量子力学Ⅲ

1. 時間に依存しない摂動論，角運動量の合成（復習）
2. 変分法
3. 虚時間発展法
4. 時間に依存する摂動論
   摂動による遷移
5. 衝突の理論
6. 多体論入門
   多粒子系の記述
7. 半古典論
8. 経路積分法

1. 摂動論

$$H = H_0 + \lambda V$$

$$\boxed{(H_0 + \lambda V)\psi_n = E_n \psi_n}$$ を解きたい。

suppose $\quad H_0 \phi_n = E_n^{(0)} \phi_n$

$$\psi_n = \psi_n^{(0)} + \lambda \psi_n^{(1)} + \lambda^2 \psi_n^{(2)} + \cdots$$
$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots$$

$\downarrow$

$$(H_0 + \lambda V)(\psi_n^{(0)} + \lambda \psi_n^{(1)} + \lambda^2 \psi_n^{(2)} + \cdots)$$
$$= (E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots)(\psi_n^{(0)} + \lambda \psi_n^{(1)} + \lambda^2 \psi_n^{(2)} + \cdots)$$

$O(\lambda^0)$:

$$H_0 \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)} \longrightarrow \psi_n^{(0)} = \phi_n$$

$O(\lambda^1)$:

$$H_0 \psi_n^{(1)} + V \psi_n^{(0)} = E_n^{(0)} \psi_n^{(1)} + E_n^{(1)} \psi_n^{(0)}$$

(note) $\quad \psi_n^{(1)} = \sum_m C_{nm}^{(1)} \phi_m$

$\downarrow$

$$\sum_m C_{nm}^{(1)} E_m^{(0)} \phi_m + V \phi_n = E_n^{(0)} \sum_m C_{nm}^{(1)} \phi_m + E_n^{(1)} \phi_n$$

$$\langle \phi_n | \phi_m \rangle = \delta_{n,m}$$

$\Downarrow$

$\langle \phi_n | \rightarrow$

$$\cancel{C_{nn}^{(1)} E_n^{(0)}} + \langle \phi_n | V | \phi_n \rangle = \cancel{E_n^{(0)} C_{nn}^{(1)}} + E_n^{(1)}$$

$\Downarrow$

$$\boxed{E_n^{(1)} = \langle \phi_n | V | \phi_n \rangle}$$

$\langle \phi_\ell | \rightarrow \qquad (\ell \neq n)$

$$C_{n\ell}^{(1)} E_\ell^{(0)} + \langle \phi_\ell | V | \phi_n \rangle = E_n^{(0)} C_{n\ell}^{(1)}$$

$\Downarrow$

$$\boxed{C_{n\ell}^{(1)} = \frac{\langle \phi_\ell | V | \phi_n \rangle}{E_n^{(0)} - E_\ell^{(0)}}}$$

$O(\lambda^2)$:

$$V \psi_n^{(1)} + H_0 \psi_n^{(2)} - E_n^{(0)} \psi_n^{(2)} + E_n^{(1)} \psi_n^{(1)} + E_n^{(2)} \psi_n^{(0)}$$

$\langle \phi_n | \rightarrow$

$$\boxed{E_n^{(2)} = \langle \phi_n | V | \psi_n^{(1)} \rangle = \sum_{l \neq n} \frac{\langle \phi_n | V | \phi_l \rangle \langle \phi_l | V | \phi_n \rangle}{E_n^{(0)} - E_l^{(0)}}}$$

Remarks:

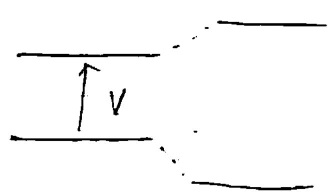
1) for $n = 0$, $E_n^{(0)} - E_l^{(0)} < 0$ for all $l \neq n$

$\Downarrow$

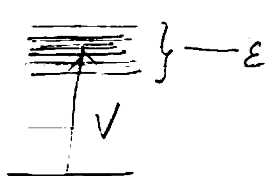
$E_n^{(2)} < 0$

2) if $\langle \phi_n | V | \phi_l \rangle \sim$ similar, the larger $E_n^{(2)}$ is for the smaller $E_n^{(0)} - E_l^{(0)}$

