(複習)

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

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

$$H_0\phi_k = \varepsilon_k\phi_k$$

$V(t)$ が小さい時 摂動的に方程式を解く。

$V(t) = V(x)e^{\pm i\omega t}$ のとき

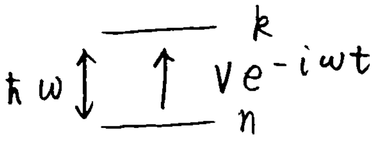
$$P_k(t) = |\langle\phi_k|\psi(t)\rangle|^2$$

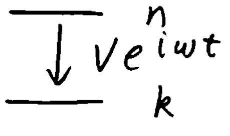
$$\xrightarrow[t\to\infty]{} \frac{2\pi}{\hbar}t\,|\langle\phi_k|V(x)|\phi_n\rangle|^2$$

$$\times\underbrace{\delta(\varepsilon_k-\varepsilon_n\pm\hbar\omega)}$$

↕

エネルギー保存則





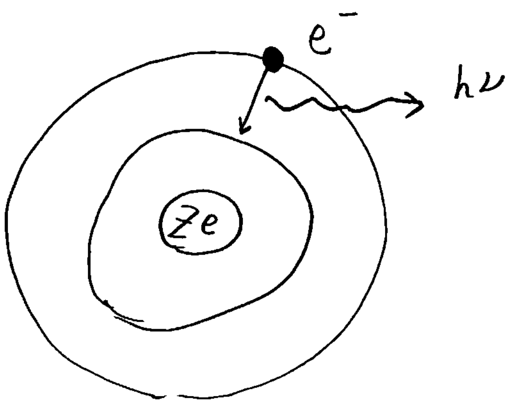
単位時間当りの遷移確率(遷移率)

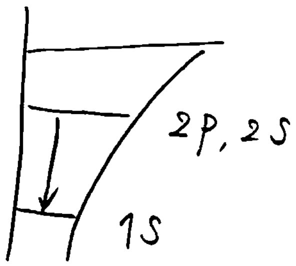
$$T_k = \frac{1}{t}P_k(t) = \frac{2\pi}{\hbar}N_{kn}|^2\delta(\varepsilon_k-\varepsilon_n\pm\hbar\omega)$$

$E=\varepsilon_k$ を持つ終状態をすべて足す

⇃ $T = \frac{2\pi}{\hbar}|V_{kn}|^2\rho(\varepsilon_n\mp\hbar\omega)$

◦ 原子と電磁場の相互作用





電磁場のハミルトニアン

$$\frac{1}{8\pi}\int d\mathbf{r}\,(\mathbb{E}^2+\mathbb{B}^2)$$

$$H=\frac{\vec{p}^{\,2}}{2m}+V(r)$$

$$\longrightarrow \frac{1}{2m}\left(\mathbb{P}+\frac{e}{c}\mathbb{A}(\mathbf{r},t)\right)^2+V(r)+\boxed{H_{em}}$$

(note)

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

"minimum principle"

$$=\frac{\mathbb{P}^2}{2m}+V(r)+H_{em}$$

$$+\frac{e}{2mc}(\mathbb{P}\cdot\mathbb{A}+\mathbb{A}\cdot\mathbb{P})+\underbrace{\frac{e^2}{2mc^2}\mathbb{A}^2}$$

$\downarrow$

$O(e^2)$ ムシ

クーロン・ゲージ $\nabla\cdot\mathbb{A}=0$ をとる。

$\downarrow$

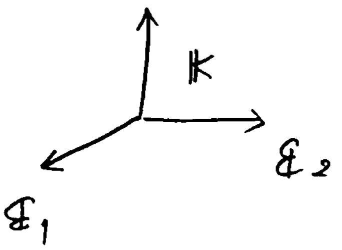
$$H=\underbrace{\frac{\mathbb{P}^2}{2m}+V(r)+H_{em}}+\underbrace{\frac{e}{mc}\mathbb{A}\cdot\mathbb{P}}$$

