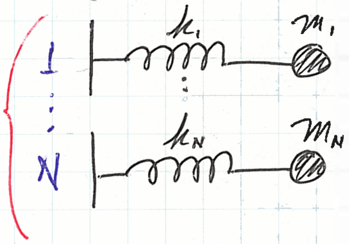
4. 調和振動子；4-1. 古典力学

2012-06-01

$$\mathcal{H} = \frac{p^2}{2m} + \frac{k}{2}x^2 \quad \cdots \quad \mathcal{H} = \sum_{i=1}^{N}\left(\frac{p_i^2}{2m_i} + \frac{k_i}{2}x_i^2\right)$$



$$Z_{(1)} = \sum_{\text{ALL STATES}} e^{-\beta\mathcal{H}} = \int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dx\, e^{-\beta\frac{p^2}{2m} - \beta\frac{k}{2}x^2}$$

$$Z_{(N)} = \quad 〃 \quad = \prod_{i=1}^{N} \int dp_i \int dx_i\, e^{-\beta\mathcal{H}_i}$$

$$Z_{(1)} = \sqrt{2\pi m k_B T}\sqrt{2\pi\frac{k_B T}{k}}$$

$$\Rightarrow Z_{(N)} = \prod_{i=1}^{N} \sqrt{2\pi m_i k_B T}\sqrt{2\pi\frac{k_B T}{k_i}}$$

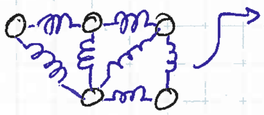
$$F_{(N)} = -k_B T \ln Z_{(N)} = -k_B T \ln \prod_{i=1}^{N}\left(2\pi m_i \cdot 2\pi\frac{1}{k_i}(k_B T)^2\right)^{1/2}$$

$$= -k_B T \ln \prod_{i=1}^{N}\left(2\pi m_i\, 2\pi\frac{1}{k_i}\right)^{1/2} - k_B T N \ln k_B T$$

$$E_{(N)} = -\frac{\partial}{\partial\beta}\ln Z_{(N)} = -\frac{\partial}{\partial\beta}\ln (k_B T)^N$$

$$= -N\frac{\partial}{\partial\beta}\ln\frac{1}{\beta} = +N\frac{1}{\beta} = N k_B T \cdots$$ エネルギーの等分配則（古典）

Dulong-Petit の法則



$$(x_i - x_{i+1})^2 = x_i^2 - 2x_i x_{i+1} + x_{i+1}^2$$

$$(x_i - y_j)^2 = x_i^2 - 2x_i y_j + y_j^2$$

↓ 結合の仕方

$$\rightarrow \mathcal{H} = \sum_{i=1}^{3N}\frac{p_i^2}{2m_i} + \sum_{ij} a_{ij}x_i x_j$$, x_i : i番目の自由度

$$Z = \int dp_1 \cdots dp_{3N} \int dx_1 \cdots dx_{3N}\, e^{-\beta\sum_{i=1}^{3N}\frac{p_i^2}{2m_i} - \beta\sum_{ij}^{3N} a_{ij}x_i x_j}$$

$$= \left(\prod_{i=1}^{3N}\sqrt{2\pi k_B T m_i}\right)\int_{-\infty}^{\infty} dx_1 \cdots dx_{3N}\, e^{-\beta\sum_{ij}^{3N} a_{ij}x_i x_j}$$

$$\sum_{ij}^{3N} a_{ij} x_i x_j = (x_1 \cdots x_{3N}) \begin{pmatrix} a_{11} & \frac{1}{2}a_{12} & \cdots & \\ \frac{1}{2}a_{21} & \ddots & & \\ \vdots & & & \\ & & & a_{3N,3N} \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_{3N} \end{pmatrix} = {}^t\vec{x} A \vec{x}$$

$$= {}^t\vec{x}\, U U^{-1} A U U^{-1} \vec{x}$$

$$= {}^t\xi D \xi$$

${}^t\vec{x}$ $\quad$ $\overset{\shortparallel}{A}$ $\quad$ $\vec{x}$

$\xi = U^{-1}\vec{x}$

${}^t\xi = {}^t\vec{x}\,{}^tU^{-1} = {}^t\vec{x}\,U$

$\xi_i = \sum_{j=1}^{3N} (U^{-1})_{ij} x_j$

ξ_i: i番目の基準振動
(NORMAL MODE)

A ⋮ $a_{ij} = a_{ji} \Rightarrow$ 対称行列

$U^{-1} A U = D$ とできる。 $D = \begin{pmatrix} \lambda_1 & & \bigcirc \\ & \ddots & \\ \bigcirc & & \lambda_{3N} \end{pmatrix}$

U ⋮ 直交行列 $\Rightarrow {}^tU = U^{-1}$

$\det U = 1$.

