4. 時間に依存する摂動論

4.1. 時間に依存する結合チャンネル方程式

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

suppose $H_0\phi_n = \varepsilon_n\phi_n$

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

$\downarrow$

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

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？

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

を解く。

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

$\downarrow$ $c_m(t=0)=\delta_{n,m}$

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

$$= i\hbar\sum_m \dot{c}_m e^{-i\varepsilon_m t/\hbar}\phi_m + \underline{\sum_m \varepsilon_m c_m e^{-i\varepsilon_m t/\hbar}\phi_m}$$

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

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

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

$\langle \phi_k | \longrightarrow$

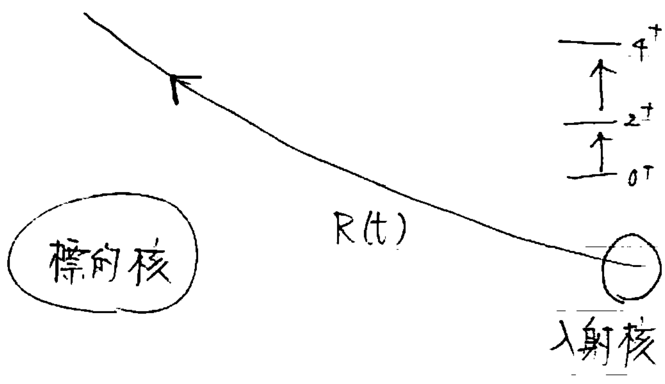
$$i\hbar \dot{c}_k e^{-i\varepsilon_k t/\hbar} - \sum_m c_m \langle \phi_k | V | \phi_m \rangle e^{-i\varepsilon_m t/\hbar} = 0$$

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

(時間に依存する結合チャンネル方程式)

$C_k(0) = \delta_{k,n}$

例)



$$V(t) \propto Z_p Z_T e^2 \frac{R_T^2}{R(t)^3} \cdot x$$

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

ニュートリノ振動

$\nu_e \leftrightarrow \nu_\mu$

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

4.2. 時間に依存する摂動論

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

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

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

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

$\varepsilon_k - \varepsilon_m$

$$= \sum_m \left(c_m^{(0)} + \lambda c_m^{(1)} + \lambda^2 c_m^{(2)} + \cdots \right) e^{i\varepsilon_{km} t/\hbar} \times \langle \phi_k | \lambda V | \phi_m \rangle$$

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

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

$$= e^{i\varepsilon_{kn} t/\hbar} \langle \phi_k | V | \phi_n \rangle$$

$$\rightsquigarrow \quad \boxed{c_k^{(1)} = \frac{1}{i\hbar} \int_0^t e^{i\varepsilon_{kn} t'/\hbar} V_{kn}(t')\, dt'}$$

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

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

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

$\longleftrightarrow$ 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 $n \to k$ へ遷移した」

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

$\downarrow$

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

(遷移確率)

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

$$\downarrow$$

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

$$\| $$

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

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

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

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

$$= \left(C_k^{(0)} + \lambda C_k^{(1)} + \lambda^2 C_k^{(2)} + \cdots\right)^* \left(C_k^{(0)} + \lambda C_k^{(1)} + \lambda^2 C_k^{(2)} + \cdots\right)$$

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

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

$$+ \lambda^2 \left\{ -\delta_{k,n} \cdot \frac{1}{\hbar^2} \sum_m \int_0^t dt'\, e^{i\varepsilon_{km}t'/\hbar} V_{km}(t') \int_0^{t'} dt''\, e^{i\varepsilon_{mn}t''/\hbar} V_{mn}(t'') \right.$$

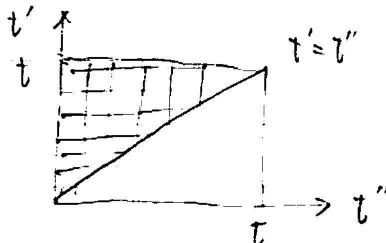
$$- \delta_{k,n} \cdot \frac{1}{\hbar^2} \sum_m \int_0^t dt'\, e^{-i\varepsilon_{km}t'/\hbar} \underbrace{V_{km}^*(t')}_{V_{mk}(t')} \int_0^{t'} dt''\, e^{-i\varepsilon_{mn}t''/\hbar} V_{mn}^*(t'')$$

$$\left. + \frac{1}{\hbar^2} \left| \int_0^t dt'\, e^{i\varepsilon_{kn}t'/\hbar} V_{kn}(t') \right|^2 \right\}$$

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

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

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



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

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

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

$$- \delta_{k,n} \cdot \frac{1}{\hbar^2} \sum_m \int_0^t dt'' \, e^{-i\varepsilon_{mn} t''/\hbar} V_{mn}^*(t'') \int_{t''}^t dt' \, e^{i\varepsilon_{mn} t'/\hbar} V_{mn}(t') \Big\}$$

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

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

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

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

$$\Downarrow$$

$$P_k(t) = \frac{1}{\hbar^2} \lambda^2 \Big| \int_0^t dt' \, e^{i\varepsilon_{kn} t'/\hbar} V_{kn}(t') \Big|^2 \quad \text{for } k \neq n$$

$$= 1 - \frac{\lambda^2}{\hbar^2} \sum_{m \neq n} \Big| \int_0^t dt' \, e^{i\varepsilon_{mn} t'/\hbar} V_{mn}(t') \Big|^2 = 1 - \sum_{m \neq n} P_m \quad \text{for } k=n$$