量子電気力学 (QED) : 第2量子化

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

$a_{\mathbf{k}\alpha}^{+}$, $a_{\mathbf{k}\alpha}$; 運動量 $\mathbf{k}$、偏極 α をもつ
フォトンの生成・消滅 演算子

$\boldsymbol{\varepsilon}_\alpha$: 偏極ベクトル （フォトンのスピンは 1）



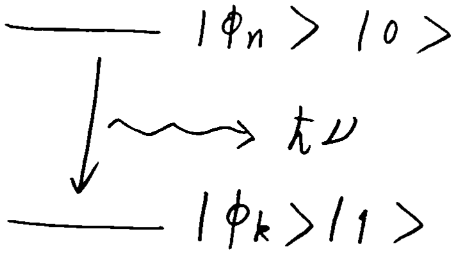
$\nabla\cdot\mathbf{A} = 0 \rightarrow \mathbf{k}\cdot\boldsymbol{\varepsilon} = 0$

$\omega_k = c\,k$

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

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

- photon emission (bound → bound)



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

$$\uparrow$$

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

終状態における状態の数 = photonの状態数

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

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

$$\downarrow$$

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

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

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

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

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

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

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

$$= \sum_{\alpha} \int d\Omega_p \ \frac{1}{2\pi} \cdot \frac{e^2}{\hbar c} \ \frac{\varepsilon_n - \varepsilon_k}{\hbar} \ \left| \frac{1}{mc} \langle \phi_k | e^{-i\mathbb{k}\cdot\mathbb{r}} \ \mathcal{E}_{\alpha} \cdot \mathbb{p} \ | \phi_n \rangle \right|^{\cdot}$$

10/20 ↑

- dipole approximation

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

$$k \ll \frac{1}{r} \qquad (長波長近似)$$

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

$$k = \frac{p}{\hbar} \sim \frac{10\,\text{eV}}{\hbar c} \sim \frac{1}{200\,\text{Å}}, \ \lambda \sim \frac{\hbar c}{10\,\text{eV}} \ \sim 200 \ \text{Å}$$

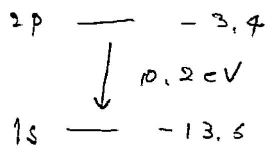
$$\left(\begin{aligned} \hbar c &\sim 200 \ \text{MeV} \cdot \text{fm} \\ &= 2000 \ \ \text{eV} \cdot \text{Å} \end{aligned} \right)$$

↓

$$\boxed{\langle \phi_k | e^{-i\mathbb{k}\cdot\mathbb{r}} \ \mathcal{E} \cdot \mathbb{p} \ | \phi_n \rangle \sim \langle \phi_k | \mathcal{E} \cdot \mathbb{p} \ | \phi_n \rangle}$$

(note) Hydrogen-like atom

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



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

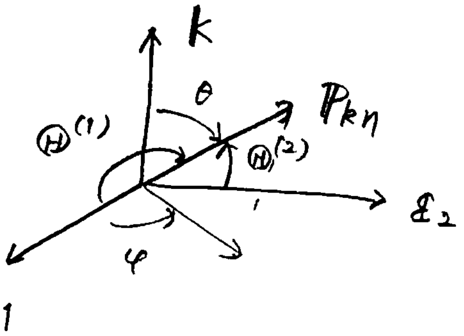
$$E_n = -\frac{1}{2} mc^2 \frac{Z^2\alpha^2}{n^2} \ \leadsto \ E_2 - E_1 = -\frac{mc^2}{2} \cdot Z^2\alpha^2 \left(\frac{1}{4} - 1\right) \simeq 10.2 \ \text{eV}$$

$$\Gamma \sim \sum_{\alpha=1,2} \int d\Omega_p \, \frac{e^2 \omega_{nk}}{2\pi m^2 \hbar c^3} \, | \langle \phi_k | \boldsymbol{\varepsilon}_\alpha \cdot \mathbb{P} | \phi_n \rangle |^2$$

$$\omega_{nk} = (\mathcal{E}_n - \mathcal{E}_k)/\hbar$$

$$= \sum_{\alpha=1,2} \int d\Omega_p \, \frac{e^2 \omega_{nk}}{2\pi m^2 \hbar c^3} \, |\langle \phi_k | \mathbb{P} | \phi_n \rangle|^2 \cos^2 \Theta^{(\alpha)}$$

