

## 2. 時間に依存する摂動論

### 2.1. 時間に依存する結合項を有する方程式

時間を含む Schrödinger eq.:  $(i\hbar \partial_t - H_0) \psi(t) = 0$

suppose  $H_0 \phi_n = \epsilon_n \phi_n$

and at  $t=0$   $\psi(t) = \phi_n$

↓

$$\psi(t) = e^{-i\epsilon_n t/\hbar} \phi_n \quad (\text{定常解})$$

問題: (時間に依存する) ポテンシャル  $V(t)$  が加わった時, 系はどのように時間発展するか?

$$(i\hbar \partial_t - H_0 - V(t)) \psi(t) = 0 \quad \text{with } \psi(t=0) = \phi_n$$

を解く

$$\psi(t) = \sum_m c_m(t) e^{-i\epsilon_m t/\hbar} \phi_m \quad \text{と展開}$$

↓  $c_m(t=0) = \delta_{n,m}$

$$\begin{aligned} i\hbar \dot{\psi} &= i\hbar \sum_m \dot{c}_m e^{-i\epsilon_m t/\hbar} \phi_m + i\hbar \sum_m c_m \left(\frac{-i\epsilon_m}{\hbar}\right) e^{-i\epsilon_m t/\hbar} \phi_m \\ &= i\hbar \sum_m \dot{c}_m e^{-i\epsilon_m t/\hbar} \phi_m + \sum_m \epsilon_m c_m e^{-i\epsilon_m t/\hbar} \phi_m \end{aligned}$$

$$H_0 \psi = \sum_m c_m e^{-i\epsilon_m t/\hbar} H_0 \phi_m$$

$$= \sum_m \epsilon_m c_m e^{-i\epsilon_m t/\hbar} \phi_m$$

$$\rightarrow \left( i\hbar \sum_m \dot{c}_m e^{-i\varepsilon_m t/\hbar} \phi_m - V \sum_m c_m e^{-i\varepsilon_m t/\hbar} \phi_m \right) = 0$$

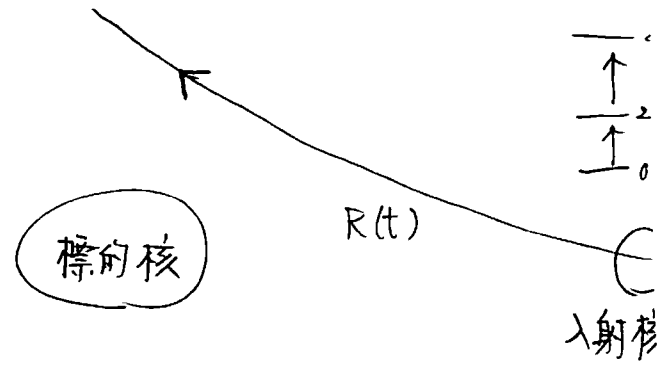
$\langle \phi_k | \rightarrow$

$$i\hbar \dot{c}_k e^{-i\varepsilon_k t/\hbar} - \sum_m c_m \langle \phi_k | V | \phi_m \rangle e^{-i\varepsilon_m t/\hbar} = 0$$

$$\rightarrow \boxed{i\hbar \dot{c}_k = \sum_m c_m e^{i(\varepsilon_k - \varepsilon_m)t/\hbar} \langle \phi_k | V | \phi_m \rangle}$$

(時間に依存する結合項を補う方程式)  
 $c_k(0) = \delta_{k,n}$

例)



$$V(t) \propto z_p z_T e^2 \frac{R_T^2}{R(t)^3} \cdot \chi$$

二つの振動  
 $\nu_e \leftrightarrow \nu_\mu$

$$H_0 = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 \chi^2$$

$$i\hbar \partial_t \begin{pmatrix} c_e \\ c_\mu \end{pmatrix} = \begin{pmatrix} V_{ee} & V_{e\mu} \\ V_{\mu e} & V_{\mu\mu} \end{pmatrix} \begin{pmatrix} c_e \\ c_\mu \end{pmatrix}$$