3) 2準位系



4) closure approximation

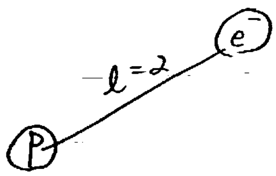


$$E_n^{(2)} \sim \sum_{l \neq n} \frac{\langle \phi_n | V | \phi_l \rangle \langle \phi_l | V | \phi_n \rangle}{E_n^{(0)} - \varepsilon}$$

$$\sim \frac{\langle \phi_n | V^2 | \phi_n \rangle}{E_n^{(0)} - \varepsilon}$$

◦ 縮退がある場合

ex. 角運動量 $l=2$



$$\psi_{nlm}(\vec{r}) = \frac{1}{r} u_{nl}(r) Y_{lm}(\hat{r})$$

$$m = -l, \cdots, l$$

$$H_0 = -\frac{\hbar^2}{2m}\nabla^2 - \frac{Ze^2}{r}$$

$$\Psi = \sum_{nl}\sum_{m} C_{nlm}\psi_{nlm}$$

$$(H_0 + \lambda V)\Psi = E\Psi$$

$$C_{nlm} E_{nl}^{(0)} + \sum_{n'l'm'} \langle \psi_{nlm} | \lambda V | \psi_{n'l'm'} \rangle C_{n'l'm'} = E C_{nlm}$$

0次: $\cancel{C_{nlm}^{(0)}} E_{nl}^{(0)} = E^{(0)} \cancel{C_{nlm}^{(0)}}$

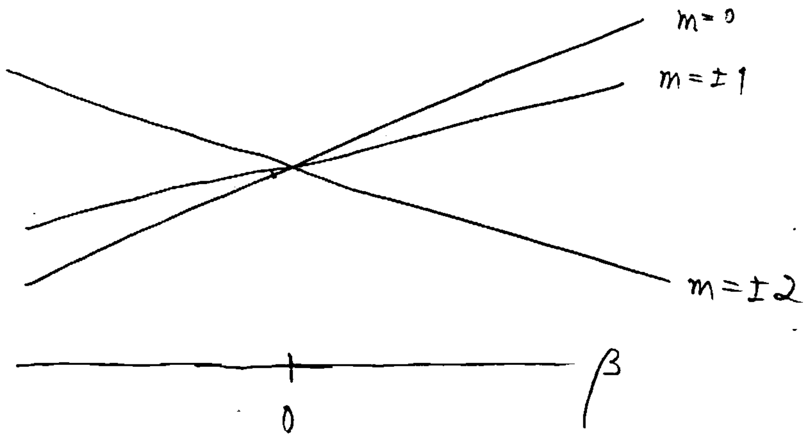
1次: $\cancel{C_{nlm}^{(1)} E_{nl}^{(0)}} + \sum_{n'l'm'} \langle \psi_{nlm} | \lambda V | \psi_{n'l'm'} \rangle C_{n'l'm'}^{(0)}$ $\delta_{nn'}$

$$= E^{(1)} C_{nlm}^{(0)} + \cancel{E^{(0)} C_{nlm}^{(1)}}$$

$$\rightarrow \boxed{\sum_{m'} \langle \psi_{nlm} | \lambda V | \psi_{nlm'} \rangle C_{nlm'}^{(0)} = E^{(1)} C_{nlm}^{(0)}}$$

