

[復習]

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

$$H_0 \phi_n = E_n \phi_n$$

$$\begin{cases} i\hbar \frac{\partial}{\partial t} \psi(t) = (H_0 + V(t)) \psi(t) \\ \psi(t=0) = \phi_n \end{cases}$$

$$\psi(t) = \sum_k C_k(t) e^{-iE_k t/\hbar} \phi_k$$

時間に依存する摂動論:

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

$$E_{kn} \equiv E_k - E_n$$

$$V_{kn}(t) \equiv \langle \phi_k | V(t) | \phi_n \rangle$$

$$\text{遷移確率: } P_{n \rightarrow k}(t) = |C_k(t)|^2.$$

1.4 周期的な摂動による遷移

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

$$C_k(t) = \frac{1}{i\hbar} \int_0^t dt' e^{iE_{kn}t'/\hbar} \underbrace{V_{kn}(t')}_{\text{F}_{kn} (e^{i\omega t'} + e^{-i\omega t'})}$$

$$(k \neq n)$$

$$= \frac{F_{kn}}{i\hbar} \int_0^t dt' (e^{i(\omega_{kn} + \omega)t'} + e^{i(\omega_{kn} - \omega)t'})$$

$$\omega_{kn} \equiv E_{kn} / \hbar$$

(note) $\int_0^t dt' e^{i\tilde{\omega}t'} = \frac{1}{i\tilde{\omega}} (e^{i\tilde{\omega}t} - 1)$

$$= \frac{1}{i\tilde{\omega}} e^{i\tilde{\omega}t/2} \underbrace{(e^{i\tilde{\omega}t/2} - e^{-i\tilde{\omega}t/2})}_{2i \sin(\tilde{\omega}t/2)}$$

$$= \frac{2}{\tilde{\omega}} e^{i\tilde{\omega}t/2} \sin(\tilde{\omega}t/2)$$

$$= \frac{2 F_{kn}}{i\hbar} \left\{ e^{i(\omega_{kn} + \omega)t/2} \frac{\sin((\omega_{kn} + \omega)t/2)}{\omega_{kn} + \omega} \right.$$

$$\left. + e^{i(\omega_{kn} - \omega)t/2} \frac{\sin((\omega_{kn} - \omega)t/2)}{\omega_{kn} - \omega} \right\}$$

$$\int_{-\infty}^{\infty} d\alpha D(\alpha) = \int_{-\infty}^{\infty} \frac{2}{t} dy \cdot t^2 \frac{\sin^2 y}{y^2} = \frac{2}{t} \cdot t^2 \cdot \pi = 2\pi t$$

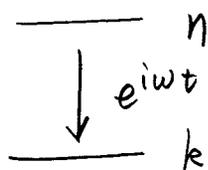
$$y = \frac{\alpha t}{2}$$

$$P_{n \rightarrow k}(t) = |C_k(t)|^2$$

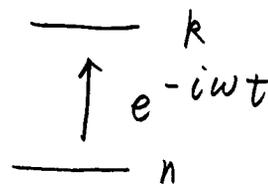
• $\omega = 0$ のとき, 1.3 の結果 $[V(t) = \hat{V} (0 \leq t \leq T)]$ に帰着 (ただし, 1.3 の式で $2\hat{H} = \hat{V}$ とする必要がある)

• $\omega_{kn} \pm \omega = 0$ の場合, "共鳴的遷移"

$$\omega = \begin{matrix} \nearrow e^{i\omega t} \\ \omega_{kn} \\ \searrow e^{-i\omega t} \end{matrix} = \mp (E_k - E_n) / \hbar$$

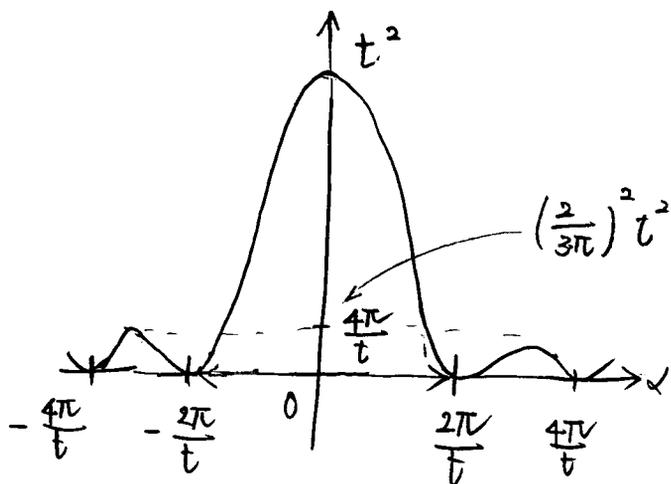


$$E_n - E_k = \hbar\omega$$



$$E_k = E_n + \hbar\omega$$

• $|C_k(t)|^2$ の中に $D(\alpha) = \left(\frac{\sin(\alpha t/2)}{\alpha/2}\right)^2 = t^2 \left(\frac{\sin(\alpha t/2)}{\alpha t/2}\right)^2$ ($\alpha = \omega_{kn} \pm \omega$) という項



