(複習)

$$\left(i\hbar\,\partial_t - H_0 - V(t)\right)\psi(t) = 0 \quad , \quad \psi(t=0) = \phi_n$$

$$H_0\,\phi_n = \varepsilon_n\,\phi_n$$

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

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

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

$$c_m^{(1)}(t) = \frac{1}{i\hbar}\int_0^t e^{i\varepsilon_{mn}t'/\hbar}\,V_{mn}(t')\,dt'$$

遷移確率:

$$P_m(t) = |c_m(t)|^2$$

$$= \begin{cases} \dfrac{1}{\hbar^2}\left|\displaystyle\int_0^t dt'\, e^{i\varepsilon_{mn}t'/\hbar}\,V_{mn}(t')\right|^2 & \text{for } m \neq n \\ 1 - \displaystyle\sum_{k\neq n} P_k & \text{for } m = n \end{cases}$$

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

4.4. 周期的な摂動による遷移.

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

$\downarrow$

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

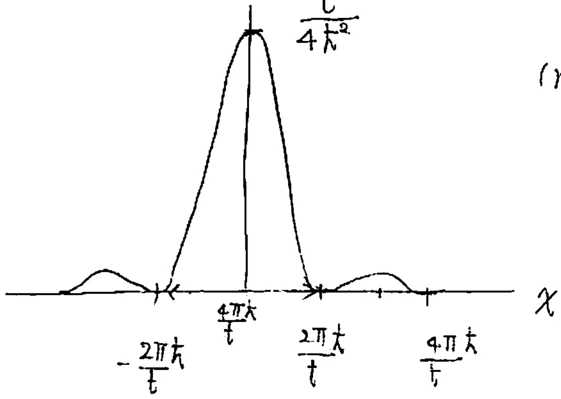
$$= V_{kn} \frac{\hbar}{i(\varepsilon_{kn} \mp \hbar\omega)} \left(\underbrace{e^{i(\varepsilon_{kn} \mp \hbar\omega)t/\hbar} - 1}_{= \, 2i \, e^{\frac{i\Delta t}{2\hbar}} \frac{e^{i\frac{\Delta t}{2\hbar}} - e^{-i\frac{\Delta t}{2\hbar}}}{2i}} \right)$$

$\downarrow$

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

$$\Delta = \varepsilon_k - \varepsilon_n \mp \hbar\omega$$

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

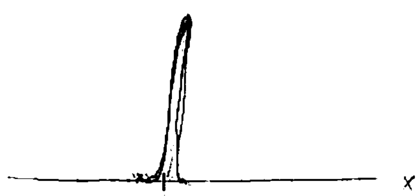


(note) $\int_{-\infty}^{\infty} dx \, \frac{1}{x^2} \sin^2\left(\frac{xt}{2\hbar}\right)$

$$= \frac{t}{2\hbar} \int_{-\infty}^{\infty} dy \, \frac{1}{y^2} \sin^2 y$$

$$= \frac{\pi t}{2\hbar}$$

$\downarrow$



(note)

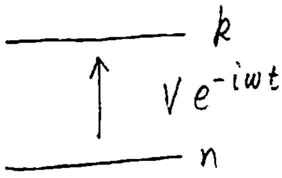
$\Delta E \cdot \Delta t \sim \hbar$

$\downarrow$

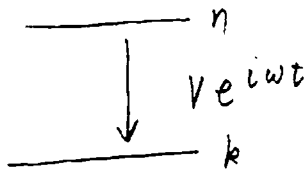
$$\boxed{P_k(t) \longrightarrow \frac{2\pi}{\hbar} t \, \lambda^2 |V_{kn}|^2 \delta(\varepsilon_k - \varepsilon_n \mp \hbar\omega)}$$

単位時間当たりの遷移確率：

$$\boxed{\Gamma_k = P_k / t = \frac{2\pi}{\hbar} \lambda^2 |V_{kn}|^2 \, \delta(\varepsilon_k - \varepsilon_n \mp \hbar\omega)}$$



$\varepsilon_k = \varepsilon_n + \hbar\omega$



$\varepsilon_k = \varepsilon_n - \hbar\omega$

。いくつかの状態が ε_k に縮退している時
(終状態が ε_k だけで指定できない時)

(例) 3次元の散乱状態 $\quad \varepsilon = \dfrac{\vec{p}^{\,2}}{2m} = \dfrac{p^2}{2m}$

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

$$\begin{pmatrix} p_x = p \\ p_y = p_z = 0 \end{pmatrix} \quad \begin{pmatrix} p_x = p_y = 0 \\ p_z = p \end{pmatrix} \quad \begin{pmatrix} p_x = p_y = \frac{p}{\sqrt{2}} \\ p_z = 0 \end{pmatrix}$$ など