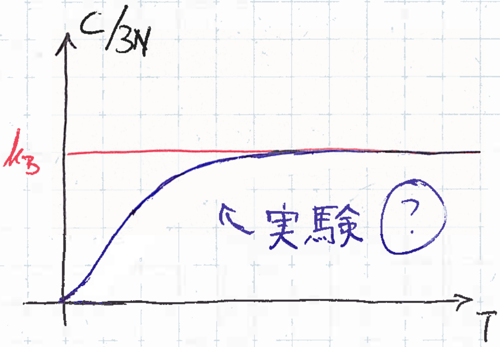
$\lambda_i > 0$

$$\Rightarrow Z = \left(\prod_{i=1}^{3N} \sqrt{2\pi m_i k_B T}\right) \int_{-\infty}^{\infty} d\xi_1 \cdots d\xi_{3N}\, e^{-\beta \sum_{i=1}^{3N} \lambda_i \xi_i^2} = \left(\prod_{i=1}^{3N} \sqrt{2\pi k_B T m_i}\right) \left(\prod_{i=1}^{3N} \sqrt{\pi \frac{k_B T}{\lambda_i}}\right)$$

$$= \prod_{i=1}^{3N} \sqrt{2\pi m_i \pi \frac{1}{\lambda_i}} \cdot (k_B T)^{3N}$$

$$\Rightarrow E = -\frac{\partial}{\partial \beta} \ln Z = -\frac{\partial}{\partial \beta} \ln (k_B T)^{3N} = 3N k_B T.$$

$$C = \frac{\partial E}{\partial T} = 3N k_B \quad \cdots \text{比熱}$$



4-2. 量子力学 … $\mathcal{H}|\psi_i\rangle = E_i|\psi_i\rangle$

$|\psi_i\rangle$: i番目の固有ベクトル

E_i : 〃 の固有値

$$\mathcal{H} = \frac{p^2}{2m} + \frac{k}{2}x^2$$

$$Z = \sum_{\substack{\text{all}\\\text{states}}} e^{-\beta\mathcal{H}} \qquad |\Psi\rangle = \sum c_i|\psi_i\rangle$$

全状態のヒルベルト空間に関する基底について和をとる。

$$Z = \sum_{i=1}^{N}\langle\psi_i|e^{-\beta\mathcal{H}}|\psi_i\rangle = \sum_{i=1}^{N} e^{-\beta E_i}$$

all states

$$Z = \mathrm{Tr}\, e^{-\beta\mathcal{H}}$$ …（基底の取り方に依らない）.

$$= \sum_i \langle\phi_i|e^{-\beta\mathcal{H}}|\phi_i\rangle = \sum_{ijm}\langle\phi_i|\psi_j\rangle\langle\psi_j|e^{-\beta\mathcal{H}}|\psi_m\rangle\langle\psi_m|\phi_i\rangle$$

$$= \sum_{ij}\langle\phi_i|\psi_j\rangle e^{-\beta E_j}\underbrace{\langle\psi_j|\phi_i\rangle}_{\text{UNITARY}} = \sum_{j=1}^{N} e^{-\beta E_j}$$

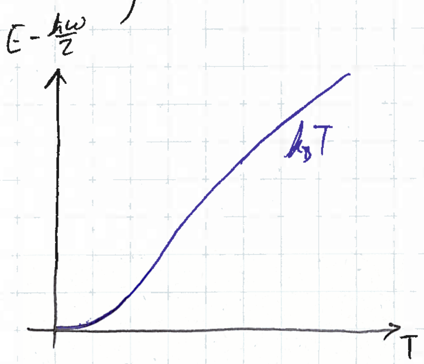
$$\begin{cases} E_n = \hbar\omega\left(n+\frac{1}{2}\right), \quad \omega = \sqrt{\frac{k}{m}}\,;\ n = 0, 1, \dots \\ |\psi_n\rangle = \cdots \end{cases}$$

∴ 零点振動

$$\Longrightarrow Z = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(n+\frac{1}{2}\right)} = e^{-\frac{1}{2}\hbar\beta\omega}\frac{1}{1-e^{-\beta\hbar\omega}}$$

$$E = -\frac{\partial}{\partial\beta}\ln Z = \frac{1}{2}\hbar\omega + \frac{\partial}{\partial\beta}\ln\left(1-e^{-\beta\hbar\omega}\right) = \frac{1}{2}\hbar\omega + \frac{\hbar\omega\, e^{-\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}}$$

