(復習) $V(x) = \frac{1}{2} m\omega^2 x^2$

$$\phi(x) = f(x)\, e^{-\frac{x^2}{2b^2}} \quad ; \quad b = \sqrt{\frac{\hbar}{m\omega}}$$

$x \to \pm\infty$ での振るまい

$$\downarrow \quad \frac{d^2 f}{dy^2} - 2y\frac{df}{dy} + \left(\frac{2E}{\hbar\omega} - 1\right) f(y) = 0 \qquad \left(y = \frac{x}{b}\right)$$

$\longleftrightarrow$ エルミート多項式

$$\left(\frac{d^2}{dx^2} - 2x\frac{d}{dx} + 2n\right) H_n(x) = 0$$

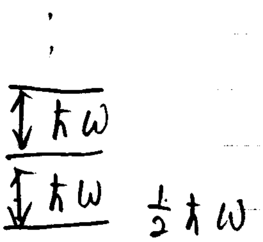
$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}$$

$$H_0(x) = 1$$
$$H_1(x) = 2x$$
$$H_2(x) = 4x^2 - 2$$
$$\vdots$$

$$\int_{-\infty}^{\infty} dx\, H_n(x) H_{n'}(x)\, e^{-x^2} = \sqrt{\pi}\, 2^n n!\, \delta_{n,n'}$$

$$\downarrow \quad f(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n\left(\frac{x}{b}\right)$$

$$\frac{2E}{\hbar\omega} - 1 = 2n \longrightarrow E = \left(n + \frac{1}{2}\right)\hbar\omega$$



← ゼロ点振動

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別解： $f(y)=\sum_{n=0}^{\infty} C_n y^n$ と展開する。

$$\downarrow$$

$$\underbrace{\sum_{n=0}^{\infty} n(n-1)C_n y^{n-2}} - 2\sum_{n=0}^{\infty} n C_n y^n + \left(\frac{2E}{\hbar\omega}-1\right)\sum_n C_n y^n = 0$$

$$\| $$

$$2C_2 + 6C_3 y + 12 C_4 y^2 + \cdots$$

$$\|$$

$$\sum_{n=0}^{\infty} (n+2)(n+1) C_{n+2} y^n$$

$$\rightarrow \sum_{n=0}^{\infty}\left[(n+2)(n+1)C_{n+2} - \left(2n - \left(\frac{2E}{\hbar\omega}-1\right)\right)C_n\right] y^n = 0$$

$$\Downarrow \quad \frac{C_{n+2}}{C_n} = \frac{2n-\left(\frac{2E}{\hbar\omega}-1\right)}{(n+2)(n+1)} \sim \frac{2}{n} \quad (n が大きいとき)$$

(note) $C_{2n+2} \sim \frac{1}{n} C_{2n} \sim \frac{1}{n(n-1)} C_{2n-2} \sim \frac{1}{n!}$

$$\Downarrow \quad f(y) = \sum_{n'=0}^{\infty} C_{2n'} y^{2n'} \sim \sum_{n'} \frac{y^{2n'}}{(n'-1)!} = \sum_{n'} n' \frac{y^{2n'}}{n'!} > e^{y^2}$$

$$\phi(x) = e^{-\frac{y^2}{2}} f(y) > e^{-\frac{y^2}{2}} e^{y^2} = e^{\frac{y^2}{2}}$$

(発散)

- 発散が起きないためには

どこかの n で $2n = \frac{2E}{\hbar\omega} - 1 \rightarrow C_{n+2} = 0$ 及び
$C_k = 0 \quad (k > n+2)$

y^n の和は途中で止まり波動関数が発散しない。

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$$\int_{-\infty}^{\infty} dx\, e^{-\alpha x^2} = \sqrt{\frac{\pi}{\alpha}}$$

$$\int_{-\infty}^{\infty} dx\, x^2 e^{-\alpha x^2} = \frac{1}{2\alpha}\sqrt{\frac{\pi}{\alpha}}$$

Ⅳ ビリアル定理

$$\phi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$$

$$\phi_0'(x) = -\frac{m\omega}{\hbar}x\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$$