全遷移確率：

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

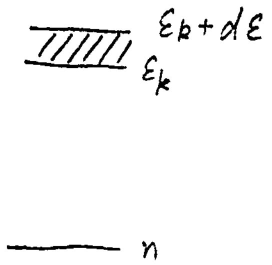
$$\approx \frac{2\pi}{\hbar} \lambda^2 |V_{kn}|^2 \underbrace{\sum_k \delta(\varepsilon_k - \varepsilon_n \mp \hbar\omega)}_{= \rho(\varepsilon_n \pm \hbar\omega)}$$

(状態密度)
単位エネルギー間隔にある状態の数

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

Fermi の Golden Rule

(note)　ε_k が連続スペクトルの場合



$\varepsilon_k \le E \le \varepsilon_k + dE$ にある状態数

$\rightarrow \rho(\varepsilon_k)dE$

$\varepsilon_k \le E \le \varepsilon_k + dE$ の間に遷移する確率

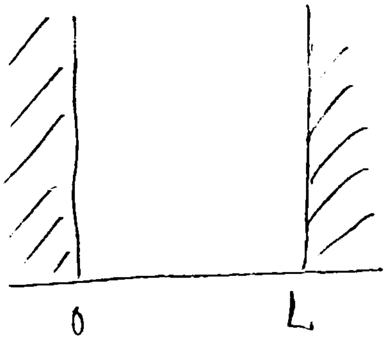
$$T = \int dE\, \rho(E) \cdot \underbrace{T(E)}_{=\frac{2\pi}{\hbar}|\lambda V_{kn}|^2 \delta(\varepsilon_k - \varepsilon_n \mp \hbar\omega)}$$

$$= \frac{2\pi}{\hbar} |\lambda V_{kn}|^2 \rho(\varepsilon_n \pm \hbar\omega)$$

。位相空間 (phase space) : 自由粒子に対する状態密度

$$H = \frac{\vec{P}^2}{2m}$$

P : 連続量



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

$$E = E_x + E_y + E_z$$

$$\left(\frac{P_x^2}{2m} - E_x\right)\psi_{E_x}(x) = 0$$

$$\psi_{E_x}(x) = A e^{ik_x x} + B e^{-ik_x x}$$

- box discretization
- periodic b.c.

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

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

$$\downarrow \qquad \psi(x) = C \sin kx$$

$$kL = 2n\pi$$

3次元 : $k_x = \frac{2\pi}{L} n_x,\quad k_y = \frac{2\pi}{L} n_y,\quad k_z = \frac{2\pi}{L} n_z.$

$$T_{tot}^{(k)} = \sum_{n_x, n_y, n_z} T_k$$

$$= \sum_{n_x, n_y, n_z} \frac{2\pi}{\hbar} \lambda^2 |V_{kn}|^2 \delta(\varepsilon_k - \varepsilon_n - \hbar\omega)$$

$$\varepsilon_k = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2)$$
$$= \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2)$$

$$\sim \int d^3n \, \frac{2\pi}{\hbar} \lambda^2 |V_{kn}|^2 \delta(\varepsilon_k - \varepsilon_n - \hbar\omega)$$

$$= \left(\frac{L}{2\pi}\right)^3 \int d^3k \, \frac{2\pi}{\hbar} \lambda^2 |V_{kn}|^2 \delta(\varepsilon_k - \varepsilon_n - \hbar\omega)$$

$$= \int \frac{V d^3p}{(2\pi\hbar)^3} \frac{2\pi}{\hbar} \lambda^2 |V_{kn}|^2 \delta(\varepsilon_k - \varepsilon_n - \hbar\omega)$$

the phase space : $\boxed{d^3n = \frac{V d^3p}{(2\pi\hbar)^3}}$

光子の場合にも使える

(note) $|V_{kn}|^2 = |\langle \phi_k | V | \phi_n \rangle|^2$

$$\phi_k \sim \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$$

$\leadsto$ V はキャンセルされる.

