Chapter 42 Time dependent perturbation Masatsugu Sei Suzuki Department of Physics, SUNY at Binghamton (Date: December 20, 2010)

Dirac picture Fermi's golden rule

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

42.1. Dirac picture (Interaction picture) The Hamiltonian is given by

The Hamiltonian is given by

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

where \hat{H}_0 is independent of *t*. The wavefunctions in the Schrödinger picture and in the Dirac picture are related by

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

or

$$\left|\psi_{I}(t)\right\rangle = e^{\frac{i}{\hbar}\hat{H}_{0}t}\left|\psi_{s}(t)\right\rangle.$$

The Schrodinger equation is given by

$$i\hbar\frac{\partial}{\partial t}|\psi_{I}(t)\rangle = i\hbar\frac{\partial}{\partial t}e^{\frac{i}{\hbar}\hat{H}_{0}t}|\psi_{s}(t)\rangle = -\hat{H}_{0}e^{\frac{i}{\hbar}\hat{H}_{0}t}|\psi_{s}(t)\rangle + e^{\frac{i}{\hbar}\hat{H}_{0}t}i\hbar\frac{\partial}{\partial t}|\psi_{s}(t)\rangle$$

Since

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

we get

$$i\hbar\frac{\partial}{\partial t}|\psi_{I}(t)\rangle = -\hat{H}_{0}e^{\frac{i}{\hbar}\hat{H}_{0}t}|\psi_{s}(t)\rangle + e^{\frac{i}{\hbar}\hat{H}_{0}t}[\hat{H}_{0} + \hat{V}_{s}(t)]|\psi_{s}(t)\rangle$$

or

$$i\hbar\frac{\partial}{\partial t}|\psi_{I}(t)\rangle = e^{\frac{i}{\hbar}\hat{H}_{0}t}\hat{V}(t)e^{-\frac{i}{\hbar}\hat{H}_{0}t}|\psi_{I}(t)\rangle = \hat{V}_{I}(t)|\psi_{I}(t)\rangle$$

or

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

where

$$\hat{V}_{I}(t) = e^{\frac{i}{\hbar}\hat{H}_{0}t}\hat{V}_{s}(t)e^{-\frac{i}{\hbar}\hat{H}_{0}t}$$
(Heisenberg-like)

which is a Schrödinger equation with the total \hat{H} replaced by \hat{V}_{I} .

Here we assume that

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

satisfies the equation

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

Then we have the following relation for the Unitary operator,

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

with the initial condition

$$\hat{U}_{I}(t,t_{0}) = \hat{1} - \frac{i}{\hbar} \int_{t_{0}}^{t} \hat{V}_{I}(t') \hat{U}_{I}(t',t_{0}) dt'.$$

We can obtain an approximate solution to this equation [Dyson series].

$$\hat{U}_{I}(t,t_{0}) = 1 - \frac{i}{\hbar} \int_{t_{0}}^{t} \hat{V}_{I}(t') [1 - \frac{i}{\hbar} \int_{t_{0}}^{t'} \hat{V}_{I}(t'') \hat{U}_{I}(t'',t_{0}) dt''] dt'$$

= 1 + (- $\frac{i}{\hbar}$) $\int_{t_{0}}^{t} \hat{V}_{I}(t') dt'$ + (- $\frac{i}{\hbar}$)² $\int_{t_{0}}^{t} \hat{V}_{I}(t') dt' \int_{t_{0}}^{t'} dt'' \hat{V}_{I}(t'')$ + ...