$\Theta^{(\alpha)}$: angle between $\mathbb{P}_{kn}$ and $\boldsymbol{\varepsilon}_\alpha$



$$\cos \Theta^{(1)} = \sin\theta \cos\varphi$$
$$\cos \Theta^{(2)} = \sin\theta \sin\varphi$$

↓

$$\sum_{\alpha=1,2} \int d\Omega_p \cos^2 \Theta^{(\alpha)} = \int_0^\pi \sin\theta \, d\theta \int_0^{2\pi} d\varphi \, \sin^2\theta$$
$$= 2\pi \int_{-1}^{1} d(\cos\theta) \, (1 - \cos^2\theta)$$
$$= 2\pi \cdot \left[x - \frac{x^3}{3} \right]_{-1}^{1} = \frac{8\pi}{3}$$

↓

$$\boxed{\Gamma = \frac{4}{3} \cdot \frac{e^2}{\hbar c} \cdot \frac{\omega_{nk}}{m^2 c^2} \, |\langle \phi_k | \mathbb{P} | \phi_n \rangle|^2}$$

$$Y_{20} = \sqrt{\frac{5}{4\pi}} \cdot \frac{1}{2}(3\cos^2\theta - 1)$$
$$Y_{00} = \frac{1}{\sqrt{4\pi}}$$

$$|j_1 m_1\rangle |j_2 m_2\rangle = \sum_{JM} \langle j_1 m_1 j_2 m_2 | JM \rangle \times |(j_1 j_2) JM \rangle$$

- r - representation

$$[\mathbb{P}^2, \mathbb{r}] = -[\mathbb{r}, \mathbb{P}^2] = -[i\hbar \nabla_p, \mathbb{P}^2] = -2i\hbar\, \mathbb{P}.$$

↓

$$\langle \phi_k | \mathbb{P} | \phi_n \rangle = \langle \phi_k | \frac{1}{-2i\hbar} [\mathbb{P}^2, \mathbb{r}] | \phi_n \rangle$$
$$= \frac{im}{\hbar} \langle \phi_k | [H_0, \mathbb{r}] | \phi_n \rangle$$

$$H_0 = \frac{\mathbb{P}^2}{2m} + V_0(r) \qquad = \frac{im}{\hbar} \langle \phi_k | (H_0 \mathbb{r} - \mathbb{r} H_0) | \phi_n \rangle$$
$$= \frac{im}{\hbar} (\varepsilon_k - \varepsilon_n) \langle \phi_k | \mathbb{r} | \phi_n \rangle$$

E1 遷移

(note)
$$x = r\sin\theta\cos\varphi = r \cdot \frac{1}{2}\sqrt{\frac{8\pi}{3}}(-Y_{11} + Y_{1-1})$$
$$y = r\sin\theta\sin\varphi = r \cdot \frac{i}{2}\sqrt{\frac{8\pi}{3}}(Y_{11} + Y_{1-1})$$
$$z = r\cos\theta = r \cdot \sqrt{\frac{4\pi}{3}}\, Y_{10}$$

◦選択則

角度成分 $\langle Y_{l_k m_k} | Y_{1m} | Y_{l_n m_n} \rangle$

$$= \langle Y_{l_k m_k} | \left(Y_{1m} | Y_{l_n m_n} \rangle \right)$$
$$= \sqrt{\frac{3}{4\pi}} \frac{\hat{l}_n}{\hat{l}_k} \langle 1\, 0\, l_n\, 0 | l_k\, 0 \rangle \langle 1\, m\, l_n\, m_n | l_k\, \overset{m_k}{\boxed{m+m_n}} \rangle$$