縮退した状態の線形結合をとり λV を対角化

$$V = \beta \, Y_{20}(\hat{r})$$



$$\langle Y_{2m} | Y_{20} | Y_{2m} \rangle = -\frac{1}{21} \cdot (3m^2 - 6) \cdot \sqrt{\frac{5}{4\pi}}$$

$$\langle Y_{20} | Y_{20} | Y_{20} \rangle = \frac{2}{7} \sqrt{\frac{5}{4\pi}}$$

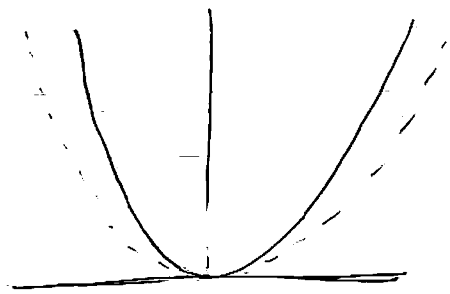
$$\langle Y_{2\pm1} | Y_{20} | Y_{2\pm1} \rangle = \frac{1}{7} \sqrt{\frac{5}{4\pi}}$$

$$\langle Y_{2\pm2} | Y_{20} | Y_{2\pm2} \rangle = -\frac{2}{7} \sqrt{\frac{5}{4\pi}}$$

(note) $\langle Y_{\ell m} | Y_{20} | Y_{\ell m'} \rangle = C_{\ell m} \, \delta_{m,m'}$

例題

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 + \beta x^4$$



$$\phi_n(x) = N\, H_n\left(\frac{x}{b}\right) e^{-\frac{x^2}{2b^2}}$$

$$b^2 = \frac{\hbar}{m\omega}$$

$$\Delta E_n = \langle n | \beta x^4 | n \rangle$$

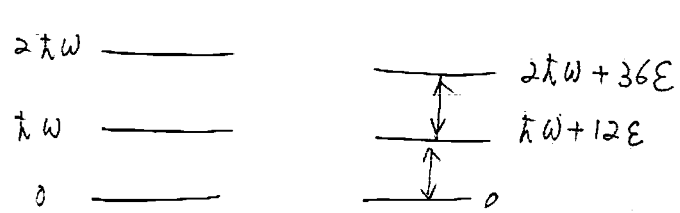
$$x = \alpha_0 (a + a^\dagger) \qquad \alpha_0 = \sqrt{\frac{\hbar}{2m\omega}}$$

$$a|n\rangle = \sqrt{n}\,|n-1\rangle$$
$$a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

$$x|n\rangle = \alpha_0 \left(\sqrt{n}\,|n-1\rangle + \sqrt{n+1}\,|n+1\rangle\right)$$
$$x^2|n\rangle = \alpha_0^2 \Big(\sqrt{n}\sqrt{n-1}\,|n-2\rangle + n|n\rangle + (n+1)|n\rangle + \sqrt{n+1}\sqrt{n+2}\,|n+2\rangle\Big)$$

$$\Downarrow \quad \langle n|x^4|n\rangle = \alpha_0^4 \left\{ n(n-1) + (2n+1)^2 + (n+1)(n+2) \right\}$$
$$= \alpha_0^4 \left(n^2 - n + 4n^2 + 4n + 1 + n^2 + 3n + 2 \right)$$
$$= \alpha_0^4 \left(6n^2 + 6n + 3 \right)$$

$$\Downarrow \quad E_n \sim n\hbar\omega + \beta \left(\frac{\hbar}{2m\omega}\right)^2 (6n^2 + 6n + 3)$$