42.2. Transition probability-I

Once $\hat{U}_I(t,t_0)$ is obtained, we have

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

where

$$|\psi_s(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}_0t}|\psi_I(t)\rangle,$$

or

$$\left|\psi_{I}(t)\right\rangle = e^{\frac{i}{\hbar}\hat{H}_{0}t}\left|\psi_{s}(t)\right\rangle$$

and

$$\left|\psi_{s}(t)\right\rangle = \hat{U}_{s}(t,t_{0})\left|\psi_{s}(t_{0})\right\rangle,$$

$$|\psi_{I}(t)\rangle = e^{\frac{i}{\hbar}\hat{H}_{0}t}\hat{U}_{s}(t,t_{0})|\psi_{s}(t_{0})\rangle = e^{\frac{i}{\hbar}\hat{H}_{0}t}\hat{U}_{s}(t,t_{0})e^{-\frac{i}{\hbar}\hat{H}_{0}t_{0}}|\psi_{I}(t_{0})\rangle.$$

Then we get

$$\hat{U}_{I}(t,t_{0}) = e^{\frac{i}{\hbar}\hat{H}_{0}t}\hat{U}_{s}(t,t_{0})e^{-\frac{i}{\hbar}\hat{H}_{0}t_{0}}.$$

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

$$\hat{H}_{0}|n\rangle = E_{n}|n\rangle,$$

$$\langle n|\hat{U}_{I}(t,t_{0})|m\rangle = e^{\frac{i}{\hbar}(E_{n}t-E_{m}t_{0})}\langle n|\hat{U}_{s}(t,t_{0})|m\rangle,$$

$$|\langle n|\hat{U}_{I}(t,t_{0})|m\rangle|^{2} = |\langle n|\hat{U}_{s}(t,t_{0})|m\rangle|^{2}.$$

((Note)) Suppose that

$$[\hat{H}_0, \hat{A}] \neq 0$$
 and $[\hat{H}_0, \hat{B}] \neq 0$
 $\hat{A}|a'\rangle = a'|a'\rangle$ and $\hat{B}|b'\rangle = b'|b'\rangle$.

In this case,

$$\left|\left\langle b'|\hat{U}_{I}(t,t_{0})|a'\right\rangle\right|^{2}\neq\left|\left\langle b'|\hat{U}_{s}(t,t_{0})|a'\right\rangle\right|^{2}$$

since

$$\langle b' | \hat{U}_{I}(t,t_{0}) | a' \rangle = \sum_{n,m} \langle b' | e^{\frac{i}{\hbar} \hat{H}_{0}t} | n \rangle \langle n | \hat{U}_{s}(t,t_{0}) | m \rangle \langle m | e^{-\frac{i}{\hbar} \hat{H}_{0}t_{0}} | a' \rangle$$

$$= \sum_{n,m} e^{\frac{i}{\hbar} (E_{n}t - E_{m}t_{0})} \langle b' | n \rangle \langle n | \hat{U}_{s}(t,t_{0}) | m \rangle \langle m | a' \rangle$$

42.3 Transition probability II. We now consider the case 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

$$\left|\psi_{s}(t_{0})\right\rangle = e^{-\frac{i}{\hbar}\hat{H}_{0}t_{0}}\left|\psi_{I}(t_{0})\right\rangle,$$

from the definition, we have

$$|\psi_{I}(t_{0})\rangle = e^{\frac{i}{\hbar}\hat{H}_{0}t_{0}}|\psi_{s}(t_{0})\rangle = e^{\frac{i}{\hbar}\hat{H}_{0}t_{0}}e^{-\frac{i}{\hbar}\hat{H}_{0}t_{0}}|i\rangle = |i\rangle,$$

At a later time 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

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

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

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

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

$$\begin{split} c_{n}(t) &= \left\langle n \left| \hat{U}_{I}(t,t_{0}) \right| i \right\rangle \\ &= \left\langle n \left| 1 + \lambda \left(-\frac{i}{\hbar} \right) \int_{t_{0}}^{t} \hat{V}_{I}(t') dt' + \lambda^{2} \left(-\frac{i}{\hbar} \right)^{2} \int_{t_{0}}^{t} dt'' \hat{V}_{I}(t') \hat{V}_{I}(t'') + \dots \right| i \right\rangle \\ c_{n}^{(0)}(t) &= \left\langle n \left| i \right\rangle = \delta_{n,i} , \\ c_{n}^{(1)} &= \left(-\frac{i}{\hbar} \right) \int_{t_{0}}^{t} dt' \left\langle n \left| \hat{V}_{I}(t') \right| i \right\rangle . \end{split}$$

