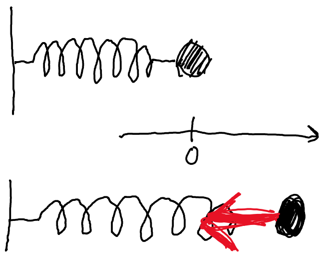
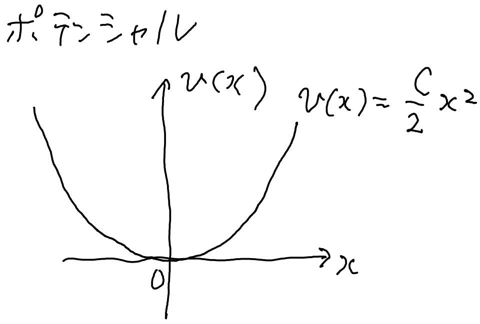
2. 調和振動子（フォノン）

※いったん電子系から離れる

2.1 一次元、単一調和振動子



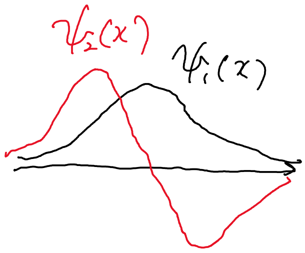
復元力：$F = -Cx$
最低次の展開



Schrödinger方程式

$$\left(-\frac{1}{2M}\frac{\partial^2}{\partial x^2} + \frac{C}{2}x^2\right)\psi(x) = E\,\psi(x)$$

↳ この解は Hermite 多項式になるが
ここでは別の解き方をする。



2.2 演算子の交換関係を使う方法

$$\hat{H}|\psi\rangle = E|\psi\rangle \qquad \hat{H} \equiv \left(\frac{\hat{p}^2}{2M} + \frac{C}{2}\hat{x}^2\right)$$

交換関係 $[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x} = i$

$\hat{H} = A\,\hat{b}^\dagger\hat{b} + B$ の形にしたい（対角化）
↳ $[\hat{b}, \hat{b}^\dagger] = 1$ を満たす演算子

二次形式（p, x の二次）→ 二次形式（b, b† の二次）なので、
線形変換で出来る

$$\left.\begin{aligned}\hat{x} &= a_1\hat{b} + a_1^*\hat{b}^\dagger \\ \hat{p} &= a_2\hat{b} + a_2^*\hat{b}^\dagger\end{aligned}\right\} \hat{x}, \hat{p}\text{ は Hermite }(\hat{x}^\dagger = \hat{x})\text{ なので。}$$

$[b, b] = [b^\dagger, b^\dagger] = 0$

$$\underset{i}{\underset{\parallel}{[\hat{x}, \hat{p}]}} = [a_1\hat{b} + a_1^*\hat{b}^\dagger, a_2\hat{b} + a_2^*\hat{b}^\dagger] = a_1a_2^*[b, \hat{b}^\dagger] + a_1^*a_2[\hat{b}^\dagger, b]$$

$$= a_1a_2^* - a_1^*a_2 = i$$

$$\mathcal{H} = \frac{\hat{p}^2}{2M} + \frac{C}{2}\hat{x}^2 = \frac{1}{2}\left\{\frac{(a_2b + a_2^*b^\dagger)^2}{M} + C(a_1b + a_1^*b^\dagger)^2\right\}$$

$$= \frac{1}{2}\left\{\hat{b}^2\underset{0}{\underset{\parallel}{\left(\frac{a_2^2}{M} + Ca_1^2\right)}} + \hat{b}^{\dagger 2}\left(\frac{a_2^{*2}}{M} + Ca_1^{*2}\right) + \left(\frac{|a_2|^2}{M} + C|a_1|^2\right)(bb^\dagger + b^\dagger b)\right\}$$

になって欲しい $\Longrightarrow |a_2| = i\sqrt{CM}|a_1|$

$a_2 = -ia_1\sqrt{CM}$

$$2i\sqrt{CM}|a_1|^2 = i$$

$$|a_1|^2 = \frac{1}{2\sqrt{CM}} \qquad |a_2|^2 = \frac{\sqrt{CM}}{2}$$

$$a_1 = \frac{(CM)^{-1/4}}{\sqrt{2}} \qquad a_2 = \frac{-i(CM)^{1/4}}{\sqrt{2}}$$

$$\boxed{\hat{\mathcal{H}} = \frac{1}{2}\sqrt{\frac{C}{M}}(bb^\dagger + b^\dagger b) \overset{bb^\dagger - b^\dagger b = 1}{=} \omega\left(b^\dagger b + \frac{1}{2}\right)} \qquad \omega \equiv \sqrt{\frac{C}{M}}$$

・なぜこの形が良いのか?