☒ 電磁場との相互作用

$$H = \frac{1}{2m}\left(p + \frac{e}{c}A(r,t)\right)^2 + V(r) + H_{em}$$

(note)

$$m\ddot{r} = -e\left[E(r,t) + \frac{1}{c}v \times B(r,t)\right]$$

"minimum principle"

Coulomb gauge $\quad \nabla \cdot A(r,t) = 0$

$$B = \nabla \times A$$
$$E = -\frac{1}{c}\frac{\partial A}{\partial t}$$
$$\nabla^2 A - \frac{1}{c^2}\frac{\partial^2 A}{\partial t^2} = 0.$$

$$H_{em} = \frac{1}{8\pi}\int dr\left(|B|^2 + |E|^2\right)$$
$$= \frac{1}{8\pi}\int dr\left(\frac{1}{c^2}|\dot{A}|^2 + |\nabla \times A|^2\right)$$

$$H = \frac{1}{2m}\left(\mathbb{P} + \frac{e}{c}A\right)^2 + V(r) + H_{em}$$

$$= \underbrace{\frac{1}{2m}\mathbb{P}^2 + V(r)}_{H_0} + H_{em} + \underbrace{\frac{1}{2m}\cdot\frac{e}{c}\left(\mathbb{P}\cdot A + A\cdot\mathbb{P}\right) + \frac{e^2}{2mc^2}A^2}_{H_{int}}$$

$$H_{int} = \frac{e}{2mc}\left(\cancel{\frac{\hbar}{i}(\nabla\cdot A)} + \frac{\hbar}{i}A\cdot\nabla + A\cdot\mathbb{P}\right) + \frac{e^2}{2mc^2}A^2$$

$$= \underbrace{\frac{e}{mc}A\cdot\mathbb{P}}_{\downarrow\ 摂動} + \underbrace{\frac{e^2}{2mc^2}A^2}_{\downarrow\ 2次}$$

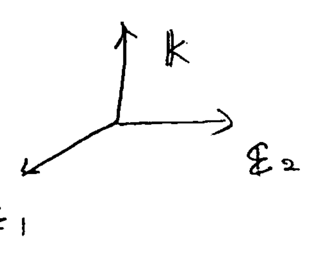
$$\alpha = \frac{e^2}{\hbar c} = \frac{1}{137}$$

量子電気力学 (QED) ： 第2量子化

$$A(r,t) = \sum_{k}\sum_{\alpha=1,2}\sqrt{\frac{2\pi c^2\hbar}{\omega V}}\left(a_{k\alpha}\,\varepsilon_\alpha\, e^{ik\cdot r - i\omega_k t} + a^{\dagger}_{k\alpha}\,\varepsilon_\alpha\, e^{-ik\cdot r + i\omega_k t}\right)$$

$a^{\dagger}_{k\alpha}, a_{k\alpha}$: photon の生成・消滅演算子

ε_α : 偏極 (polarization) ベクトル



$$\nabla\cdot A = 0 \longrightarrow k\cdot\varepsilon = 0$$

$$\varepsilon_\alpha\cdot\varepsilon_{\alpha'} = \delta_{\alpha,\alpha'}$$

$$\omega = c\,|k|.$$

$$\omega = ck = \frac{c}{\hbar} p$$

$$\left(\nabla^2 - \frac{1}{c^2} \partial_t^2\right) e^{\pm(i\mathbb{k}\cdot\mathbb{r} - i\omega_k t)} = \left(-k^2 + \frac{\omega_k^2}{c^2}\right) e^{\pm i(\mathbb{k}\cdot\mathbb{r} - \omega_k t)}$$

$$= 0$$

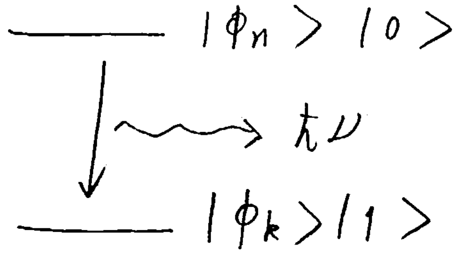
$$H_{em} = \frac{1}{8\pi} \int d\mathbb{r} \left(|\mathbb{E}|^2 + |\mathbb{B}|^2 \right)$$

$$= \sum_{\mathbb{k}} \sum_{\alpha} \left(a^{\dagger}_{\mathbb{k}\alpha} a_{\mathbb{k}\alpha} + \frac{1}{2} \right) \hbar \omega_k$$

$$\omega = ck = \frac{c}{\hbar}p$$

$$p = \frac{\hbar}{c}\omega$$

∘ photon emission (bound → bound)



$$H_{int} = \frac{e}{mc}\sqrt{\frac{2\pi c^2\hbar}{\omega V}}\,\boldsymbol{\varepsilon}\cdot\mathbb{p}\,e^{-i(\mathbb{k}\cdot\mathbb{r}-\omega t)}$$

$$\frac{e}{mc}\mathbb{A}\cdot\mathbb{p}$$

終状態における状態の数 = photon の状態数

$$d^3n = \frac{V d^3p}{(2\pi\hbar)^3} = \frac{V}{(2\pi\hbar)^3}p^2dp\,d\Omega_p$$

$$= \frac{V}{(2\pi\hbar)^3}\left(\frac{\hbar\omega}{c}\right)^2\frac{1}{c}d(\hbar\omega)\,d\Omega_p$$