$$i\hbar \dot{c}_k(t) = \sum_m c_m(t) e^{i\varepsilon_{km}t/\hbar} V_{km}(t)$$

↓

$$c_k(t) = \delta_{k,n} + \frac{1}{i\hbar} \int_0^t dt' \sum_m \underbrace{c_m(t')} e^{i\varepsilon_{km}t'/\hbar} V_{km}(t')$$

$$\parallel$$

$$\delta_{m,n} + \frac{1}{i\hbar} \int_0^{t'} dt'' \sum_{m'} c_{m'}(t'') e^{i\varepsilon_{mm'}t''/\hbar} \times V_{mm'}(t'')$$

$$= \delta_{k,n} + \frac{1}{i\hbar} \int_0^t dt' e^{i\varepsilon_{kn}t'/\hbar} V_{kn}(t')$$

$$+ \left(\frac{1}{i\hbar}\right)^2 \int_0^t dt' \int_0^{t'} dt'' \sum_{m,m'} e^{i\varepsilon_{km}t'/\hbar} e^{i\varepsilon_{mm'}t''/\hbar} V_{km}(t') V_{mm'}(t'')$$

$$\cdot c_{m'}(t'')$$

## 2.2. 時間に依存する擾動論

$$i\hbar \dot{c}_k = \sum_m c_m e^{i(\epsilon_k - \epsilon_m)t/\hbar} \langle \phi_k | \lambda V | \phi_m \rangle$$

$$c_k(t) = c_k^{(0)} + \lambda c_k^{(1)} + \lambda^2 c_k^{(2)} + \dots$$

$$c_k^{(0)}(t) = c_k(0) = \delta_{k,n}$$

$$i\hbar (\dot{c}_k^{(0)} + \lambda \dot{c}_k^{(1)} + \lambda^2 \dot{c}_k^{(2)} + \dots)$$

$$= \sum_m (c_m^{(0)} + \lambda c_m^{(1)} + \lambda^2 c_m^{(2)} + \dots) e^{i(\epsilon_k - \epsilon_m)t/\hbar} \times \langle \phi_k | \lambda V | \phi_m \rangle$$

$$O(\lambda^0): i\hbar \dot{c}_k^{(0)} = 0 \quad \rightarrow \quad c_k^{(0)} = \text{const.} = \delta_{k,n}$$

$$O(\lambda^1): i\hbar \dot{c}_k^{(1)} = \sum_m c_m^{(0)} e^{i\epsilon_k t/\hbar} \langle \phi_k | V | \phi_m \rangle \\ = e^{i\epsilon_k t/\hbar} \langle \phi_k | V | \phi_n \rangle$$

↪

$$c_k^{(1)} = \frac{1}{i\hbar} \int_0^t e^{i\epsilon_k t'/\hbar} V_{kn}(t') dt'$$

$$O(1^2): i\hbar \dot{c}_k^{(2)} = \sum_m c_m^{(1)} e^{i\epsilon_{km}t/\hbar} V_{km}(t)$$

$$\begin{aligned} c_k^{(2)} &= \frac{1}{i\hbar} \sum_m \int_0^t dt' c_m^{(1)}(t') e^{i\epsilon_{km}t'/\hbar} V_{km}(t') \\ &= -\frac{1}{\hbar^2} \sum_m \int_0^t dt' e^{i\epsilon_{km}t'/\hbar} V_{km}(t') \\ &\quad \times \int_0^{t'} dt'' e^{i\epsilon_{mn}t''/\hbar} V_{mn}(t'') \end{aligned}$$

at time  $t$ ,  $c_k(t) \neq 0$  for  $k \neq n$ .

