

時間に依存する摂動論

$$H = H_0 + V(t)$$

$$H_0 \phi_n = \epsilon_n \phi_n$$

$$i\hbar \frac{\partial}{\partial t} \Psi(t) = (H_0 + V) \Psi(t)$$

$$\Psi(t=0) = \phi_n$$

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

↓

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

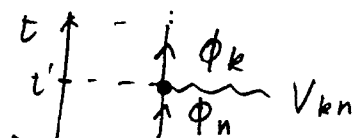
↷

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

+ ...

$$\begin{cases} P_k(t) = |\langle \phi_k | \Psi(t) \rangle|^2 = |c_k(t)|^2 & (k \neq n) \\ P_n(t) = 1 - \sum_{k \neq n} P_k(t) \end{cases}$$

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



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

$$V(t) = \begin{cases} \lambda x & (0 \leq t \leq T) \\ 0 & (t > T) \end{cases}$$

(note) $V(t) = \lambda x = \lambda \alpha_0 (a + a^\dagger)$; $\alpha_0 = \sqrt{\frac{\hbar}{2m\omega}}$

$$\Downarrow \lambda x |0\rangle = \lambda \alpha_0 |1\rangle$$

\Downarrow

$$C_1 = \frac{1}{i\hbar} \int_0^T dt e^{i(k\omega - 0)t/\hbar} \cdot \lambda \alpha_0$$

$$= \frac{\lambda \alpha_0}{i\hbar} \int_0^T dt e^{i\omega t}$$

$$= \frac{\lambda \alpha_0}{i\hbar} \cdot \frac{1}{i\omega} (e^{i\omega T} - 1)$$

$$= -\frac{\lambda \alpha_0}{\hbar \omega} e^{i\omega T/2} \cdot 2i \sin\left(\frac{\omega T}{2}\right)$$

\Downarrow

$$P_1 = |C_1|^2 = \left(\frac{\lambda \alpha_0}{\hbar \omega}\right)^2 \cdot 4 \sin^2\left(\frac{\omega T}{2}\right)$$

$$P_k = 0 \quad (k > 1)$$

$$P_0 = 1 - P_1 = 1 - \left(\frac{\lambda \alpha_0}{\hbar \omega}\right)^2 \cdot 4 \sin^2\left(\frac{\omega T}{2}\right)$$

(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.

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

$\int_0^t dt' e^{i\epsilon_{kn}t'/\hbar} V_{kn}(t') dt' = V_{kn} \int_0^t dt' e^{i(\epsilon_{kn} \mp \hbar\omega)t'/\hbar}$

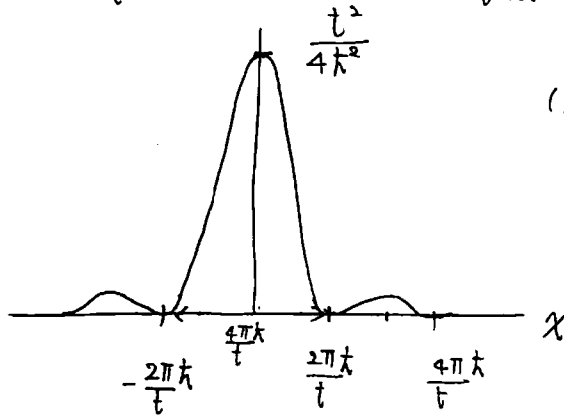
$= V_{kn} \frac{\hbar}{i(\epsilon_{kn} \mp \hbar\omega)} (e^{i(\epsilon_{kn} \mp \hbar\omega)t/\hbar} - 1)$

$\frac{e^{i\frac{\Delta t}{\hbar}} - e^{-i\frac{\Delta t}{\hbar}}}{2i}$

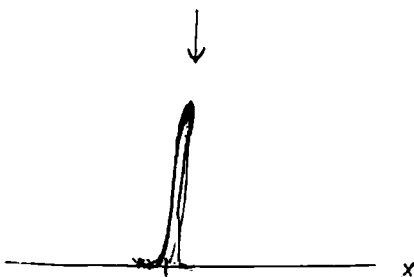
$P_k(t) = \frac{4\lambda^2}{\Delta^2} |V_{kn}|^2 \sin^2\left(\frac{\Delta t}{2\hbar}\right)$