Since

$$\hat{V}_{I}(t) = {}^{\frac{i}{\hbar}\hat{H}_{0}t} \hat{V}_{s}(t) e^{-\frac{i}{\hbar}\hat{H}_{0}t},$$

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

$$\langle n | \hat{V}_{I}(t') | i \rangle = \langle n | e^{\frac{i}{\hbar} \hat{H}_{0}t} \hat{V}_{s}(t) e^{-\frac{i}{\hbar} \hat{H}_{0}t} | i \rangle$$

$$= e^{\frac{i}{\hbar} (E_{n} - E_{i})t'} \langle n | \hat{V}_{s}(t') | i \rangle = e^{i\omega_{ni}t'} V_{ni}(t')$$

where

$$\omega_{ni} = \frac{E_n - E_i}{\hbar} \, .$$

Then

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

Similarly, we get

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

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 $\left|i\right\rangle \rightarrow \left|f\right\rangle$

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

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

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

Note that this probability is clearly only valid provided

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

42.4. Transition probability in the Schrödinger picture In the Schrödinger picture, we have

$$\begin{split} \left| \psi_{s}(t) \right| &\leq e^{-\frac{i}{\hbar} \hat{H}_{0}t} \left| \psi_{I}(t) \right| \\ &= e^{-\frac{i}{\hbar} \hat{H}_{0}t} \sum_{n} c_{n}(t) \left| n \right| \\ &= \sum_{n} c_{n}(t) e^{-\frac{i}{\hbar} \hat{H}_{0}t} \left| n \right| \\ &= \sum_{n} c_{n}(t) e^{-\frac{i}{\hbar} E_{n}t} \left| n \right| \\ &= \sum_{n} c_{n}(t) e^{-\frac{i}{\hbar} E_{n}t} \left| n \right| \\ &d_{n}(t) = \left\langle n \left| \psi_{s}(t) \right\rangle = c_{n}(t) e^{-\frac{i}{\hbar} E_{n}t} = e^{-\frac{i}{\hbar} E_{n}t} \left\langle n \left| \psi_{I}(t) \right\rangle \right\rangle \end{split}$$

$$\left|\left\langle n\left|\psi_{s}(t)\right\rangle\right|^{2}=\left|\left\langle n\left|\psi_{I}(t)\right\rangle\right|^{2}\right|^{2}$$

42.5. Exact solution

In the Dirac picture,

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

$$\langle n | \hat{V}_I(t) | m \rangle = e^{\frac{i}{\hbar} (E_n - E_m)t} \langle n | \hat{V}_s(t) | m \rangle = e^{i\omega_{nm}t} V_{nm},$$

where

$$V_{nm} = \langle n | \hat{V}_s(t) | m \rangle,$$

$$\omega_{nm} = \frac{E_n - E_m}{\hbar}.$$
 (Bohr frequency)

Then we have

$$i\hbar \frac{\partial}{\partial t}c_n(t) = \sum_m e^{i\omega_{nm}t}V_{nm}c_m(t).$$

42.6. Time dependent perturbation: Schrödinger picture

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

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

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

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

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

$$\left|\psi_{s}(t)\right\rangle = \sum_{n} d_{n}(t)\left|n\right\rangle$$

with

$$d_n(t) = \langle n | \psi_s(t) \rangle = e^{-\frac{i}{\hbar}E_n t} \langle n | \psi_I(t) \rangle = e^{-\frac{i}{\hbar}E_n t} c_n(t)$$

We introduce

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

Recall that

$$\langle n | \hat{H}_0 | k \rangle = E_n \delta_{n,k}$$

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

$$= [H_0 + \lambda \hat{V}(t)] \sum_n d_n(t) | n \rangle$$

$$= \sum_n d_n(t) E_n | n \rangle + \sum_k \lambda d_k(t) \hat{V}(t) | k \rangle$$

or

$$i\hbar \frac{d}{dt}d_n(t) = E_n d_n(t) + \sum_n \lambda V_{nk}(t) d_k(t)$$
(1)