↓

$$\left\langle \frac{1}{2}m\omega^2 x^2 \right\rangle = \frac{m\omega^2}{2}\sqrt{\frac{m\omega}{\pi\hbar}}\int_{-\infty}^{\infty} dx\, x^2 e^{-\frac{m\omega}{2\hbar}x^2}$$

$$= \frac{m\omega^2}{2}\cancel{\sqrt{\frac{m\omega}{\pi\hbar}}}\,\frac{\hbar}{2m\omega}\cancel{\sqrt{\frac{\pi\hbar}{m\omega}}} = \frac{1}{4}\hbar\omega$$

$$\left\langle \frac{p^2}{2m} \right\rangle = \frac{\hbar^2}{2m}\int_{-\infty}^{\infty} dx\, [\phi_0'(x)]^2$$

$$= \frac{\hbar^2}{2m}\left(\frac{m\omega}{\hbar}\right)^2\sqrt{\frac{m\omega}{\pi\hbar}}\int_{-\infty}^{\infty} x^2 e^{-\frac{m\omega}{\hbar}x^2} = \frac{1}{4}\hbar\omega$$

↓

$$\langle T \rangle = \langle V \rangle = \frac{1}{4}\hbar\omega$$

一般には $\langle T \rangle = \frac{1}{2}\left\langle x\frac{dV}{dx}\right\rangle$

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3.9. 調和振動子ポテンシャル：代数学的解法

$$a^{\dagger} = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} - i\frac{\hat{p}}{\sqrt{2m\omega\hbar}}$$

$$\rightarrow \quad a = (a^{\dagger})^{\dagger} = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} + i\frac{\hat{p}}{\sqrt{2m\omega\hbar}}$$

(note) $$[a, a^{\dagger}] = \sqrt{\frac{m\omega}{2\hbar}}\cdot\left(\frac{-i}{\sqrt{2m\omega\hbar}}\right)[x, p] + \frac{i}{\sqrt{2m\omega\hbar}}\cdot\sqrt{\frac{m\omega}{2\hbar}}\,[p, x]$$

$$= -\frac{i}{\hbar}[x, p] = 1.$$

$\downarrow$

$$[a, (a^{\dagger})^{n}] = n(a^{\dagger})^{n-1}$$

- $[a, a^{\dagger}] = 1$
- $[a, (a^{\dagger})^{n}] = n(a^{\dagger})^{n-1}$ とすると

$$[a, (a^{\dagger})^{n+1}] = (a^{\dagger})^{n}[a, a^{\dagger}] + [a, (a^{\dagger})^{n}]a^{\dagger}$$

$$= (a^{\dagger})^{n} + n(a^{\dagger})^{n} = (n+1)(a^{\dagger})^{n}$$

任意の関数 $f(a^{\dagger})$ に対して

$$f(a^{\dagger}) = \sum_{n=0}^{\infty}\frac{1}{n!}f^{(n)}(0)(a^{\dagger})^{n}$$

$$\rightarrow \quad [a, f(a^{\dagger})] = \sum_{n=0}^{\infty}\frac{1}{n!}f^{(n)}(0)\cdot n(a^{\dagger})^{n-1}$$

$$= f'(a^{\dagger})$$

すなわち $a = \frac{d}{da^{\dagger}}$ としてよい。

同様に $a^{\dagger} = -\frac{d}{da}$; : $[a^{\dagger}, g(a)] = -g'(a)$

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$$a + a^\dagger = 2 \cdot \sqrt{\frac{m\omega}{2\hbar}}\, \hat{x} \quad \rightarrow \quad \hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\, (a + a^\dagger)$$

$$a^\dagger - a = -2 \cdot \frac{i}{\sqrt{2m\omega\hbar}}\, \hat{p} \quad \rightarrow \quad \hat{p} = i \sqrt{\frac{m\omega\hbar}{2}}\, (a^\dagger - a)$$

$\downarrow$

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}^2$$

$$= -\frac{1}{\cancel{2m}} \cdot \frac{\cancel{m}\omega\hbar}{2} (a^\dagger - a)^2 + \frac{1}{\cancel{2}} \cancel{m}\omega^2 \cdot \frac{\hbar}{\cancel{2m\omega}} (a + a^\dagger)^2$$

$$= \frac{\hbar\omega}{4} \Big(\cancel{-a^\dagger a^\dagger} + a^\dagger a + a a^\dagger \cancel{- a a}$$
$$+ \cancel{a^\dagger a^\dagger} + a^\dagger a + a a^\dagger \cancel{+ a a} \Big) = \frac{\hbar\omega}{2} (a a^\dagger + a^\dagger a)$$