$\Delta = \epsilon_k - \epsilon_n \mp \hbar\omega$

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



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

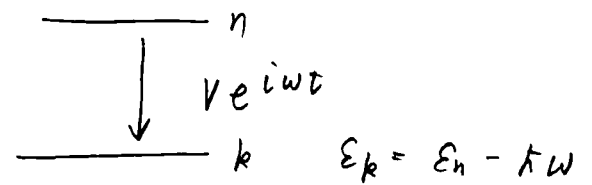
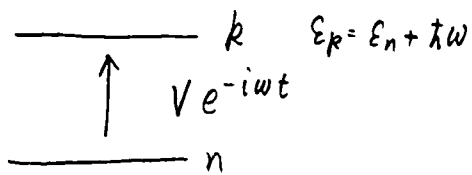


(note) $\Delta E \cdot \Delta t \sim \hbar$

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

単位時間当たりの遷移確率:

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



- いくつかの状態が ϵ_k に縮退している時
(終状態が ϵ_k として指定できない時)

(例) 3次元の散乱状態 $\epsilon = \frac{\vec{p}^2}{2m} = \frac{p^2}{2m}$

$$p = \sqrt{2m\epsilon}$$

$$\left(\begin{array}{l} p_x = p \\ p_y = p_z = 0 \end{array} \right) \quad \left(\begin{array}{l} p_x = p_y = 0 \\ p_z = p \end{array} \right) \quad \left(\begin{array}{l} p_x = p_y = \frac{p}{\sqrt{2}} \\ p_z = 0 \end{array} \right) \quad \text{etc.}$$

全遷移確率:

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

$$\approx \frac{2\pi}{\hbar} \lambda^2 |V_{fn}|^2 \underbrace{\sum_k \delta(\epsilon_k - \epsilon_n \mp \hbar\omega)}_{\rho(\epsilon_n \pm \hbar\omega)}$$

(状態密度)

単位エネルギー間隔にある状態の数

$$\boxed{T = \frac{2\pi}{\hbar} |\lambda V_{fn}|^2 \rho(\epsilon_n \pm \hbar\omega)}$$

Fermi の Golden Rule

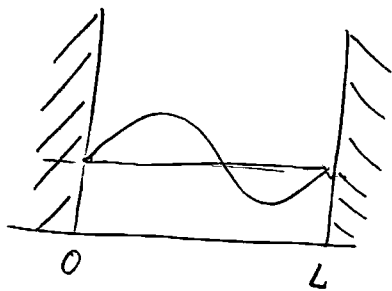
例) 終状態が散乱状態の場合 (E_f だけ指定)

$$H = \frac{\vec{P}^2}{2m} \quad \vec{P}: \text{連続量}$$

$$H \psi_f(\vec{x}) = E_f \psi_f(\vec{x})$$

$$\psi_f(\vec{x}) = \psi_{E_x}(x) \psi_{E_y}(y) \psi_{E_z}(z)$$

$$\left(\frac{P_x^2}{2m} - E_x \right) \psi_{E_x}(x) = 0 \quad \text{1D と}$$



周期境界条件

$$\psi(0) = \psi(L) = 0$$

$$\psi'(0) = \psi'(L)$$

↓

$$\psi(x) = c \sin kx$$

$$kL = 2n\pi$$

↓

$$k_x = \frac{2\pi}{L} n_x, \quad k_y = \frac{2\pi}{L} n_y, \quad k_z = \frac{2\pi}{L} n_z$$

$$T_{fi} = \sum_{n_x, n_y, n_z} \frac{2\pi}{\hbar} \lambda^2 |V_{fi}|^2 \delta(\epsilon_f - \epsilon_i \mp \hbar\omega)$$

\uparrow

$$\epsilon_f = \frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2)$$

$$= \frac{\hbar^2}{2m} \left(\frac{2\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2)$$
 を満たすような (n_x, n_y, n_z) を足す。

$$\begin{aligned} &\sim \int d^3n \frac{2\pi}{\hbar} \lambda^2 |V_{fi}|^2 \delta(\epsilon_f - \epsilon_i \mp \hbar\omega) \\ &= \left(\frac{L}{2\pi}\right)^3 \int d^3k \frac{2\pi}{\hbar} \lambda^2 |V_{fi}|^2 \delta(\epsilon_f - \epsilon_i \mp \hbar\omega) \\ &= \int \underbrace{\left[\frac{d^3k}{(2\pi)^3} \cdot L^3 \right]}_{\substack{\parallel \\ d^3n}} \frac{2\pi}{\hbar} \lambda^2 |V_{fi}|^2 \delta(\epsilon_f - \epsilon_i \mp \hbar\omega) \end{aligned}$$

$$\phi_f \sim \frac{1}{\sqrt{L^3}} e^{i\vec{k} \cdot \vec{r}}$$

↓
 L^3 は \vec{r} -セルの体積。