When $\lambda \hat{V}_1(t)$ is zero

$$d_n(t) = c_n(t)e^{-iE_n t/\hbar}, (c_n: \text{ const}).$$
⁽²⁾

If, now, $\lambda \hat{V}(t)$ is not zero, $d_n(t)$ of Eq.(1) is expected to be very close to Eq.(2).

$$d_n(t) \equiv c_n(t)e^{-iE_nt/\hbar}$$
(3)

Substituting Eq.(3) into Eq.(1), we obtain

$$i\hbar\left\{\dot{c}_n(t)e^{-iE_nt/\hbar}+c_n(t)\left(-\frac{i}{\hbar}E_n\right)e^{-iE_nt/\hbar}\right\}$$

$$=E_nc_n(t)e^{-iE_nt/\hbar}+\sum_k\lambda V_{nk}(t)c_k(t)e^{-iE_kt/\hbar}$$

Then

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

42.7. Perturbation equation

$$c_{n}(t) \equiv c_{n}^{(0)}(t) + \lambda c_{n}^{(1)}(t) + \lambda^{2} c_{n}^{(2)}(t) + \cdots$$
$$i\hbar [\dot{c}_{n}^{(0)}(t) + \lambda \dot{c}_{n}^{(1)}(t) + \lambda^{2} \dot{c}_{n}^{(2)}(t) + \cdots] = \lambda \sum_{k} e^{i\omega_{nk}t} V_{nk}(t) [c_{k}^{(0)}(t) + \lambda c_{k}^{(1)}(t) + \cdots]$$

For the coefficient of λ^0

$$i\hbar \dot{c}_n^{(0)}(t) = 0$$
 (4)

For the coefficient of λ^r

$$i\hbar \dot{c}_{n}^{(r)}(t) = \sum_{k} e^{i\omega_{nk}t} V_{nk}(t) c_{k}^{(r-1)}(t)$$
(5)

Solution

Switch-on

$$|i>$$
 state
 $V=0$ state
 $t=0$
 $t=t_0$

At $t < t_0$, the system is assumed to be in the state $|i\rangle$. At $t = t_0$, $c_n(t = t_0) = \delta_{n,i}$ (continuous at $t = t_0$). This relation is valid for all λ .

$$c_n(t=t_0) = c_n^{(0)}(t=t_0) + \lambda c_n^{(1)}(t=t_0) + \lambda^2 c_n^{(2)}(t=t_0) + \cdots$$

Consequently,

$$c_n^{(0)}(t=t_0)=\delta_{n,i}$$

$$c_n^{(r)}(t=t_0) = 0$$
 for $r \ge 1$.

From Eq.(4)

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

For r = 1

$$i\hbar \dot{c}_{n}^{(1)}(t) = \sum_{k} e^{i\omega_{nk}t} V_{nk}(t) \delta_{k,i} = e^{i\omega_{ni}t} V_{ni}(t)$$
$$c_{n}^{(1)}(t) = \frac{1}{i\hbar} \int_{t_{0}}^{t} e^{i\omega_{ni}t} V_{ni}(t') dt'$$

For r = 2

$$i\hbar \dot{c}_{n}^{(2)}(t) = \sum_{k} e^{i\omega_{nk}t} V_{nk}(t) c_{k}^{(1)}(t)$$

For r = 3

$$i\hbar \dot{c}_{n}^{(3)}(t) = \sum_{k} e^{i\omega_{nk}t} V_{nk}(t) c_{k}^{(2)}(t)$$

42.8 Transition probability

$$P_{if}(t) = |d_f(t)|^2 = |c_f(t)|^2$$

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.