(note)
$$Y_{1m}(\Omega)\, Y_{l_n m_n}(\Omega) = \sum_{L=|l_n-1|}^{l_n+1} \sqrt{\frac{3\cdot(2l_n+1)}{4\pi(2L+1)}} \langle 1\, 0\, l_n\, 0 | L\, 0 \rangle \times \langle 1\, m\, l_n\, m_n | L\;\; m+m_n \rangle \times Y_{L\, m+m_n}(\Omega)$$

$\downarrow$

$$\langle Y_{l_k m_k} | Y_{1m} | Y_{l_n m_n} \rangle$$

$$= \sum_{L=|l_n-1|}^{l_n+1} \langle 1 m\ l_n\ m_n | l_k\ m+m_n \rangle \underbrace{\int d\Omega\ Y^*_{l_k m_k}(\Omega) Y_{L\ m+m_n}}_{\delta_{L,l_k}\delta_{m_k,\ m+m_n}}$$

$$\times \frac{\sqrt{3}\ \hat{l}_n}{\sqrt{4\pi}\ \hat{L}} \langle 1 0\ l_n 0 | L 0 \rangle$$

$$\rightarrow \quad l_k = \cancel{l_n,}\ l_n \pm 1$$

$$m_k = m_n,\ m_n \pm 1$$

$$\boxed{\begin{array}{l} \text{パリティ変化: } + \\ \Delta S = 0. \end{array}}$$

$2P \rightarrow 1S$

(note)

- $\ddot{r}$ - representation

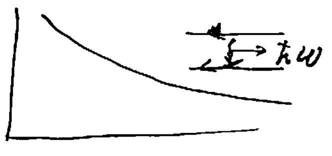
$$[H_0, \mathbb{P}] = [V_0(r), \mathbb{P}] = i\hbar\,(\nabla V_0)$$

$\downarrow$

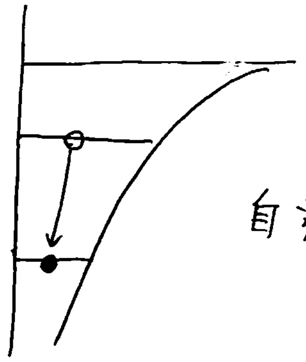
$$\langle \phi_k | \mathbb{P} | \phi_n \rangle = \frac{1}{\varepsilon_k - \varepsilon_n} \langle \phi_k | \underbrace{\varepsilon_k \mathbb{P} - \mathbb{P} \varepsilon_n}_{= [H_0, \mathbb{P}]} | \phi_n \rangle$$

$$= \frac{i\hbar}{\varepsilon_k - \varepsilon_n} \langle \phi_k | \underbrace{\nabla V_0}_{\downarrow\ -\text{加速度}/m} | \phi_n \rangle$$

→ 加速度運動する荷電粒子はフォトンを自発的に放出する（制動輻射 : bremsstrahlung）



寿命



自発的にフォトンを放出して崩壊

単位時間当りの崩壊確率：Γ

↓

Δt たった時にもとの状態にある確率：

$$1-\Delta t\cdot\Gamma \sim e^{-\Gamma\Delta t}$$

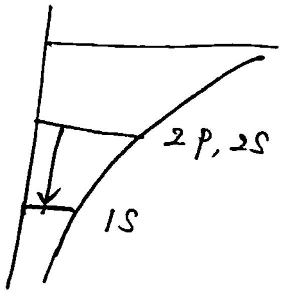
↓

これを少しずつ（Δt ずつ）続けると、

$$P(t)\sim e^{-\Gamma t}$$

↓ $t\sim\frac{1}{\Gamma}$ の時間がたつとほぼ完全に崩壊 → 状態の寿命

∘ 2p → 1s transition



$$T = \frac{4}{3}\cdot\frac{e^2}{\hbar c}\cdot\frac{\omega_{nk}^{3}}{c^2} \quad |\langle \phi_k | \mathbf{r} | \phi_n \rangle|^2 .$$