固有状態 $|0\rangle, |1\rangle, |2\rangle, \cdots |n\rangle, \cdots$

$|1\rangle = b^\dagger|0\rangle$, $|2\rangle = b^{\dagger 2}|0\rangle, \cdots \sim (b^\dagger)^n|0\rangle, \cdots$

$b|0\rangle = 0$ (真空状態)

$\mathcal{H}|0\rangle = \omega(b^\dagger b + \frac{1}{2})|0\rangle = \frac{\omega}{2}|0\rangle \Longrightarrow$ 固有エネルギー $E_0 = \frac{\omega}{2}$

$$\mathcal{H}|n\rangle = \omega\left(b^\dagger b + \frac{1}{2}\right)|n\rangle = \omega b^\dagger b(b^\dagger)^n|0\rangle + \frac{\omega}{2}(b^\dagger)^n|0\rangle$$

$$b^\dagger b(b^\dagger)^n = b^\dagger(bb^\dagger)(b^\dagger)^{n-1} = (b^\dagger)^n + (b^\dagger)^2 b(b^\dagger)^{n-1} = 2(b^\dagger)^n + (b^\dagger)^3 b(b^\dagger)^{n-2}$$

$bb^\dagger = 1 + b^\dagger b$

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

$$H|n\rangle = \left(n+\frac{1}{2}\right)\omega(b^\dagger)^n|0\rangle + \omega(b^\dagger)^{n+1}\underbrace{b|0\rangle}_{=0}$$

$$= \left(n+\frac{1}{2}\right)\omega|n\rangle$$

固有値 $E_n = \left(n+\frac{1}{2}\right)\omega$

・規格化

$$\langle n|n\rangle = \langle 0|\, b^n (b^\dagger)^n|0\rangle = \langle 0|b^{n-1}\{n(b^\dagger)^{n-1} + (b^\dagger)^n b\}|0\rangle$$

$$= n\langle 0|b^{n-1}(b^\dagger)^{n-1}|0\rangle = \cdots = n!\langle 0|0\rangle$$

$|0\rangle$ が規格化されているならば $|n\rangle = \dfrac{(b^\dagger)^n}{\sqrt{n}}|0\rangle$ とすれば規格子

・直交性

$\langle n|m\rangle \quad (n > m)$

$$= \langle 0|\, b^n (b^\dagger)^m|0\rangle = \langle 0|b^{n-m}\, b^m (b^\dagger)^m|0\rangle$$

$$= m!\langle 0|b^{n-m}|0\rangle = 0$$

$n < m$ に関しては $\langle m|n\rangle^* = \langle n|m\rangle$ を考えれば良い

$$\boxed{\langle n|m\rangle = \delta_{nm}\, n!}$$

・いろいろな期待値

平均位置

$$\langle n|\hat{x}|n\rangle = \frac{1}{n!}\langle 0|b^n \frac{(CM)^{-1/4}}{\sqrt{2}}(b+b^\dagger)(b^\dagger)^n|0\rangle$$

$$= \frac{1}{n!}\frac{(CM)^{-1/4}}{\sqrt{2}}\left\{\langle 0|b^{n+1}(b^\dagger)^n|0\rangle + \langle 0|b^n(b^\dagger)^{n+1}|0\rangle\right\} = 0$$