◦ 別の導出法：相互作用表示

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

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

↓

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

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

$$= \underbrace{e^{iH_0 t/\hbar} V(t) e^{-iH_0 t/\hbar}}_{\equiv \tilde{V}(t)} \underbrace{e^{iH_0 t/\hbar} |\psi(t)\rangle}_{= |\tilde{\psi}(t)\rangle}$$

<u>define</u>

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

↓

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

Supplement 15-B

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

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

We can write this in the form

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle \tag{15B-2}$$

where

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

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

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

$$|\psi_I(t)\rangle = e^{iH_0t/\hbar}|\psi(t)\rangle \tag{15B-4}$$

It follows that

$$\begin{aligned}\frac{d}{dt}|\psi_I(t)\rangle &= \frac{i}{\hbar}H_0|\psi_I(t)\rangle + e^{iH_0t/\hbar}\left(-\frac{i}{\hbar}\right)(H_0 + H_1)|\psi(t)\rangle \\ &= e^{iH_0t/\hbar}\left(-\frac{i}{\hbar}\right)H_1e^{-iH_0t/\hbar}|\psi_I(t)\rangle\end{aligned}$$

If we now define

$$V(t) = e^{iH_0t/\hbar}H_1e^{-iH_0t/\hbar} \tag{15B-5}$$

we end up with the equation

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

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

$$|\psi_I(0)\rangle = |\phi\rangle \tag{15B-7}$$

is to write

$$|\psi_I(t)\rangle = U_I(t)|\phi\rangle \tag{15B-8}$$

Equation (15B-6) takes the form

$$\frac{dU_I(t)}{dt} = -\frac{i}{\hbar}V(t)U_I(t) \tag{15B-9}$$

Since $U_I(0) = 1$, we can convert the differential equation into an integral equation

$$U_I(t) = 1 - \frac{i}{\hbar}\int_0^t dt'\, V(t')U_I(t') \tag{15B-10}$$

This can be solved by iteration. In the first step we replace the U_I under the integral by 1. In the second step, we take the $U_I(t)$ so obtained and insert it on the right-hand side, and so on. We thus get

$$U_I(t) = 1 - \frac{i}{\hbar}\int_0^t dt'\, V(t') + \left(-\frac{i}{\hbar}\right)^2 \int_0^t dt'\, V(t') \int_0^{t'} dt''\, V(t'') + \cdots \tag{15B-11}$$

This is a nice compact form, but working out the integrals in the second term is still very tedious. That is all we have to say about this, other than to say that the first-order expression is very handy for dealing with two- and three-level systems, as we shall see in Chapter 18.

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

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

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

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

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

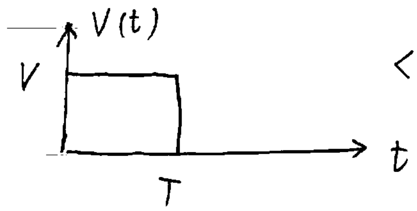
$$= |\underbrace{\langle\phi_k|\, e^{-iH_0 t/\hbar}}_{\langle\phi_k|\, e^{-i\varepsilon_k t/\hbar}}\ \underbrace{e^{iH_0 t/\hbar}\,|\Psi(t)\rangle}_{|\tilde{\Psi}(t)\rangle}|^2$$

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

$$= \left|\frac{1}{i\hbar}\int_0^t dt'\, \underbrace{\langle\phi_k|\tilde{V}(t')|\phi_n\rangle}_{\substack{\parallel \\ e^{i\varepsilon_{kn}t'/\hbar}\, V_{kn}(t')}}\right|^2 \qquad (k \neq n)$$

4.3. 時間を含まない摂動による遷移

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



$$\langle \varphi_k | V(t) | \varphi_n \rangle = V_{kn} \quad (0 \le t \le T)$$

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

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

$\downarrow$

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

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

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

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

$$P_k(t) = \frac{\lambda^2}{\hbar^2} |V_{kn}|^2 \cdot \left| \frac{\hbar}{i\varepsilon_{kn}} (e^{i\varepsilon_{kn}T/\hbar} - 1) \right|^2 \quad (\text{if } \varepsilon_{kn} \neq 0)$$

$$= \frac{\lambda^2}{\varepsilon_{kn}^2} |V_{kn}|^2 \cdot \left| e^{i\varepsilon_{kn}T/2\hbar} (e^{i\varepsilon_{kn}T/2\hbar} - e^{-i\varepsilon_{kn}T/2\hbar}) \right|^2$$

$$= \frac{4\lambda^2}{\varepsilon_{kn}^2} |V_{kn}|^2 \sin^2\left(\frac{\varepsilon_{kn}T}{2\hbar}\right)$$

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

○ 収束の条件:

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

$\downarrow$

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

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

$\downarrow$

- $|\lambda V_{kn}| \ll |\varepsilon_{kn}|$

or

- $|\varepsilon_{kn} T/\hbar| \ll 1$