非調和性

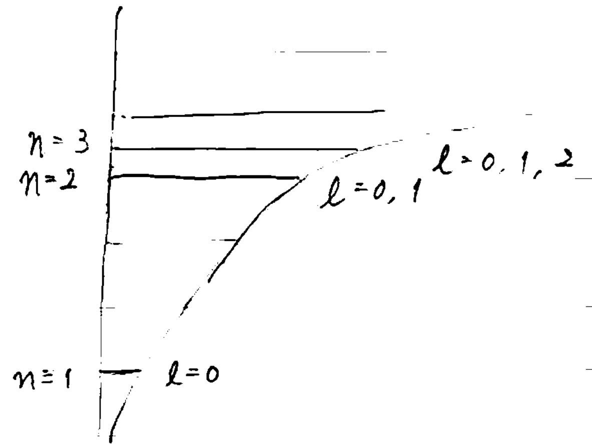
■ 水素原子に対する相対論的補正

$$H = \frac{\vec{p}^{\,2}}{2m} - \frac{Ze^2}{r}$$

$$E_n = -\frac{1}{2}\mu c^2 \frac{(Z\alpha)^2}{n^2}$$

$(n = 1, \cdots)$

$(l = 0, 1, \cdots, n-1)$



相対論：Dirac 方程式（量力 IV）

$\longrightarrow$ 非相対論近似（→シュレーディンガー方程式）

$\downarrow$

$$H = \frac{\vec{p}^{\,2}}{2m} - \frac{Ze^2}{r} \underbrace{- \frac{\vec{p}^{\,4}}{8m^3c^2} + \frac{Ze^2}{2m^2c^2}\frac{1}{r^3}\vec{S}\cdot\vec{L}}_{= \Delta H}$$

。第1項：運動エネルギーに対する相対論的補正

$$K = \sqrt{\vec{p}^{\,2}c^2 + (mc^2)^2} - mc^2 \sim \frac{p^2}{2m} - \frac{p^4}{8m^3c^2}$$

$$\Delta E_1 = \langle \phi_{nlm} | -\frac{\vec{p}^{\,4}}{8m^3c^2} | \phi_{nlm} \rangle$$

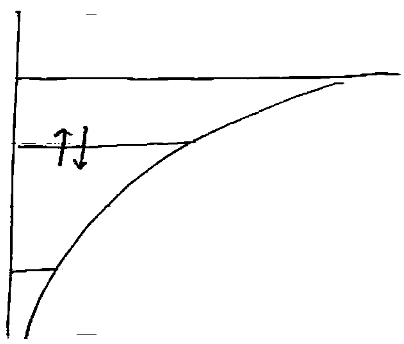
$$= \cdots = -\frac{1}{2} mc^2 (Z\alpha)^2 \left[\frac{(Z\alpha)^2}{n^3(l+\frac{1}{2})} - \frac{3(Z\alpha)^2}{4n^4} \right]$$

◦第2項：スピン-軌道力

陽子の作る電場中を電子が運動

→ 磁場が発生

→ 磁場と電子スピンの相互作用



軌道角運動量 $\vec{l}$ とスピン $\vec{s}$ の合成：

$$\vec{j} = \vec{l} + \vec{s}$$

$$j_z = l_z + s_z$$

$$j = l \pm \frac{1}{2}$$

$$\left\{ |Y_{lm_l}\rangle |\chi_{m_s}\rangle \right\} \longleftrightarrow \left\{ |j\, m_z\rangle \right\}$$

$$\rightarrow |\mathcal{Y}_{jlm}\rangle = \sum_{m_l m_s} \boxed{\langle l\, m_l\, \tfrac{1}{2}\, m_s | j\, m_z \rangle} \times Y_{lm_l}\, \chi_{m_s}$$

Clebsch-Gordan 係数

スピン波動関数

(例) $l=1 \otimes s$

$$Y_{11} \otimes \chi_\uparrow \qquad Y_{11} \otimes \chi_\downarrow$$
$$Y_{10} \otimes \chi_\uparrow \qquad Y_{10} \otimes \chi_\downarrow$$
$$Y_{1-1} \otimes \chi_\uparrow \qquad Y_{1-1} \otimes \chi_\downarrow$$

$$\Updownarrow$$

$$|\tfrac{3}{2}\ \tfrac{3}{2}\rangle\ |\tfrac{3}{2}\ \tfrac{1}{2}\rangle\ |\tfrac{3}{2}\ -\tfrac{1}{2}\rangle\ |\tfrac{3}{2}\ -\tfrac{3}{2}\rangle$$
$$|\tfrac{1}{2}\ \tfrac{1}{2}\rangle\ |\tfrac{1}{2}\ -\tfrac{1}{2}\rangle$$