↔ 摂動を加えた後で系の状態を観測すれば

最初の状態  $n$  と異なる状態  $k$  に系が存在する確率がある

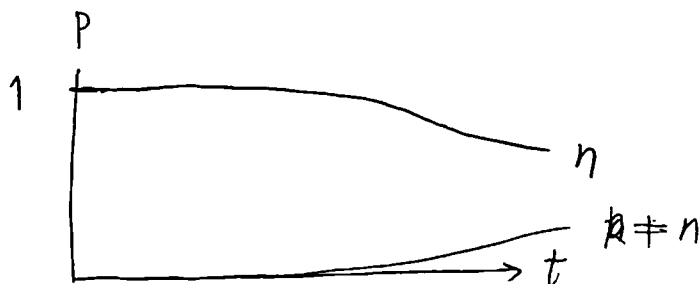
「摂動により  $n \rightarrow k$  の遷移」

(note)  $\psi(t) = \sum_m c_m(t) e^{-i\epsilon_m t/\hbar} \phi_m$

↓

$$P_k(t) = |\langle \phi_k | \psi(t) \rangle|^2 = |c_k(t)|^2$$

(遷移確率)



$$P_k(t) = |C_k(t)|^2$$

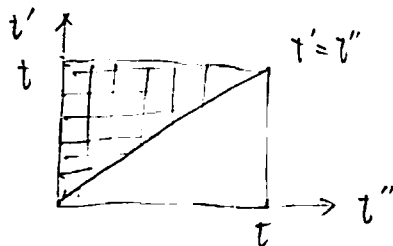
$$= (C_k^{(0)} + \lambda C_k^{(1)} + \lambda^2 C_k^{(2)} + \dots)^* (C_k^{(0)} + \lambda C_k^{(1)} + \lambda^2 C_k^{(2)} + \dots)$$

$$= |C_k^{(0)}|^2 + \lambda (C_k^{(1)*} C_k^{(0)} + C_k^{(0)*} C_k^{(1)}) + \lambda^2 (C_k^{(0)*} C_k^{(2)} + C_k^{(1)*} C_k^{(1)} + C_k^{(2)*} C_k^{(0)}) + \dots$$

$$= \delta_{k,n} + \lambda \left\{ \delta_{k,n} \left[ -\frac{1}{i\hbar} \int_0^t e^{-i\epsilon_{kn}t'/\hbar} V_{kn}(t') dt' + \frac{1}{i\hbar} \int_0^t e^{i\epsilon_{kn}t'/\hbar} V_{kn}(t') dt' \right] + \lambda^2 \left[ \delta_{k,n} \cdot \frac{1}{\hbar^2} \sum_m \int_0^t dt' e^{i\epsilon_{kn}t'/\hbar} V_{km}(t') \int_0^{t'} dt'' e^{i\epsilon_{mn}t''/\hbar} V_{mn}(t'') - \delta_{k,n} \cdot \frac{1}{\hbar^2} \sum_m \int_0^t dt' e^{-i\epsilon_{kn}t'/\hbar} V_{km}^*(t') \int_0^{t'} dt'' e^{-i\epsilon_{mn}t''/\hbar} V_{mn}^*(t'') + \frac{1}{\hbar^2} \left| \int_0^t dt' e^{i\epsilon_{kn}t'/\hbar} V_{kn}(t') \right|^2 \right] \right\}$$

$$= \delta_{k,n} + \lambda^2 \left\{ \frac{1}{\hbar^2} \left| \int_0^t dt' e^{i\epsilon_{kn}t'/\hbar} V_{kn}(t') \right|^2 \right.$$

$$- \delta_{k,n} \frac{1}{\hbar^2} \sum_m \int_0^t dt' e^{i\epsilon_{nm}t'/\hbar} V_{nm}(t') \int_0^{t'} dt'' e^{i\epsilon_{mn}t''/\hbar} V_{mn}(t'') - \delta_{k,n} \frac{1}{\hbar^2} \sum_m \int_0^t dt' e^{-i\epsilon_{nm}t'/\hbar} V_{mn}(t') \int_0^{t'} dt'' e^{-i\epsilon_{mn}t''/\hbar} V_{nm}(t'')$$