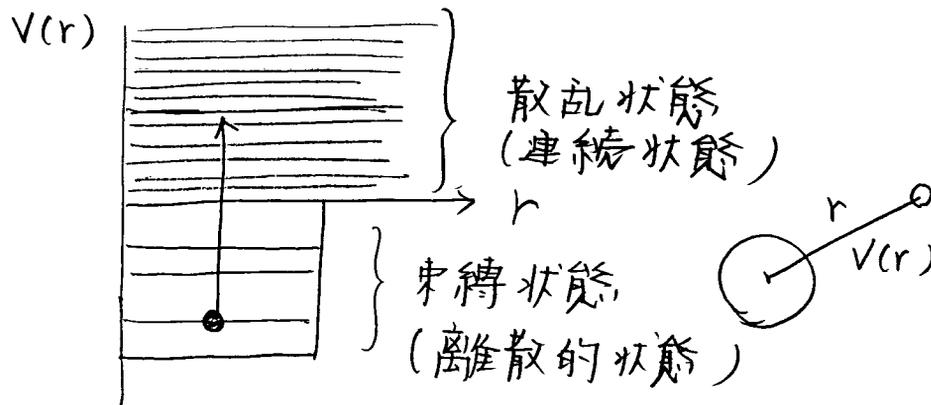
(note)

$$D(\alpha) \rightarrow 2\pi t \delta(\alpha) \quad t \rightarrow \infty$$

$$\text{cf. } \int_{-\infty}^{\infty} dx \frac{\sin^2 x}{x^2} = \pi$$

連続状態への遷移の場合

具体的な例) 3次元ポテンシャル中の粒子の運動



$$\psi(t) = \underbrace{\sum_{\mathbf{k}} c_{\mathbf{k}}(t) e^{-iE_{\mathbf{k}}t/\hbar} \phi_{\mathbf{k}}}_{\text{束縛状態}} + \underbrace{\int \frac{d^3P}{(2\pi\hbar)^3} C(E_P) e^{-iE_P t/\hbar} \phi_P}_{\text{連続状態}}$$

$$E_P = \frac{1}{2m} (P_x^2 + P_y^2 + P_z^2)$$

$$\phi_P(\mathbf{r}) \sim e^{i\mathbf{P} \cdot \mathbf{r}/\hbar}$$

(note) 自由粒子の運動

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

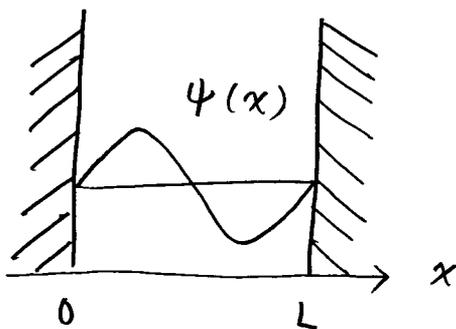
$$= \frac{1}{2m} (\hat{P}_x^2 + \hat{P}_y^2 + \hat{P}_z^2)$$

$$H \psi(\mathbf{r}) = E \psi(\mathbf{r})$$

$$\psi(\mathbf{r}) = \psi_{E_x}(x) \psi_{E_y}(y) \psi_{E_z}(z) \quad \text{と変数分離}$$

$$\left(\frac{\hat{P}_x^2}{2m} - E_x \right) \psi_{E_x}(x) = 0 \quad \text{など}$$

$$E = E_x + E_y + E_z$$



周期境界条件

$$\begin{cases} \psi(0) = \psi(L) = 0 \\ \psi'(0) = \psi'(L) \end{cases}$$

$$\downarrow \quad \psi(x) = \sqrt{\frac{2}{L}} \sin kx \quad ; \quad kL = 2n\pi$$

