\varepsilon(t')dt'\right|^2$$

$$P(0 \to 1, t = \infty) = \frac{P_0^{\,2}\tau^2}{2\pi^2 m\hbar\omega_0}\left|\int_{-\infty}^{\infty} \frac{\exp(i\omega_{10}t')}{t'^2 + \tau^2}dt'\right|^2$$

((**Residue theorem**))

We use the upper-half plane of the complex plane. There is a simple pole at $z = i\tau$.

$$\int_{-\infty}^{\infty} \frac{\exp(i\omega_{10}t')}{t'^2 + \tau^2}dt = 2\pi i \,\mathrm{Res}[i\tau] = 2\pi i\frac{\exp(-\omega_{10}\tau)}{2i\tau} = \frac{\pi}{\tau}\exp(-\omega_{10}\tau).$$

Then we have

$$P(0 \to 1, t = \infty) = \frac{P_0^{\,2}}{2m\hbar\omega_0}\exp(-2\omega_{10}\tau).$$

15.3 Solve the preceding problem for a field proportional to

$$\varepsilon(t) = Ae^{-t/\tau} \text{ for } t>0.$$

corresponding to a given total classical imparted impulse *P*.

((**Solution**))

$$P_0 = \int_0^\infty e\varepsilon(t)dt = \int_0^\infty eAe^{-t/\tau}dt = eA\tau \ ,$$

or

$$A = \frac{P_0}{e\tau} \ ,$$

$$\begin{aligned} P(0 \to 1) &= \left| c_f^{(1)}(t) \right|^2 \\ &= \frac{1}{\hbar^2} \frac{e^2\hbar}{2m\omega_0} \left| \int_0^\infty \exp(i\omega_{10}t')\varepsilon(t')dt' \right|^2 \\ &= \frac{1}{\hbar^2} \frac{e^2\hbar}{2m\omega_0} A^2 \left| \int_0^\infty \exp(i\omega_{10}t')e^{-t'/\tau}dt' \right| \end{aligned}$$

or

$$P(0 \to 1) = \frac{P_0^{\ 2}}{2\tau^2 m\hbar\omega_0} \left| \int_0^\infty \exp(i\omega_{10}t' - t'/\tau)dt' \right| = \frac{P_0^{\ 2}}{2\tau^2 m\hbar\omega_0} \left| \frac{1}{-i\omega_{10} + 1/\tau} \right| ,$$

or

$$P(0 \to 1) = \frac{P_0^{\ 2}}{2m\hbar\omega_0} \left(\frac{1}{1 + \omega_{10}^{\ 2}\tau^2} \right) .$$

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APPENDIX-I

Equivalence of the probability amplitude in the Dirac picture and Schrodinger picture

$$\left|\psi_I(t)\right\rangle = \sum_n c_n(t)\left|n\right\rangle , \qquad \text{(Dirac picture)}$$

$$\left|\psi_S(t)\right\rangle = \sum_n a_n(t)\left|n\right\rangle \qquad \text{(Schrodinger picture)}$$

Here we show that

$$\left|c_n(t)\right|^2 = \left|a_n(t)\right|^2$$

We note that

$$\left|\psi_I(t)\right\rangle = \exp(\frac{i}{\hbar}\hat{H}_0 t)\left|\psi_S(t)\right\rangle .$$

Then we get

$$\begin{aligned} c_n(t) &= \left\langle n\middle|\psi_I(t)\right\rangle \\ &= \left\langle n\right|\exp(\frac{i}{\hbar}\hat{H}_0 t)\left|\psi_S(t)\right\rangle \\ &= \exp(\frac{i}{\hbar}E_n t)\left\langle n\middle|\psi_S(t)\right\rangle \\ &= \exp(\frac{i}{\hbar}E_n t)a_n(t) \end{aligned}$$

or

$$\left|c_n(t)\right|^2 = \left|a_n(t)\right|^2 .$$

APPENDIX II

Dirac delta function

$$\delta(x) = \lim_{\eta\to\infty}\frac{1}{\pi}\frac{\sin(\eta x)}{x}$$

$$\delta(\omega) = \lim_{t\to\infty} \frac{1}{2\pi t} \frac{\sin^2\left(\frac{\omega t}{2}\right)}{\left(\frac{\omega}{2}\right)^2}$$

$$\frac{2\pi}{t}\delta(\omega) = \lim_{t\to\infty} \frac{\sin^2\left(\frac{\omega t}{2}\right)}{\left(\frac{\omega t}{2}\right)^2}$$