原点から対称に振動するので

平均二乗変位

$$\langle n|(\hat{x}-\langle x\rangle)^2|n\rangle = \langle n|\hat{x}^2|n\rangle = \frac{1}{n!}\frac{(CM)^{-1/2}}{2}\langle 0|b^n(b+b^\dagger)^2 b^{\dagger n}|0\rangle$$

$$= \frac{1}{n!}\frac{(CM)^{-1/2}}{2}\Big(\underbrace{\langle 0|b^n b b^\dagger b^{\dagger n}|0\rangle}_{(n+1)!} + \langle 0|b^n \underbrace{b^\dagger b}_{bb^\dagger - 1} b^{\dagger n}|0\rangle\Big)$$

$$= \frac{1}{n!}\frac{(CM)^{-1/2}}{2}\left\{2(n+1)! - n!\right\} = \frac{(CM)^{-1/2}}{2}(2n+2-1) = (CM)^{-1/2}\left(n+\frac{1}{2}\right)$$

2.3 3次元単一調和振動子

$$\mathcal{H} = \frac{1}{2M}(\hat{P}_x^2 + \hat{P}_y^2 + \hat{P}_z^2) + \frac{C_x}{2}\hat{x}^2 + \frac{C_y}{2}\hat{y}^2 + \frac{C_z}{2}\hat{z}^2$$

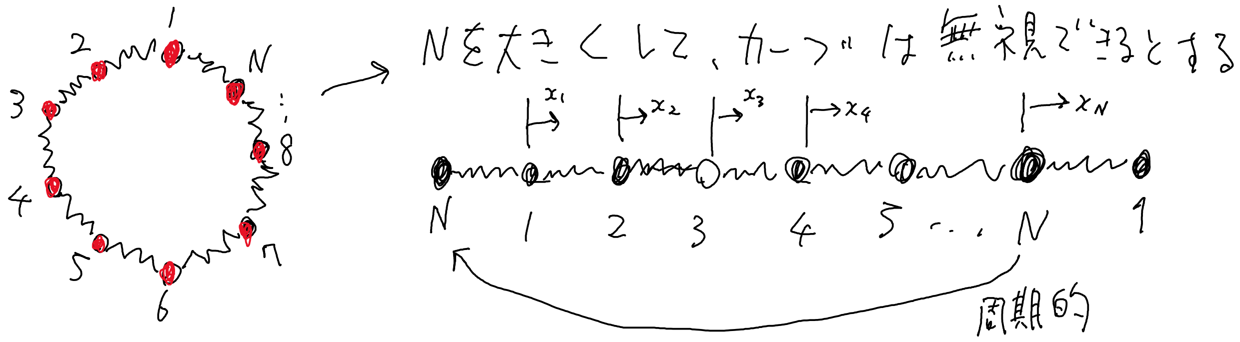
$[x, P_x] = [y, P_y] = [z, P_z] = i$, その他 $[x, y]$, $[x, P_y]$ などは0

$$\hat{x} = \frac{(C_x M)^{-1/4}}{\sqrt{2}}(\hat{b}_x + \hat{b}_x^\dagger) \qquad \hat{P}_x = \frac{(C_x M)^{1/4}}{i\sqrt{2}}(b_x - b_x^\dagger)$$

$$y = \frac{(C_y M)^{-1/4}}{\sqrt{2}}(\hat{b}_y + \hat{b}_y^\dagger) \qquad P_y = \frac{(C_y M)^{1/4}}{i\sqrt{2}}(b_y - b_y^\dagger)$$

$$z = \frac{(C_z M)^{-1/4}}{\sqrt{2}}(b_z + b_z^\dagger) \qquad P_z = \frac{(C_z M)^{1/4}}{i\sqrt{2}}(b_z - b_z^\dagger)$$

2.4 一次元連成調和振動子



$$\mathcal{H} = \frac{1}{2M}\sum_{j=1}^{N}\hat{p}_j^2 + \frac{C}{2}\sum_{j=1}^{N}(\hat{x}_{j+1} - \hat{x}_j)^2$$

まずはFourier変換

$$\hat{x}_q \equiv \frac{1}{\sqrt{N}}\sum_{j=1}^{N}\hat{x}_j e^{2\pi iqj/N} \qquad \hat{p}_q \equiv \frac{1}{\sqrt{N}}\sum_{j=1}^{N}\hat{p}_j e^{2\pi iqj/N}$$

$$\hat{x}_j = \frac{1}{\sqrt{N}}\sum_{q=1}^{N}\hat{x}_q e^{-2\pi iqj/N} \qquad \hat{p}_j = \frac{1}{\sqrt{N}}\sum_{q=1}^{N}\hat{p}_q e^{-2\pi iqj/N}$$