$$\int_0^t dt' \int_0^{t'} dt'' = \int_0^t dt'' \int_{t''}^t dt'$$

$$\begin{aligned}
&= \delta_{k,n} + \lambda^2 \left\{ \frac{1}{\hbar^2} \left| \int_0^t dt' e^{i\epsilon_{kn}t'/\hbar} V_{kn}(t') \right|^2 \right. \\
&\quad - \delta_{k,n} \cdot \frac{1}{\hbar^2} \sum_m \int_0^t dt' e^{-i\epsilon_{mn}t'/\hbar} V_{mn}^*(t') \int_0^{t'} dt'' e^{i\epsilon_{mn}t''/\hbar} V_{mn}(t'') \\
&\quad \left. - \delta_{k,n} \cdot \frac{1}{\hbar^2} \sum_m \int_0^t dt'' e^{-i\epsilon_{mn}t''/\hbar} V_{mn}^*(t'') \int_{t''}^t dt' e^{i\epsilon_{mn}t'/\hbar} V_{mn}(t') \right\}
\end{aligned}$$

$$\begin{aligned}
\left[ \right. &= \delta_{k,n} + \lambda^2 \left\{ \frac{1}{\hbar^2} \left| \int_0^t dt' e^{i\epsilon_{kn}t'/\hbar} V_{kn}(t') \right|^2 \right. \\
&\quad \left. - \delta_{k,n} \cdot \frac{1}{\hbar^2} \sum_m \int_0^t dt' e^{-i\epsilon_{mn}t'/\hbar} V_{mn}^*(t') \cdot \int_0^t dt' e^{i\epsilon_{mn}t'/\hbar} V_{mn}(t') \right\}
\end{aligned}$$

$$\begin{aligned}
&= \delta_{k,n} + \lambda^2 \left\{ \frac{1}{\hbar^2} \left| \int_0^t dt' e^{i\epsilon_{kn}t'/\hbar} V_{kn}(t') \right|^2 \right. \\
&\quad \left. - \delta_{k,n} \cdot \frac{1}{\hbar^2} \sum_m \left| \int_0^t dt' e^{i\epsilon_{mn}t'/\hbar} V_{mn}(t') \right|^2 \right\}
\end{aligned}$$

$$\begin{aligned}
\left[ \right. &\downarrow \\
P_k(t) &= \frac{1}{\hbar^2} \lambda^2 \left| \int_0^t dt' e^{i\epsilon_{kn}t'/\hbar} V_{kn}(t') \right|^2 \quad \text{for } k \neq n \\
&= 1 - \frac{\lambda^2}{\hbar^2} \sum_{m \neq n} \left| \int_0^t dt' e^{i\epsilon_{mn}t'/\hbar} V_{mn}(t') \right|^2 = 1 - \sum_{m \neq n} P_m \quad \text{for } k
\end{aligned}$$

$$|\lambda C_k^{(1)}|^2$$

• 別の導出法: 相互作用表示

$$i\hbar \partial_t |\psi(t)\rangle = (H_0 + V(t)) |\psi(t)\rangle$$

define  $|\tilde{\psi}(t)\rangle = e^{iH_0 t/\hbar} |\psi(t)\rangle$

↓

$$i\hbar \partial_t |\tilde{\psi}(t)\rangle = -H_0 e^{iH_0 t/\hbar} |\psi(t)\rangle + e^{iH_0 t/\hbar} \cdot \underbrace{i\hbar \partial_t |\psi(t)\rangle}_{}$$

$$= e^{iH_0 t/\hbar} V(t) |\psi(t)\rangle$$

$$= \underbrace{e^{iH_0 t/\hbar} V(t) e^{-iH_0 t/\hbar}}_{\parallel}$$

$$\tilde{V}(t)$$

$$\underbrace{e^{iH_0 t/\hbar} |\psi(t)\rangle}_{\parallel}$$

$$|\tilde{\psi}(t)\rangle$$

define

$$|\tilde{\psi}(t)\rangle = \tilde{U}(t) |\tilde{\psi}(0)\rangle$$

↓

$$\underbrace{[i\hbar \dot{\tilde{U}} - \tilde{V} \tilde{U}]}_{\parallel} |\tilde{\psi}(0)\rangle = 0 \quad \text{with } \tilde{U}(0) = 1.$$