(note) $\vec{j} = \vec{l} + \vec{s}$

$$\downarrow \quad \vec{j}^{\,2} = l^2 + s^2 + 2\vec{l}\cdot\vec{s}$$

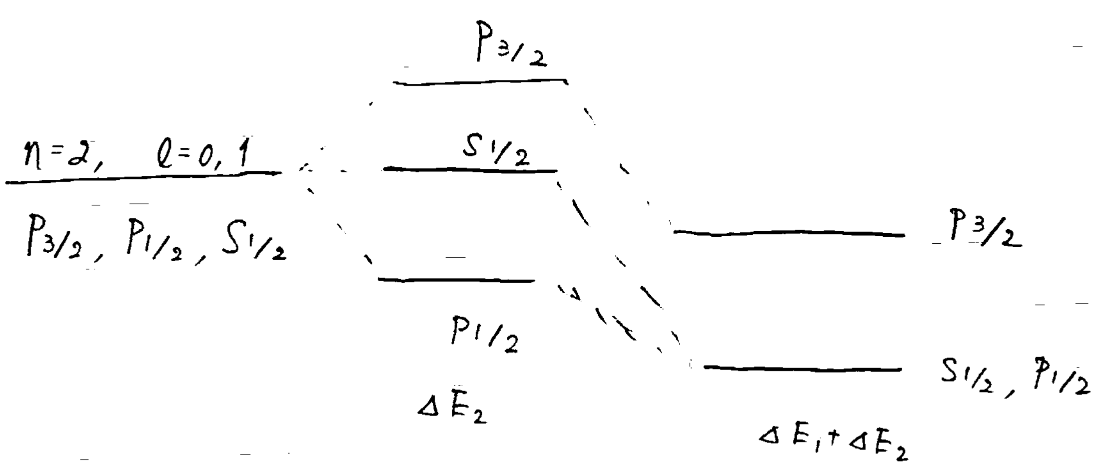
$$\therefore \quad \vec{l}\cdot\vec{s} = \frac{1}{2}\left[j(j+1) - l(l+1) - \frac{3}{4} \right]$$

$$= \begin{cases} \dfrac{l}{2} & (j = l + \frac{1}{2}) \\ -\dfrac{l+1}{2} & (j = l - \frac{1}{2}) \end{cases}$$

$$\Delta E_2 = \langle \phi_{njlm} | \frac{Ze^2}{2m^2c^2} \frac{1}{r^3} \vec{l}\cdot\vec{s} | \phi_{njlm} \rangle$$

$$= \frac{Ze^2}{2m^2c^2} \langle \phi_{njl} | \frac{1}{r^3} | \phi_{njl} \rangle \cdot \underline{\langle \mathcal{Y}_{ljm} | \vec{l}\cdot\vec{s} | \mathcal{Y}_{ljm} \rangle}$$

$$= \frac{1}{4} mc^2 (Z\alpha)^4 \frac{\left\{ \begin{matrix} l \\ -l-1 \end{matrix} \right\}}{n^3 l (l+\frac{1}{2})(l+1)}$$



$$\Delta E = \Delta E_1 + \Delta E_2$$

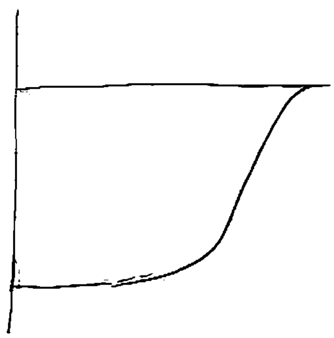
$$= -\frac{1}{2} mc^2 (Z\alpha)^4 \cdot \frac{1}{n^3} \left(\frac{1}{j+\frac{1}{2}} - \frac{3}{4n} \right)$$

