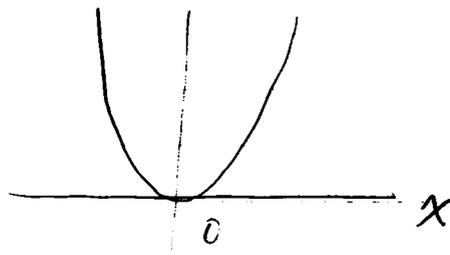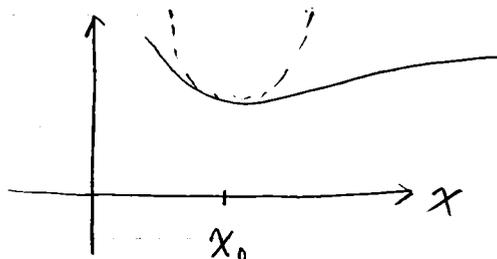## 3.8. 調和振動子ポテンシャル

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

(note)

$$V(x) \sim V(x_0) + \frac{1}{2} V''(x_0)(x-x_0)^2 + \cdots$$

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 \right) \phi(x) = E \phi(x)$$

・$x \to \pm\infty$ での解の様子：

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 \right) \phi(x) \sim 0$$

解： $\phi(x) \sim e^{-\frac{m\omega}{2\hbar} x^2}$

$$\phi'(x) = -\frac{m\omega}{\hbar} x \, e^{-\frac{m\omega}{2\hbar} x^2}$$

$$\phi''(x) = -\frac{m\omega}{\hbar} e^{-\frac{m\omega}{2\hbar} x^2} + \left(\frac{m\omega}{\hbar}\right)^2 x^2 e^{-\frac{m\omega}{2\hbar} x^2}$$

$$\sim \left(\frac{m\omega}{\hbar}\right)^2 x^2 e^{-\frac{m\omega}{2\hbar} x^2}$$

⇩ $\phi(x) = f(x) \, e^{-\frac{m\omega}{2\hbar} x^2}$ とおいて f について解く.

$$\to \quad -\frac{\hbar^2}{2m} f'' + \hbar\omega \, x f' = \left(E - \frac{\hbar\omega}{2} \right) f$$

$$\text{or} \quad y = \sqrt{\frac{m\omega}{\hbar}}\, x$$

$$\to \quad f'' - 2y f' + \left(\frac{2E}{\hbar\omega} - 1\right) f(y) = 0$$

(note) エルミート多項式

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

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

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

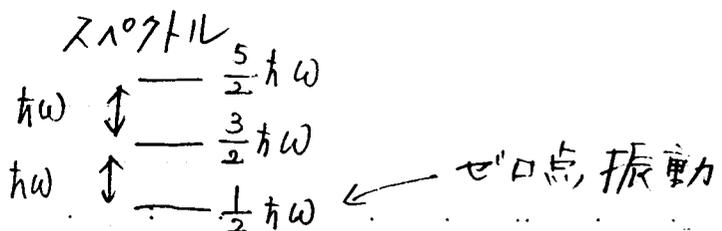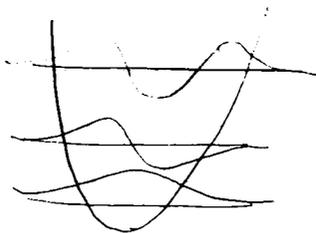$$H_0(x) = 1$$
$$H_1(x) = 2x$$
$$H_2(x) = 4x^2 - 2$$
$$\vdots$$

$$\Downarrow \quad f(y) = H_n(y) \quad ; \quad \frac{2E}{\hbar\omega} - 1 = 2n$$

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

規格化まで含めると

$$\phi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}\, x\right) e^{-\frac{m\omega}{2\hbar} x^2}$$

スペクトル

$$\hbar\omega \updownarrow \quad \underline{\quad} \frac{5}{2}\hbar\omega$$
$$\underline{\quad} \frac{3}{2}\hbar\omega$$
$$\hbar\omega \updownarrow \quad \underline{\quad} \frac{1}{2}\hbar\omega \leftarrow ゼロ点振動$$

3.9. 調和振動子ポテンシャル : 代数学的解法

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

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

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

$$+ \frac{i}{\sqrt{2m\omega\hbar}} \cdot \sqrt{\frac{m\omega}{2\hbar}} \, [p, x]$$

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

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

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

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

$$= (a^+)^n + n(a^+)^n = (n+1)(a^+)^n$$

任意の関数 $f(a^+)$ に対して

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

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

$$= f'(a^+)$$

すなわち $a = \dfrac{d}{da^+}$ としてよい

同様に $a^+ = -\dfrac{d}{da}$ ∴ $[a^+, g(a)] = -g'(a)$

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

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

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

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

$$= \frac{\hbar\omega}{4} \left(-a^\dagger a^\dagger + a^\dagger a + a a^\dagger - aa \right.$$
$$\left. + a^\dagger a^\dagger + a^\dagger a + a a^\dagger + aa \right) = \frac{\hbar\omega}{2} (a a^\dagger + a^\dagger a)$$

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

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

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

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

$$H(a|\varphi\rangle) = (-\hbar\omega a + aH) |\varphi\rangle$$
$$= (E - \hbar\omega)(a|\varphi\rangle)$$
$$H(a^\dagger |\varphi\rangle) = (\hbar\omega a^\dagger + a^\dagger H) |\varphi\rangle$$
$$= (E + \hbar\omega)(a^\dagger |\varphi\rangle)$$

$$固有状態$$

$$\begin{array}{ll} \uparrow a^\dagger & E + \hbar\omega \\ \overline{} & E \cdots \\ \downarrow a & E - \hbar\omega \end{array}$$

基底状態（最低エネルギー状態）： $a|0\rangle = 0$

$\rightarrow$ $H|0\rangle = \hbar\omega(a^\dagger a + \frac{1}{2})|0\rangle = \underline{\frac{1}{2}\hbar\omega}|0\rangle$

固有値

$a|0\rangle = 0$

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

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

$\overset{\parallel}{\phi_0(x)}$

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

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

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

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

規格化：

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

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

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

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

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

すなわち

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

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

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

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

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

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

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

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

(ビリアル定理)