0



$$i\hbar \dot{\tilde{U}} = \tilde{V} \tilde{U} \quad \text{with } \tilde{U}(0) = 1$$

$$\downarrow \quad \tilde{U} = 1 + \frac{1}{i\hbar} \int_0^t dt' \tilde{V}(t') \underbrace{\tilde{U}(t')}_{\parallel 1 + \frac{1}{i\hbar} \int_0^{t'} dt'' \tilde{V}(t'') \tilde{U}(t'')}$$

$$= 1 + \frac{1}{i\hbar} \int_0^t dt' \tilde{V}(t') - \frac{1}{\hbar^2} \int_0^t dt' \tilde{V}(t') \int_0^{t'} dt'' \tilde{V}(t'') \tilde{U}(t')$$

$$|\tilde{\Psi}(0)\rangle = |\Psi(0)\rangle = |\phi_n\rangle$$

$$P_k(t) = |\langle \phi_k | \Psi(t) \rangle|^2$$

$$= \underbrace{|\langle \phi_k |}_{\downarrow} e^{-iH_0 t/\hbar} \underbrace{e^{iH_0 t/\hbar} |\Psi(t)\rangle}_{\downarrow}$$

$$\langle \phi_k | e^{-i\epsilon_k t/\hbar} \quad |\tilde{\Psi}(t)\rangle$$

$$= |\langle \phi_k | \tilde{\Psi}(t) \rangle|^2$$

$$= \left| \frac{1}{i\hbar} \int_0^t dt' \underbrace{\langle \phi_k | \tilde{V}(t') | \phi_n \rangle}_{\parallel}$$

$$e^{i\epsilon_{kn} t'/\hbar} V_{kn}(t')$$

( $k \neq n$ )

## The Interaction Picture

For the discussion of systems involving only two or three levels, it is particularly convenient to use a description of the time evolution of the system that lies between the Schrödinger picture and the Heisenberg picture, both of which were discussed in Chapter 6. Let us start with the Schrödinger equation, which reads

$$\frac{d}{dt} |\psi(t)\rangle = -\frac{i}{\hbar} H |\psi(t)\rangle = -\frac{i}{\hbar} (H_0 + H_1) |\psi(t)\rangle \quad (15B-1)$$

We can write this in the form

$$|\psi(t)\rangle = U(t) |\psi(0)\rangle \quad (15B-2)$$

where

$$\frac{d}{dt} U(t) = -\frac{i}{\hbar} (H_0 + H_1) U(t) \quad (15B-3)$$

The initial condition is  $U(0) = 1$ .

The procedure calls for the definition of a new state vector  $|\psi_I(t)\rangle$  defined by

$$|\psi_I(t)\rangle = e^{iH_0 t/\hbar} |\psi(t)\rangle \quad (15B-4)$$

It follows that

$$\begin{aligned} \frac{d}{dt} |\psi_I(t)\rangle &= \frac{i}{\hbar} H_0 |\psi_I(t)\rangle + e^{iH_0 t/\hbar} \left( -\frac{i}{\hbar} \right) (H_0 + H_1) |\psi(t)\rangle \\ &= e^{iH_0 t/\hbar} \left( -\frac{i}{\hbar} \right) H_1 e^{-iH_0 t/\hbar} |\psi_I(t)\rangle \end{aligned}$$

If we now define

$$V(t) = e^{iH_0 t/\hbar} H_1 e^{-iH_0 t/\hbar} \quad (15B-5)$$

we end up with the equation

$$\frac{d}{dt} |\psi_I(t)\rangle = \left( -\frac{i}{\hbar} \right) V(t) |\psi_I(t)\rangle \quad (15B-6)$$