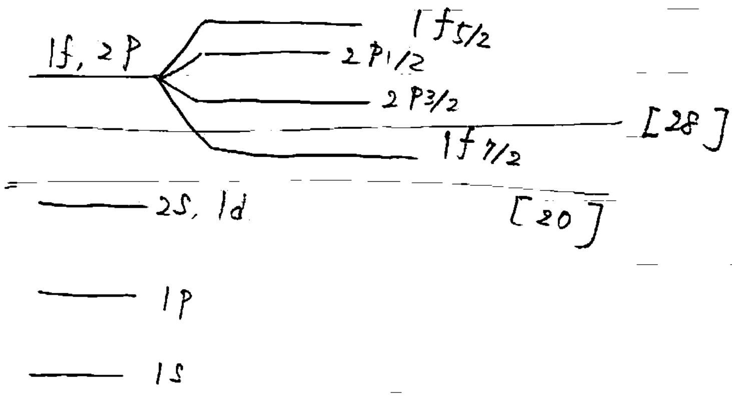
(参考) 原子核のスピン-軌道力

Nコの中性子
Zコの陽子 } 多体系

Z, N = 2, 8, 20, 28, 50, 82 の時に安定（魔法数）

└ スピン-軌道力が本質的





$\int e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}}$

$+\int e^{-\alpha x^2} x^2 dx = \sqrt{\pi}\cdot(+\frac{1}{2})\alpha^{-\frac{3}{2}}$

$e^{-\frac{x^2}{2b^2}}\cdot\left(-\frac{x}{b^2}\right)$

$-\frac{1}{b^2} e^{-\frac{x^2}{2b^2}} + \frac{x^2}{b^4} e^{-\frac{x^2}{2b^2}}$

α. 変分法 (Rayleigh - Ritzの方法)

$$E_0 \le \frac{\langle f|H|f\rangle}{\langle f|f\rangle}$$

(note) $|f\rangle = \sum_n c_n |\phi_n\rangle$

$\downarrow$

$$\text{rhs} = \frac{\sum_n c_n^2 \varepsilon_n}{\sum_n c_n^2} \ge \varepsilon_0$$

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 + \beta x^4$$

試行関数 $f(x) = (\pi b^2)^{-1/4} e^{-\frac{x^2}{2b^2}}$

$\left(\text{if } \beta = 0,\ b = \sqrt{\frac{\hbar}{m\omega}}\right)$

$\downarrow$

$$\langle f|f\rangle = \frac{1}{\sqrt{\pi b^2}}\int dx\, e^{-\frac{x^2}{b^2}} = 1$$

$$\langle f|T|f\rangle = -\frac{\hbar^2}{2m}\frac{1}{\sqrt{\pi b^2}}\int dx\left(-\frac{1}{b^2} + \frac{x^2}{b^4}\right)e^{-\frac{x^2}{b^2}}$$

$$= -\frac{\hbar^2}{2m}\frac{1}{\cancel{\sqrt{\pi b^2}}}\left(-\frac{1}{b^2}\cdot\cancel{\sqrt{\pi b^2}} + \frac{1}{b^4}\cdot\frac{\cancel{\sqrt{\pi b^2}}}{2}\cdot b^2\right)$$

$$= \frac{\hbar^2}{2m}\cdot\frac{1}{2b^2}$$

$$\langle f|\frac{1}{2}m\omega^2 x^2|f\rangle = \frac{m\omega^2}{2}\cdot\frac{1}{\cancel{\sqrt{\pi b^2}}}\cdot\frac{\cancel{\sqrt{\pi b^2}}}{2}\cdot b^2 = \frac{1}{4}m\omega^2 b^2$$

$$\int e^{-\alpha x^2} x^2 dx = \frac{\sqrt{\pi}}{2} \alpha^{-\frac{3}{2}}$$

$$\int e^{-\alpha x^2} x^4 dx = \frac{\sqrt{\pi}}{2} \cdot \frac{3}{2} \alpha^{-\frac{5}{2}}$$

$$\langle f | \beta x^4 | f \rangle = \frac{\beta}{\sqrt{\pi b^2}} \int dx \; x^4 e^{-\frac{x^2}{b^2}}$$

$$= \frac{\beta}{\sqrt{\pi b^2}} \cdot \frac{3}{4} \sqrt{\pi b^2} \cdot b^4 = \frac{3}{4} \beta b^4$$