$n : 2p, \quad k : 1s$

$$\sum_{m'} T_{nlm \to n'l'm'}$$

$$= \sum_{m'} \frac{4}{3}\cdot\frac{e^2}{\hbar c}\cdot\frac{\omega_{nk}^{3}}{c^2} \quad \langle \phi_{n'l'm'} | \mathbf{r} | \phi_{nlm} \rangle \cdot \langle \phi_{nlm} | \mathbf{r} | \phi_{n'l'm',}$$

(note)
$$x = r\cdot\frac{1}{2}\sqrt{\frac{8\pi}{3}}\,(-Y_{11} + Y_{1-1})$$
$$y = r\cdot\frac{i}{2}\sqrt{\frac{8\pi}{3}}\,(Y_{11} + Y_{1-1})$$
$$z = r\cdot\sqrt{\frac{4\pi}{3}}\,Y_{10}$$

↓

$$xx + yy + zz = r^2\cdot\frac{4\pi}{3}\left\{\frac{1}{2}(-Y_{11}+Y_{1-1})^2 - \frac{1}{2}(Y_{11}+Y_{1-1})^2 + Y_{10}^2\right.$$
$$= r^2\cdot\frac{4\pi}{3}\,(-2\,Y_{11}Y_{1-1} + Y_{10}^2)$$

$$= \cancelto{m'=0}{\sum_{m'}} \frac{4}{3}\cdot\frac{e^2}{\hbar c}\cdot\frac{\omega_{nk}^{3}}{c^2}\left(\int_0^\infty r^2 dr \; r \; R_{nl}(r)\, R_{n'l'}(r)\right)^2\cdot\frac{4\pi}{3}$$

$$\times\left\{-\langle Y_{00}|Y_{11}|Y_{1m}\rangle\langle Y_{1m}|Y_{1-1}|Y_{00}\rangle \right.$$
$$-\langle Y_{00}|Y_{1-1}|Y_{1m}\rangle\langle Y_{1m}|Y_{11}|Y_{00}\rangle$$
$$\left.+\langle Y_{00}|Y_{10}|Y_{1m}\rangle\langle Y_{1m}|Y_{10}|Y_{00}\rangle\right\}$$

(note)
$$\langle Y_{00}|Y_{1k}|Y_{1m}\rangle = \int d\hat{r}\; Y_{00}^{*}\, Y_{1k}\, Y_{1m}$$
$$= \frac{1}{\sqrt{4\pi}}\int d\hat{r}\;(-)^k\, Y_{1-k}^{*}\, Y_{1m}$$
$$= \frac{1}{\sqrt{4\pi}}\cdot(-)^k\,\delta_{m,-k}$$

$$\langle Y_{1m} | Y_{1k} | Y_{00} \rangle = \int d\hat{r}\; Y_{1m}^{*}\, Y_{1k}\, Y_{00}$$

$$= \frac{1}{\sqrt{4\pi}} \int d\hat{r}\; Y_{1m}^{*}\, Y_{1k}$$

$$= \frac{1}{\sqrt{4\pi}}\, \delta_{m,k}$$

$\downarrow$

angular part $= \frac{1}{4\pi}$ for all m

$\downarrow$

$$T = \frac{4}{9} \cdot \frac{e^2}{\hbar c} \cdot \frac{\omega^3}{c^2} \left(\int_0^\infty r^3 dr\; R_{n\ell}(r)\, R_{n'\ell'}(r) \right)^2$$

(note) in general $\sum_{m'} \rightarrow \frac{1}{2J+1} \sum_{m} \sum_{m'}$

(終状態で和, 始状態で平均.