↓

$$T = \int\frac{\cancel{V}}{(2\pi\hbar)^3}\left(\frac{\hbar\omega}{c}\right)^2\frac{1}{c}d(\hbar\omega)\,d\Omega_p$$

$$\times\frac{2\pi}{\hbar}\left(\frac{e}{mc}\right)^2\frac{2\pi c^2\hbar}{\omega\cancel{V}}\left|\langle\phi_k|\boldsymbol{\varepsilon}\cdot\mathbb{p}\,e^{-i\mathbb{k}\cdot\mathbb{r}}|\phi_n\rangle\right|$$

$$\times\delta(\varepsilon_k-\varepsilon_n+\hbar\omega)$$

$$\text{係数} = \frac{1}{\cancel{(2\pi\hbar)^3}_{\,2\pi}}\cdot\frac{(\cancel{\hbar}\omega)^2}{c^3}\cdot\frac{\cancel{2\pi}}{\hbar}\cdot\frac{e^2}{m^2\cancel{c^2}}\cdot\frac{\cancel{2\pi c^2\hbar}}{\cancel{\omega}}$$

$$= \frac{\omega e^2}{2\pi c^3m^2\hbar} = \frac{\omega}{2\pi}\cdot\frac{e^2}{\hbar c}\cdot\frac{1}{m^2c^2}$$

$$= \int_{d\Omega_p} d(\hbar\omega)\,\frac{\omega}{2\pi}\cdot\frac{e^2}{\hbar c}\,\frac{1}{m^2c^2}\left|\langle\phi_k|\boldsymbol{\varepsilon}\cdot\mathbb{p}\,e^{-i\mathbb{k}\cdot\mathbb{r}}|\phi_n\rangle\right|^2$$

$$\times\,\delta(\varepsilon_k-\varepsilon_n+\hbar\omega)$$

$$= \int d\Omega_p \, \frac{1}{2\pi} \cdot \frac{e^2}{\hbar c} \, \frac{\varepsilon_n - \varepsilon_k}{\hbar} \left| \frac{1}{mc} \underbrace{\langle \phi_k | e^{-i\mathbf{k}\cdot\mathbf{r}} \, \boldsymbol{\varepsilon}\cdot\mathbf{p} \, | \phi_n \rangle}_{} \right|^2$$

10/20

◦ dipole approximation

$$e^{-i\mathbf{k}\cdot\mathbf{r}} \sim 1 \qquad \mathbf{k}\cdot\mathbf{r} \ll 1$$

$$k \ll \frac{1}{r} \quad \text{(長波長近似)}$$

$$\hbar\omega = pc \sim 10 \text{ eV}$$

$$k = \frac{p}{\hbar} \sim \frac{10\text{eV}}{\hbar c} \qquad \lambda \sim \frac{\hbar c}{10\text{eV}} \sim 200 \text{ Å}$$

$$\left(\begin{aligned} \hbar c &\sim 200 \text{ MeV}\cdot\text{fm} \\ &= 2000 \text{ eV}\cdot\text{Å} \end{aligned} \right)$$

$$\downarrow$$

$$\boxed{\langle \phi_k | e^{-i\mathbf{k}\cdot\mathbf{r}} \, \boldsymbol{\varepsilon}\cdot\mathbf{p} \, | \phi_n \rangle \sim \langle \phi_k | \boldsymbol{\varepsilon}\cdot\mathbf{p} \, | \phi_n \rangle}$$

(note) Hydrogen-like atom

$$R_{10}(r) = 2 \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} e^{-Zr/a_0}$$

$$a_0 = \frac{\hbar}{mc\alpha} = 0.53 \text{ Å}$$

$$E_n = -\frac{1}{2} mc^2 \frac{Z^2\alpha^2}{n^2} \rightsquigarrow E_2 - E_1 = -\frac{mc^2}{2} \cdot Z^2\alpha^2 \left(\frac{1}{4} - 1\right) \simeq 10.2 \text{ eV}$$