$\downarrow$

$$\frac{\langle f | H | f \rangle}{\langle f | f \rangle} = \frac{\hbar^2}{4 m b^2} + \frac{1}{4} m \omega^2 b^2 + \frac{3}{4} \beta b^4 \equiv F(b)$$

$$F'(b) = -\frac{\hbar^2}{2 m b^3} + \frac{1}{2} m \omega^2 b + 3 \beta b^3$$

(note) if $\beta = 0$

$$F'(b) = 0 \quad \text{at} \quad b = \sqrt{\frac{\hbar}{m\omega}}$$

$$-\frac{\hbar^2}{2m} + \frac{1}{2} m \omega^2 \left(\frac{\hbar}{m\omega}\right)^2 = 0.$$

$$b = b_0 + \Delta b \qquad b_0 = \sqrt{\frac{\hbar}{m\omega}}$$

$\downarrow$

$$0 = -\frac{\hbar^2}{2m} \frac{1}{(b_0 + \Delta b)^3} + \frac{1}{2} m \omega^2 (b_0 + \Delta b) + 3 \beta (b_0 + \Delta b)^3$$

$$\sim -\frac{\hbar^2}{2m} \frac{1}{b_0^3} (\cancel{1} - \frac{3 \Delta b}{b_0}) + \frac{1}{2} m \omega^2 (\cancel{b_0} + \Delta b) + 3 \beta b_0^3$$

$$= \underbrace{\left(\frac{1}{2} m \omega^2 + \frac{3 \hbar^2}{2 m b_0^4}\right)}_{\substack{\parallel \\ \frac{1}{2} m \omega^2 + \frac{3 \hbar^2}{2m} \cdot \frac{m^2 \omega^2}{\hbar^2} \\ \parallel \\ 2 m \omega^2}} \Delta b + 3 \beta b_0^3$$

$\downarrow$

$$\boxed{\Delta b \sim -\frac{3 \beta b_0^3}{2 m \omega^2}}$$

3. 虚時間発展法

$$e^{-H\tau}|\psi\rangle \propto |\phi_0\rangle \qquad \text{as } \tau \to \infty$$

for any $|\psi\rangle$ which is not an eigen-state of H

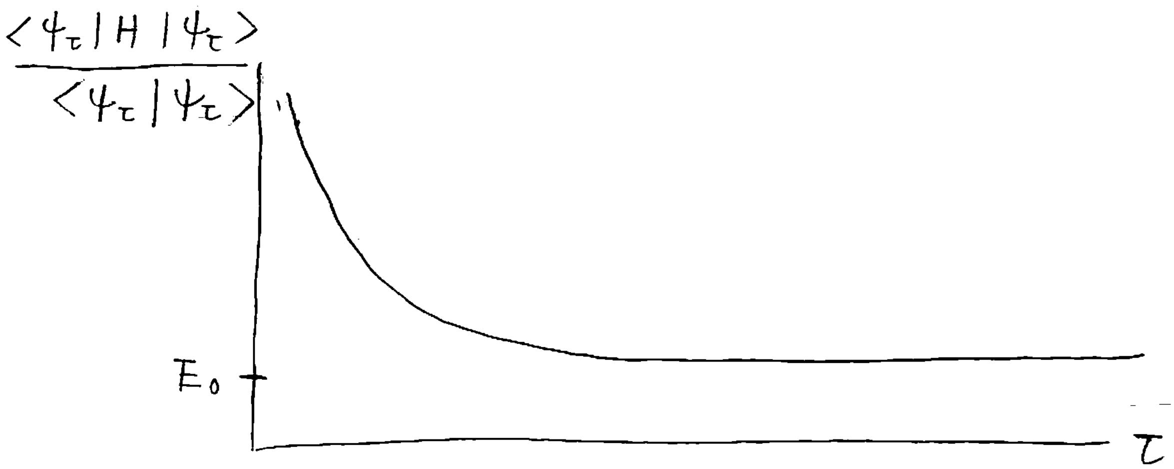
$$|\psi\rangle = \sum_n c_n |\phi_n\rangle$$

$$\downarrow$$

$$|\psi_\tau\rangle \equiv e^{-H\tau}|\psi\rangle = \sum_n c_n e^{-E_n\tau}|\phi_n\rangle$$

$$E_0 \leq 0, \quad E_n \geq 0 \quad (n \neq 0)$$

$$\rightarrow c_0 |\phi_0\rangle$$



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