- radial integral :

$$R_{1s}(r) = 2 \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} e^{-Zr/a_0} \qquad \leftarrow \text{ch. 12}$$

$$R_{2p}(r) = \frac{1}{\sqrt{3}} \left(\frac{Z}{2a_0}\right)^{\frac{3}{2}} \frac{Zr}{a_0}\, e^{-Zr/2a_0}$$

$$a_0 = \frac{\hbar}{mc\alpha}$$

$\downarrow$

$$\int_0^\infty r^3 dr\; R_{1s}(r)\, R_{2p}(r) = \frac{1}{\sqrt{6}} \left(\frac{Z}{a_0}\right)^4 \int_0^\infty r^4 e^{-3Zr/2a_0}\, dr.$$

$$x = \frac{3Z}{2a_0}\, r$$

$$= \frac{1}{\sqrt{6}} \left(\frac{Z}{a_0}\right)^4 \left(\frac{2a_0}{3Z}\right)^5 \underbrace{\int_0^\infty x^4 e^{-x}\, dx} = \frac{24}{\sqrt{6}} \left(\frac{2}{3}\right)^5 \frac{a_0}{Z}$$

$$E_n = -\frac{1}{2} mc^2 \frac{Z^2\alpha^2}{n^2} \qquad c = 3\times 10^{10}\,\mathrm{cm/sec}$$

$$\hbar\omega = -\frac{1}{2} mc^2 Z^2\alpha^2 \cdot \left(\frac{1}{4} - 1\right) = \frac{3}{8} mc^2 \cdot Z^2\alpha^2$$

$\downarrow$

$$T = \frac{4}{9}\cdot\frac{e^2}{\hbar c}\cdot\frac{1}{c^2}\left(\frac{\frac{3}{8} mc^2\cdot Z^2\alpha^2}{\hbar}\right)^3 \cdot \frac{24^2}{6}\left(\frac{2}{3}\right)^{10}\left(\frac{a_0}{Z}\right)^2$$

$$= \frac{4}{9}\cdot\frac{\alpha}{\cancel{c^2}}\cdot\frac{3^3}{8^3}(mc^2)^{\cancel{3}} Z^6\alpha^6\cdot\frac{1}{\hbar^3}\cdot\frac{24^2}{6}\left(\frac{2}{3}\right)^{10} Z^{-2}\frac{\hbar^2}{\cancel{m^2c^2\alpha^2}}$$

$$= mc^2\cdot\alpha^5\cdot Z^4\cdot\frac{1}{\hbar}\cdot\left(\frac{4}{9}\cdot\frac{3^3}{8^3}\cdot\frac{24^2}{6}\cdot\frac{4}{9}\left(\frac{2}{3}\right)^8\right.$$

$$\frac{4\cdot 4\cdot\cancel{9}\cdot\cancel{3}\cdot\cancel{24}\cdot 24}{\cancel{9}\cdot\underset{\cancel{3}}{\cancel{9}}\cdot\cancel{8}\cdot 8\cdot 8\cdot 6} = 1$$

$$= \left(\frac{2}{3}\right)^8\cdot\frac{mc^2}{\hbar}\cdot\alpha^5\cdot Z^4$$

$$\sim 0.627\times 10^9\; Z^4 \quad \mathrm{sec}^{-1} \qquad P = 1 - Tt \sim e^{-Tt}$$

$$\tau \equiv 1/T = 1.59\,(\times 10^{-9})\cdot Z^{-4}\quad \mathrm{sec}$$ (平均寿命)

(note)

$$P(t+\Delta t) \sim P(t)\,(1 - T\Delta t)$$

$$\rightarrow \boxed{P(t) = e^{-Tt}}$$

$$\left(\frac{2}{3}\right)^8 \sim 0.039$$

$$T \sim 0.039\times\frac{0.51\ \mathrm{MeV}}{197.1\times 10^{-13}\ \mathrm{MeV\cdot cm}}\cdot\left(\frac{1}{137}\right)^5\cdot 3\times 10^{10}\,\mathrm{cm/sec} \times Z^4$$

$$\sim 6.27\times 10^8\; Z^4\ \mathrm{sec}^{-1}$$