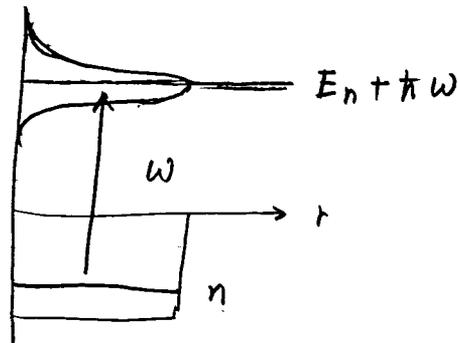
$$\leadsto \quad k_x = \frac{2\pi}{L} n_x \quad \text{など}$$

$$\leadsto \quad \text{状態数: } \sum_{n_x, n_y, n_z} \sim \int d^3n = \left(\frac{L}{2\pi}\right)^3 \int d^3k$$

$$= \left(\frac{L}{2\pi\hbar}\right)^3 \int d^3p$$

$$\Psi(t) = \sum_k C_k(t) e^{-iE_k t/\hbar} \phi_k + \int \frac{dP}{(2\pi\hbar)^3} C(E_P) e^{-iE_P t/\hbar} \phi_P$$

$$V(t) = \hat{H} e^{-i\omega t} \quad \text{に} \downarrow \text{する連続状態への遷移}$$



$$C(E_P) = \frac{2}{i\hbar} \langle \phi_P | \hat{H} | \phi_n \rangle \times e^{i(E_P - E_n - \hbar\omega)t/2\hbar} \cdot \frac{\sin((E_P - E_n - \hbar\omega)t/2\hbar)}{(E_P - E_n)/\hbar - \omega}$$

$$E_P = \frac{P^2}{2m} = \frac{|P|^2}{2m}$$

全遷移確率:

$$D(\alpha) = \left(\frac{\sin(\alpha t/2)}{\alpha/2} \right)^2$$

$$P(t) = \int \frac{dP}{(2\pi\hbar)^3} |C(E_P)|^2$$

$$\int dE P_{n \rightarrow E}(t) = \int \frac{dP}{(2\pi\hbar)^3} \cdot \frac{1}{\hbar^2} |\langle \phi_P | \hat{H} | \phi_n \rangle|^2 \cdot D((E_P - E_n - \hbar\omega)/\hbar)$$

$$\xrightarrow{t \rightarrow \infty} \int \frac{dP}{(2\pi\hbar)^3} |\langle \phi_P | \hat{H} | \phi_n \rangle|^2 \cdot \frac{2\pi}{\hbar} t \int (E_P - E_n - \hbar\omega)$$

$$\int (E_P - E_n - \hbar\omega)/\hbar = \hbar \int (E_P - E_n - \hbar\omega)$$

エネルギー保存則

単位時間当りの遷移確率

$$\frac{dP}{dt} = \frac{2\pi}{\hbar} \int \frac{dP}{(2\pi\hbar)^3} |\langle \phi_P | \hat{H} | \phi_n \rangle|^2 \delta(E_P - E_n - \hbar\omega)$$

もし、 $|\langle \phi_P | \hat{H} | \phi_n \rangle|^2$ が「終状態のエネルギー E_P には
依らない」とすると $\langle \phi_P | \hat{H} | \phi_n \rangle \equiv F_{fi}$ として

$$\frac{dP}{dt} = \frac{2\pi}{\hbar} |F_{fi}|^2 \underbrace{\int \frac{dP}{(2\pi\hbar)^3} \delta(E_P - E_n - \hbar\omega)}_{\rho(E_P = E_n + \hbar\omega)}$$

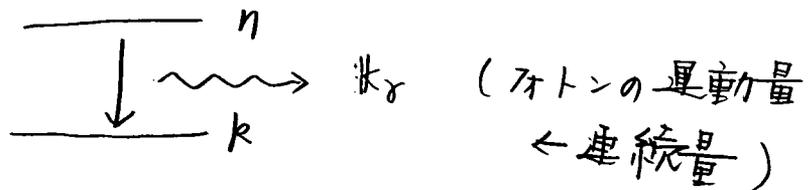
(Pの方向に依らない
という意味)

$\rho(E_P = E_n + \hbar\omega)$

終状態の状態密度
(状態の数)

$V(t) = \hat{H} e^{i\omega t}$ で遷移する場合も同様。

例)



一般に

$$W_{fi} \equiv \frac{dP}{dt} = \frac{2\pi}{\hbar} |F_{fi}|^2 \rho(E_f)$$

「フェルミの黄金則」