Solving this equation is not trivial, and in general the best one can do is to find a solution in terms of a power series in  $V(t)$ . The formal procedure for solving this in a way that incorporates the initial condition

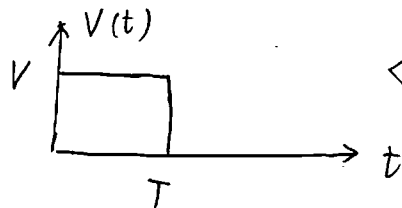
$$|\psi_I(0)\rangle = |\phi\rangle \quad (15B-7)$$

is to write

$$|\psi_I(t)\rangle = U_I(t) |\phi\rangle \quad (15B-8)$$

2.3. 時間を含むない摂動による遷移

$$V(t) = V \quad (0 \leq t \leq T)$$



$$\langle \phi_k | V(t) | \phi_n \rangle = V_{kn} \quad (0 \leq t \leq T)$$

$$\int_0^T e^{i\epsilon_{kn}t'/\hbar} V_{kn}(t') dt' = V_{kn} \frac{\hbar}{i\epsilon_{kn}} (e^{i\epsilon_{kn}T/\hbar} - 1) \quad (\epsilon_{kn} \neq 0)$$

$$= V_{kn} T \quad (\epsilon_{kn} = 0)$$

↓

$$C_k^{(1)} = -\frac{V_{kn}}{\epsilon_{kn}} (e^{i\epsilon_{kn}T/\hbar} - 1)$$

$$C_k^{(2)} = -\frac{1}{\hbar^2} \sum_m V_{km} V_{mn} \int_0^T dt' e^{i\epsilon_{km}t'/\hbar} \int_0^{t'} dt'' e^{i\epsilon_{mn}t''/\hbar}$$

$$\frac{\hbar}{i\epsilon_{mn}} (e^{i\epsilon_{mn}t'/\hbar} - 1)$$

$$= -\frac{1}{\hbar^2} \sum_m V_{km} V_{mn} \cdot \frac{\hbar}{i\epsilon_{mn}} \left\{ \frac{\hbar}{i\epsilon_{kn}} (e^{i\epsilon_{kn}T/\hbar} - 1) - \frac{\hbar}{i\epsilon_{km}} \times (e^{i\epsilon_{km}T/\hbar} - 1) \right\}$$

$$= \sum_m \frac{V_{km} V_{mn}}{\epsilon_{mn}} \left\{ \frac{e^{i\epsilon_{kn}T/\hbar} - 1}{\epsilon_{kn}} - \frac{e^{i\epsilon_{km}T/\hbar} - 1}{\epsilon_{km}} \right\}$$

$$\begin{aligned}
 P_k(T) &= \frac{\lambda^2}{\hbar^2} |V_{kn}|^2 \cdot \left| \frac{\hbar}{i\epsilon_{kn}} (e^{i\epsilon_{kn}T/\hbar} - 1) \right|^2 \quad (\text{if } \epsilon_{kn} \neq 0) \\
 &= \frac{\lambda^2}{\epsilon_{kn}^2} |V_{kn}|^2 \cdot \left| e^{i\epsilon_{kn}T/2\hbar} (e^{i\epsilon_{kn}T/2\hbar} - e^{-i\epsilon_{kn}T/2\hbar}) \right|^2 \\
 &= \frac{4\lambda^2}{\epsilon_{kn}^2} |V_{kn}|^2 \sin^2\left(\frac{\epsilon_{kn}T}{2\hbar}\right)
 \end{aligned}$$

$$P_k(T) = \lambda^2 |V_{kn}|^2 T^2 \quad (\text{if } \epsilon_{kn} = 0)$$

• 収束の条件:

$$C_k^{(1)} = -\frac{V_{kn}}{\epsilon_{kn}} (e^{i\epsilon_{kn}T/\hbar} - 1)$$

↓

$$\left| \lambda \frac{V_{kn}}{\epsilon_{kn}} (e^{i\epsilon_{kn}T/\hbar} - 1) \right| \ll 1$$