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

$$P_{if}(t) = \lambda^{2} |c_{f}^{(1)}(t)|^{2}$$

$$= \frac{\lambda^{2}}{\hbar^{2}} \left| \int_{t_{0}}^{t} e^{i\omega_{f}t'} V_{fi}(t') dt' \right|^{2}$$

42.9 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; $t_0 = 0$

$$c_{f}^{(1)}(t) = -\frac{i}{\hbar} \int_{0}^{t} e^{i\omega_{fi}t'} [\langle f | \hat{V} | i \rangle e^{i\omega t'} + \langle f | \hat{V}^{+} | i \rangle e^{-i\omega t'}] dt'$$
$$= -\frac{i}{\hbar} [(\frac{e^{i(\omega + \omega_{fi})t} - 1}{\omega + \omega_{fi}}) \langle f | \hat{V} | i \rangle + (\frac{e^{i(-\omega + \omega_{fi})t} - 1}{-\omega + \omega_{fi}}) \langle f | \hat{V}^{+} | i \rangle]$$

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

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

or

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

where

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

Therefore, we have

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

B. Resonant nature of the transition probability We consider the following case (two discrete case)



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

(i) When $E_{\rm f} > E_{\rm i}$, $\Rightarrow \omega_{\rm fi} > 0$. Under such conditions, A. dominates (absorption).

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

with

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

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

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*,

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



(ii) When $E_{\rm f} > E_{\rm i}$, $\Rightarrow \omega_{\rm fi} < 0$. A_+ dominant (emission).

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

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

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

C. Discussion of the resonant approximation



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

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

D. Limit of first-order calculation

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

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.

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

Therefore *t* should be

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

or

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

or

$$\hbar |\omega_{fi}| >> \lambda |\langle f | \hat{V}^{+} | i \rangle|.$$

42.10 Constant perturbation

$$\frac{H_0}{t_0 = 0} \rightarrow t$$

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

We consider first a perturbation

$$\hat{V}(t) = \hat{V}\Theta(t) = \begin{cases} 0 & \text{for } t < 0 \\ \hat{V} & \text{for } t \ge 0 \end{cases}$$
$$c_{f}^{(1)}(t) = -\frac{i}{\hbar} \int_{0}^{t} dt' e^{i\omega_{f}t'} V_{fi} = -\frac{V_{fi}}{\hbar\omega_{fi}} (e^{i\omega_{f}t} - 1),$$
$$\left| c_{f}^{(1)}(t) \right|^{2} = \frac{\left| V_{fi} \right|^{2}}{\hbar^{2} \omega_{fi}^{2}} \left[2 - 2\cos(\omega_{fi}t) \right]$$
$$= \frac{1}{\hbar^{2}} \left[\frac{\sin(\omega_{fi}t/2)}{\omega_{fi}/2} \right]^{2} \left| V_{fi} \right|^{2}$$
$$= 4 \frac{\sin^{2} \left(\frac{E_{fi}}{2\hbar} t \right)}{(E_{fi})^{2}} \left| V_{fi} \right|^{2}$$

or

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

A group of final states around the state with E_i . E_i is not the state in the continuous region. $E_i \neq E_n$ (or $E_i \cong E_n$)



$$P = \lambda^{2} \sum_{n, E_{n} \equiv E_{i}} \left| c_{n}^{(1)} \right|^{2} = \lambda^{2} \int dE_{n} \rho(E_{n}) \left| c_{n}^{(1)} \right|^{2}$$
$$= 4\lambda^{2} \int \sin^{2} \left[\frac{(E_{n} - E_{i})t}{2\hbar} \right] \frac{|V_{ni}|^{2}}{|E_{n} - E_{i}|^{2}} \rho(E_{n}) dE_{n}$$

where

$$\underbrace{\rho(E)}_{\uparrow} dE \Rightarrow \text{the number of states within interval } (E \sim E + dE)$$

density of states

When *t* is sufficiently large

$$\int_{-\infty}^{\infty} \sin^2 \left[\frac{(E_n - E_i)t}{2\hbar} \right] \frac{dE_n}{\left| E_n - E_i \right|^2} = \frac{t}{2\hbar} \int_{-\infty}^{\infty} \frac{\sin^2 x}{x^2} dx = \frac{\pi t}{2\hbar}$$