Hermite共役

$$x_q^\dagger = \frac{1}{\sqrt{N}}\sum_{j=1}^{N}x_j^\dagger e^{-2\pi iqj/N} = \frac{1}{\sqrt{N}}\sum_{j=1}^{N}x_j e^{2\pi i(N-q)j/N} = x_{N-q}$$

同様に $\hat{p}_q^\dagger = \hat{p}_{N-q}$

交換関係

$$[x_q, p_{q'}] = \frac{1}{N}\sum_{j=1}^{N}\sum_{j'=1}^{N}\underbrace{[x_j, p_{j'}]}_{i\delta_{jj'}} e^{2\pi iqj/N}e^{2\pi iq'j'/N}$$

$$= \frac{i}{N}\sum_{j=1}^{N}e^{2\pi i(q+q')j/N} = i\,\delta_{q,N-q}$$

ハミルトニアンの変換

$(q' = N-q \text{ のみ})$

$$\mathcal{H} = \frac{1}{2M}\frac{1}{N}\sum_{qq'} P_q P_{q'} \underbrace{\sum_j e^{-2\pi i (q+q')j/N}}_{\to N\delta_{q+q',N}}$$

$$\boxed{\sum_{j=1}^{N} e^{2\pi i q j/N} = N\delta_{q0}}$$

$$+\frac{C}{2}\frac{1}{N}\sum_{qq'} x_q x_{q'} (e^{-2\pi i q/N}-1)(e^{-2\pi i q'/N}-1)\underbrace{\sum_j e^{-2\pi i (q+q')j/N}}$$

$$= \frac{1}{2M}\sum_q P_q P_{N-q} + \frac{C}{2}\sum_q x_q x_{N-q}\underbrace{(e^{-2\pi i q/N}-1)(e^{2\pi i q/N}-1)}_{4\sin^2\left(\frac{\pi q}{N}\right)}$$

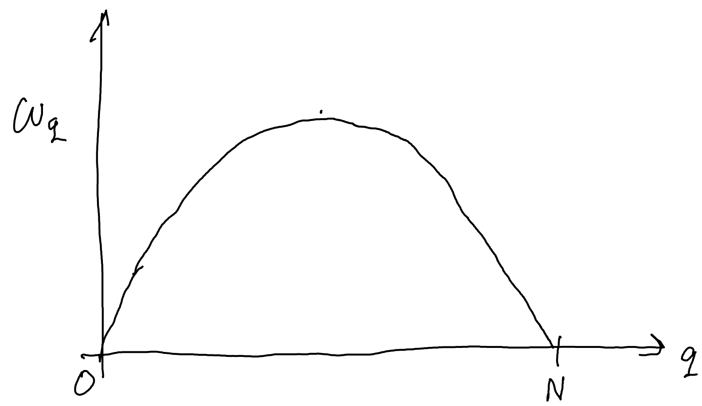
$$= \sum_{q=1}^{N}\left\{\frac{1}{2M}P_q P_q^{\dagger} + 2C\sin^2\left(\frac{\pi q}{N}\right)x_q x_q^{\dagger}\right\}$$

演算子の線形変換とハミルトニアンの対角化

$$x_q = \frac{\{4MC\cos^2(\pi q/N)\}^{-1/4}}{\sqrt{2}}(b_q + b_q^{\dagger})$$

$$P_q = \frac{\{4MC\cos^2(\pi q/N)\}^{1/4}}{i\sqrt{2}}(b_q - b_q^{\dagger})$$

$$\mathcal{H} = \sum_{q=1}^{N}\omega_q\left(b_q^{\dagger}b_q + \frac{1}{2}\right) \qquad \omega_q = \sqrt{\frac{C}{M}}\sin\left(\frac{\pi q}{N}\right)$$



$$E = E_{n_1 n_2 \cdots n_N} = \sum_{q=1}^{N}\omega_q\left(n_q + \frac{1}{2}\right)$$

b_q^{+}、b_q^{+} は生成・消滅演算子 (creator・annihilater) と呼ばれる。 ← 何故そう呼ばれるのか？