$$= \hbar\omega \left(a^\dagger a + \frac{1}{2} \right)$$

(note) $[H, a] = [\hbar\omega a^\dagger, a]\, a = -\hbar\omega a$

$[H, a^\dagger] = a^\dagger [\hbar\omega a, a^\dagger] = \hbar\omega a^\dagger$

$\downarrow$

$H|\varphi\rangle = E|\varphi\rangle$ とすると

$$H(a|\varphi\rangle) = (-\hbar\omega a + a H)|\varphi\rangle$$
$$= (E - \hbar\omega)\, (\underline{a|\varphi\rangle})$$

$$H(a^\dagger|\varphi\rangle) = (\hbar\omega a^\dagger + a^\dagger H)|\varphi\rangle$$
$$= (E + \hbar\omega)\, (\underline{a^\dagger|\varphi\rangle})$$

固有状態

$E+\hbar\omega$
$\uparrow a^\dagger$
E
$\downarrow a$
$E-\hbar\omega$

基底状態（最低エネルギー状態）：$a|0\rangle = 0$

$$\rightarrow \quad H|0\rangle = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)|0\rangle = \underbrace{\frac{1}{2}\hbar\omega}_{\text{固有値}}|0\rangle$$

$a|0\rangle = 0$

$$\rightarrow \quad 0 = \langle x|a|0\rangle = \langle x|\sqrt{\frac{m\omega}{2\hbar}}\hat{x} + i\frac{1}{\sqrt{2m\omega\hbar}}\hat{p}|0\rangle$$

$$= \left(\sqrt{\frac{m\omega}{2\hbar}}\,x + i\frac{1}{\sqrt{2m\omega\hbar}}\cdot\frac{\hbar}{i}\frac{d}{dx}\right)\underbrace{\langle x|0\rangle}_{\phi_0(x)}$$

$$\rightarrow \quad \phi_0'(x) = -\sqrt{\frac{2m\omega}{\hbar}}\cdot\sqrt{\frac{m\omega}{2\hbar}}\,x\,\phi_0(x)$$

$$= -\frac{m\omega}{\hbar}\,x\,\phi_0(x)$$

$$\rightarrow \quad \phi_0(x) \propto e^{-\frac{m\omega}{2\hbar}x^2}$$

励起状態：$|n\rangle = A\cdot(a^\dagger)^n|0\rangle$

規格化：

$$1 = \langle n|n\rangle = A^2\langle 0|a^n(a^\dagger)^n|0\rangle$$

$$a(a^\dagger)^n|0\rangle = \left((a^\dagger)^n a + n(a^\dagger)^{n-1}\right)|0\rangle = n(a^\dagger)^{n-1}|0\rangle$$

$$\Downarrow$$

$$a^2(a^\dagger)^n|0\rangle = n\,a(a^\dagger)^{n-1}|0\rangle = n(n-1)(a^\dagger)^{n-2}|0\rangle$$

$\rightarrow$ これをくり返すと $\quad a^n(a^\dagger)^n|0\rangle = n!\,|0\rangle$

$$\Downarrow$$

$$1 = A^2\cdot n! \quad \Downarrow \quad A = \frac{1}{\sqrt{n!}}$$

すなわち $|n\rangle = \frac{1}{\sqrt{n!}} (a^\dagger)^n |0\rangle$

$$\rightarrow \quad a|n\rangle = \frac{1}{\sqrt{n!}} \left[\cancel{(a^\dagger)^n a} + n (a^\dagger)^{n-1} \right] |0\rangle$$

$$= \sqrt{n} \frac{1}{\sqrt{(n-1)!}} (a^\dagger)^{n-1} |0\rangle = \sqrt{n}\, |n-1\rangle$$

$$a^\dagger |n\rangle = \sqrt{n+1} \cdot \frac{(a^\dagger)^{n+1}}{\sqrt{(n+1)!}} |0\rangle = \sqrt{n+1}\, |n+1\rangle$$