Note:

$$x \equiv \frac{t}{2\hbar} (E_n - E_i),$$

$$\int_{0}^{\infty} dx \frac{\sin^2 x}{x^2} = \frac{\pi}{2}, \qquad \int_{-\infty}^{\infty} dx \frac{\sin^2 x}{x^2} = \pi$$

$$\Rightarrow \sin^2 \left[\frac{(E_n - E_i)t}{2\hbar} \right] \frac{1}{|E_n - E_i|^2} = \frac{\pi t}{2\hbar} \delta(E_n - E_i)$$

Then we have

$$P = 4\lambda^2 \int |V_{ni}|^2 \rho(E_n) dE_n \frac{\pi t}{2\hbar} \delta(E_n - E_i)$$
$$= \frac{2\pi}{\hbar} \lambda^2 t \int |V_{ni}|^2 \rho(E_n) \delta(E_n - E_i) dE_n$$

Thus the total probability is proportional to t for large value of t.

42.11 Fermi's golden rule

We can define a transition probability per unit time

$$W_{i\to[n]} = \frac{2\pi}{\hbar} \lambda^2 |V_{ni}|^2 \delta(E_n - E_i)$$

where [n] stands for a group of final states with energy similar to *i*.

It must be understood that expression is integrated with $\int dE_n \rho(E_n)$

↓ ((Generalized Ferm's golden rule)) For the harmonic perturbation

$$w_{i\to n} = \frac{2\pi}{\hbar} \lambda^2 \left| \langle f | V^+ | i \rangle \right|^2 \delta(E_n - E_i - \hbar \omega) \qquad \text{(Fermi's Golden Rule)}$$

and

$$w_{i\to n} = \frac{2\pi}{\hbar} \lambda^2 \left| \left\langle f \left| V \right| i \right\rangle \right|^2 \delta(E_n - E_i + \hbar \omega)$$

Note that

$$\left|\left\langle f\left|V^{+}\right|i\right\rangle\right|^{2}=\left|\left\langle f\left|V\right|i\right\rangle\right|^{2}$$

((Note)) Density of states for free electrons

42.12 Free electron gas in three dimensions

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

$$H\psi_{\mathbf{k}} = \frac{\mathbf{p}^2}{2m}\psi_{\mathbf{k}} = -\frac{\hbar^2}{2m}\nabla^2\psi_{\mathbf{k}} = \varepsilon_{\mathbf{k}}\psi_{\mathbf{k}}.$$
(3)

It is convenient to introduce wavefunctions that satisfy periodic boundary conditions. Boundary condition (Born-von Karman boundary conditions).

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

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

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

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

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

with

$$k_{x} = (2\pi/L) n_{x}, (n_{x} = 0, \pm 1, \pm 2, \pm 3,), k_{y} = (2\pi/L) n_{y}, (n_{y} = 0, \pm 1, \pm 2, \pm 3,), k_{z} = (2\pi/L) n_{z}, (n_{z} = 0, \pm 1, \pm 2, \pm 3,).$$

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

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

Here

$$\mathbf{p}\psi_{k}(\mathbf{r}) = \frac{\hbar}{i} \nabla_{\mathbf{k}} \psi_{k}(\mathbf{r}) = \hbar \mathbf{k} \psi_{k}(\mathbf{r}) .$$
(6)

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

42.13 The Pauli's exclusion principle

The one-electron levels are specified by the wavevectors 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:

$$|\mathbf{k},\uparrow\rangle,|\mathbf{k},\downarrow\rangle.$$

In building up the *N*-electron ground state, we begin by placing two electrons in the oneelectron 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 *k*-space $(2\pi/L)^3$. We consider the number of oneelectron levels in the energy range from ε to ε +d ε , $D(\varepsilon)$ d ε

$$D(\varepsilon)d\varepsilon = 2\frac{L^3}{(2\pi)^3} 4\pi k^2 dk, \qquad (13)$$

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

$$D(\varepsilon) = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \sqrt{\varepsilon} .$$
(14)

42.14 Higher order term: $c_{f}^{(2)}$

$$c_n^{(2)}(t) = \left(-\frac{i}{\hbar}\right)^2 \sum_m \int_{t_0=0}^t dt' \int_{t_0=0}^t dt'' e^{i\omega_{nm}t'} V_{nm}(t') e^{i\omega_{m}t''} V_{mi}(t'').$$