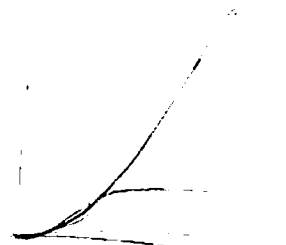
(note)  $|e^{i\epsilon_{kn}T/\hbar} - 1|^2 = 4\sin^2\left(\frac{\epsilon_{kn}T}{2\hbar}\right)$

↓

$$|\lambda V_{kn}| \ll |\epsilon_{kn}|$$

or

$$|\epsilon_{kn}T/\hbar| \ll 1$$



10/13/e  
↑

(note)  $\int_{-\infty}^{\infty} dx \frac{1}{x^2} \sin^2 x = \pi$

2.4 周期的な擾動による遷移

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

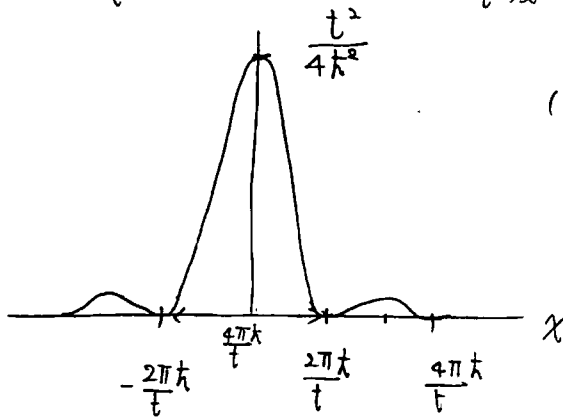
$$\downarrow \int_0^t dt' e^{iE_k t'/\hbar} V_{kn}(t') dt' = V_{kn} \int_0^t dt' e^{i(E_k - E_n \mp \hbar\omega)t'/\hbar}$$

$$= V_{kn} \frac{\hbar}{i(E_k - E_n \mp \hbar\omega)} \left( \frac{e^{i(E_k - E_n \mp \hbar\omega)t/\hbar} - 1}{2i e^{i\frac{\Delta t}{2\hbar}}} \frac{e^{i\frac{\Delta t}{2\hbar}} - e^{-i\frac{\Delta t}{2\hbar}}}{2i} \right)$$

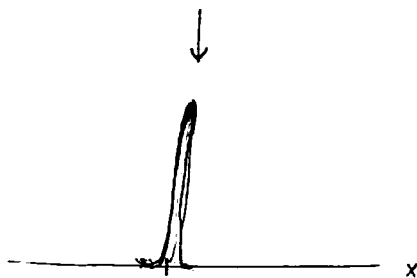
$$\rightarrow P_k(t) = \frac{4\lambda^2}{\Delta^2} |V_{kn}|^2 \sin^2\left(\frac{\Delta t}{2\hbar}\right)$$

$$\Delta = E_k - E_n \mp \hbar\omega$$

$$f(x) = \frac{1}{x^2} \sin^2\left(\frac{x t}{2\hbar}\right) \xrightarrow{t \rightarrow \infty} \frac{\pi t}{2\hbar} \delta(x)$$



(note)  $\int_{-\infty}^{\infty} dx \frac{1}{x^2} \sin^2\left(\frac{x t}{2\hbar}\right)$   
 $= \frac{t}{2\hbar} \int_{-\infty}^{\infty} dy \frac{1}{y^2} \sin^2 y$   
 $= \frac{\pi t}{2\hbar}$



(note)  $\Delta E \cdot \Delta t \sim \hbar$

$$\rightarrow P_k(t) \rightarrow \frac{2\pi}{\hbar} t \lambda^2 |V_{kn}|^2 \delta(E_k - E_n \mp \hbar\omega)$$

単位時間当たりの遷移確率:

$$T_k = P_k / t = \frac{2\pi}{\hbar} \lambda^2 |V_{kn}|^2 \delta(\epsilon_k - \epsilon_n \mp \hbar\omega)$$