(note) $n=0$ のとき $a|0\rangle = 0$, $a^\dagger |0\rangle = |1\rangle$

(note) $\hat{n} = a^\dagger a$

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

note) $\frac{1}{2} m\omega^2 x^2 = \frac{m\omega^2}{2} \cdot \frac{\hbar}{2m\omega} \left(a^{\dagger 2} + a^2 + \underbrace{a a^\dagger}_{= a^\dagger a + 1} + a^\dagger a \right)$

$$\langle n|(a^\dagger)^2|n\rangle \propto \langle n|n+2\rangle = 0$$
$$\langle n|a^2|n\rangle \propto \langle n|n-2\rangle = 0$$

$$\downarrow$$

$$\langle n| \frac{1}{2} m\omega^2 x^2 |n\rangle = \frac{\hbar\omega}{4} \cdot (2n+1) = \frac{1}{2} \cdot \underbrace{\hbar\omega \left(n + \frac{1}{2}\right)}_{= E_n}$$

$$\downarrow$$

$$\langle n| \frac{1}{2} m\omega^2 x^2 |n\rangle = \langle n| \frac{p^2}{2m} |n\rangle = \frac{1}{2} E_n.$$

(ビリアル定理)

(補足)

$$\langle x|\hat{p}|\phi\rangle = \int dx' \, \underline{\langle x|\hat{p}|x'\rangle} \underbrace{\langle x'|\phi\rangle}_{=\phi(x')}$$

(note) $[\hat{x}, \hat{p}] = i\hbar$

$$\rightarrow \langle x|\hat{x}\hat{p} - \hat{p}\hat{x}|x'\rangle = i\hbar \langle x|x'\rangle = i\hbar\,\delta(x-x')$$

$$= (x-x')\langle x|\hat{p}|x'\rangle$$

(note) $(x-x')\frac{d}{dx}\delta(x-x') = -\delta(x-x')$

(証明) $-\int dx\,\delta(x-x')f(x) = -f(x')$

$$\int dx\,(x-x')\frac{d}{dx}\delta(x-x')\cdot f(x)$$

$$= -\int dx \frac{d}{dx}\big((x-x')f(x)\big)\delta(x-x')$$

$$= -\int dx\,\big(f(x) + (x-x')f'(x)\big)\delta(x-x')$$

$$= -f(x')$$

$$\sim \langle x|\hat{p}|x'\rangle = -i\hbar\frac{d}{dx}\delta(x-x') = \frac{\hbar}{i}\frac{d}{dx}\delta(x-x')$$

$$\sim \boxed{\langle x|\hat{p}|\phi\rangle = \int dx' \frac{\hbar}{i}\frac{d}{dx}\delta(x-x')\phi(x') = \frac{\hbar}{i}\frac{d}{dx}\phi(x)}$$

(note) 超対称性量子力学

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right)\varphi_0(x)=0$$

（エネルギーのスケールは適当にとる）

$$\rightarrow \quad V\varphi_0 = \frac{\hbar^2}{2m}\varphi_0''$$

$$\therefore \quad H=\frac{\hbar^2}{2m}\left(-\frac{d^2}{dx^2}+\frac{\varphi_0''}{\varphi_0}\right)$$

$$A^\dagger = \frac{\hbar}{\sqrt{2m}}\left(-\frac{d}{dx}-\frac{\varphi_0'}{\varphi_0}\right), \quad A=\frac{\hbar}{\sqrt{2m}}\left(\frac{d}{dx}-\frac{\varphi_0'}{\varphi_0}\right)$$

とすると

$$A\varphi_0 = \frac{\hbar}{\sqrt{2m}}\left(\varphi_0' - \frac{\varphi_0'}{\varphi_0}\varphi_0\right)=0$$

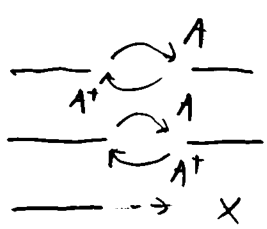
$$A^\dagger A = \frac{\hbar^2}{2m}\left(-\frac{d^2}{dx^2} + \underbrace{\left(\frac{\varphi_0'}{\varphi_0}\right)'}_{=\frac{\varphi_0\varphi_0''-\cancel{\varphi_0'^2}}{\varphi_0^2}} + \cancel{\frac{\varphi_0'}{\varphi_0}\frac{d}{dx}} - \cancel{\frac{\varphi_0'}{\varphi_0}\frac{d}{dx}} \cancel{+\left(\frac{\varphi_0'}{\varphi_0}\right)^2}\right)$$

$$= H.$$

$$\tilde{H} = AA^\dagger$$

もし $H\varphi_n = A^\dagger A\varphi_n = E_n\varphi_n$ なら

$$\tilde{H}(A\varphi_n) = A\underline{A^\dagger A}\varphi_n = E_n(A\varphi_n)$$



H $\quad\quad$ $\tilde{H}$