We assume again that

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

Then

$$c_n^{(2)}(t) = (-\frac{i}{\hbar})^2 \sum_m V_{nm} V_{mi} \int_{t_0=0}^t e^{i\omega_{nm}t'} dt' \int_{t_0=0}^t dt'' e^{i\omega_{mi}t''}$$

Note that

$$I = \int_{t_0=0}^{t} e^{i\omega_{nm}t'} dt' \int_{t_0=0}^{t'} dt'' e^{i\omega_{mi}t''} = \int_{t_0=0}^{t} dt' e^{i\omega_{nm}t'} (\frac{e^{i\omega_{mi}t'}-1}{i\omega_{mi}})$$
$$= \frac{1}{i\omega_{mi}} \int_{t_0=0}^{t} dt' (e^{i(\omega_{nm}+\omega_{mi})t'} - e^{i\omega_{nm}t'})$$
$$= \frac{1}{i\omega_{mi}} \int_{t_0=0}^{t} dt' (e^{i\omega_{ni}t} - e^{i\omega_{nm}t'})$$
$$= \frac{1}{i\omega_{mi}} \left[\left(\frac{e^{i\omega_{ni}t}-1}{i\omega_{ni}} \right) - \left(\frac{e^{i\omega_{nm}t}-1}{i\omega_{nm}} \right) \right]$$

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

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

Here note that

$$c_n^{(1)}(t) = (\frac{V_{ni}}{E_n - E_i})(1 - e^{i\omega_{ni}t}),$$

With $c^{(1)}$ and $c^{(2)}$ together, we have





42.15 Time dependent perturbation: some examples Using the following formula, we solve several problems.

$$c_{n}^{(1)} = \left(-\frac{i}{\hbar}\right)_{t_{0}}^{t} dt' e^{i\omega_{ni}t'} V_{ni}(t')$$

$$c_{n}^{(2)} = \left(-\frac{i}{\hbar}\right)^{2} \sum_{m} \int_{t_{0}}^{t} dt' \int_{t_{0}}^{t'} dt'' e^{i\omega_{nm}t'} V_{nm}(t') e^{i\omega_{mi}t''} V_{mi}(t'')$$

$$P(i \to f) = \lambda^{2} \left| c_{f}^{(1)}(t) \right|^{2} = \frac{\lambda^{2}}{\hbar^{2}} \left| \int_{t_{0}}^{t} e^{i\omega_{fi}t'} \left\langle f \left| \hat{V}(t') \right| i \right\rangle dt' \right|^{2}$$

((Selected problems))

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 $t = +\infty$).

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.

3. Solve the preceding problem for a field proportional to

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

corresponding to a given total classical imparted impulse P.

(1) 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
angle to the state |k
angle is equal to

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

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

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

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

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

When $t \rightarrow \infty$,

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

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)

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

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.

$$P(0 \rightarrow 1) = \frac{P_0^2}{2m\hbar\omega_0} \ll 1$$

or

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

 $\overline{(2)}$

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

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

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

((Residue theorem))

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

$$\int_{-\infty}^{\infty} \frac{\exp(i\omega_{10}t')}{t'^2 + \tau^2} dt = 2\pi i \operatorname{Re} s[i\tau] = 2\pi i \frac{\exp(-\omega_{10}\tau)}{2i\tau} = \frac{\pi}{\tau} \exp(-\omega_{10}\tau)$$

Then we have

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

(3)

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

or

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

$$P(0 \rightarrow 1) = \left| c_f^{(1)}(t) \right|^2$$

$$= \frac{1}{\hbar^2} \frac{e^2 \hbar}{2m\omega_0} \left| \int_0^\infty \exp(i\omega_{10}t') \varepsilon(t') dt' \right|^2$$

$$= \frac{1}{\hbar^2} \frac{e^2 \hbar}{2m\omega_0} A^2 \left| \int_0^\infty \exp(i\omega_{10}t') e^{-t'/\tau} dt \right|^2$$

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

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