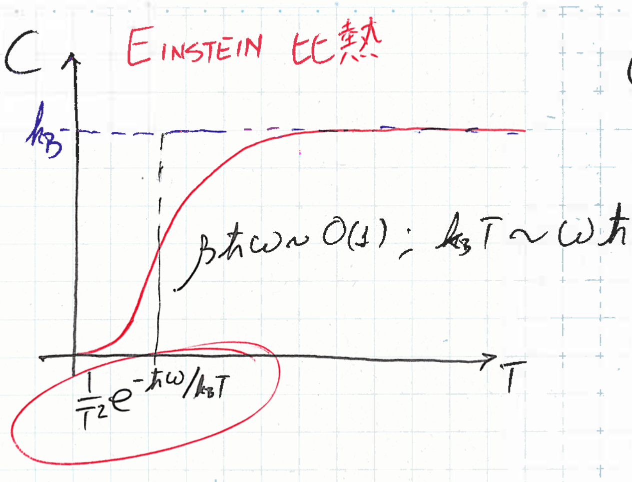
$$\xrightarrow[\beta\to 0]{\hbar\to 0} \frac{\hbar\omega}{2} + k_B T.$$



$$C = \frac{\partial E}{\partial T} = \frac{\partial}{\partial T}\left(\hbar\omega\frac{1}{e^{\beta\hbar\omega}-1}\right) = \frac{\partial\beta}{\partial T}\frac{\partial}{\partial\beta}\left(\frac{\hbar\omega}{e^{\beta\hbar\omega}-1}\right)$$

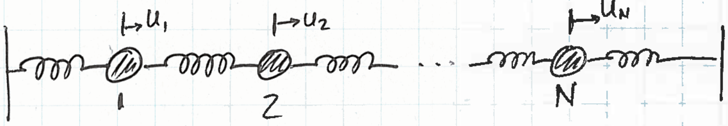
$$= +\frac{\hbar\omega}{k_B T^2}\left(\frac{\hbar\omega\, e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}\right)$$

$$= k_B(\beta\hbar\omega)^2\frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}$$



$$C \xrightarrow{\beta\to 0} k_B(\beta\hbar\omega)^2\frac{1}{(\beta\hbar\omega)^2}$$

4-3. 連成振動子の基準モード



固定端

$$m\ddot{u}_1 = -ku_1 + k(u_2-u_1) \quad \times e^{iq}$$
$$m\ddot{u}_2 = k(u_1-u_2) + k_2(u_3-u_2) \quad \times e^{i2q}$$
$$\vdots$$
$$+)\ m\ddot{u}_N = k(u_{N-1}-u_N) - ku_N \quad \times e^{iNq}$$

$$\mathcal{H} = \frac{1}{2m}\sum_{i=1}^{N} p_i^2 + \frac{k}{2}\Big(u_1^2 + (u_1-u_2)^2 + \cdots + (u_{N-1}-u_N)^2 + u_N^2\Big)$$

$$m\sum_{j=1}^{N}\ddot{u}_j e^{iqj} = k\sum_{j=1}^{N} u_{j+1}e^{iqj} - 2k\sum_{j=1}^{N} u_j e^{iqj} + k\sum_{j=1}^{N} u_{j-1}e^{iqj} \quad ; u_0 = u_{N+1} = 0.$$

$$= k\sum_{l=0}^{N-1} u_l e^{iq(l+1)} - 2k\sum_{l=0}^{N} u_l e^{iql} + k\sum_{l=2}^{N+1} u_l e^{iq(l-1)}$$

$$\boxed{\hat{u}_q = \sum_{j=1}^{N} u_j e^{iqj}} \Rightarrow m\ddot{\hat{u}}_q = k\hat{u}_q e^{iq} - 2k\hat{u}_q + k\hat{u}_q e^{-iq} - ku_N e^{iq(N+1)} - ku_1$$

$$\boxed{\hat{v}_q = \sum_{j=1}^{N} e^{-iqj}u_j} \Rightarrow m\ddot{\hat{v}}_q = k(e^{iq} - 2 + e^{-iq})v_q - ku_N e^{-iq(N+1)} - ku_1$$

$$\boxed{\xi_q = \alpha\hat{u}_q + \beta\hat{v}_q} \Rightarrow m\ddot{\xi}_q = k(e^{iq} - 2 + e^{-iq})\xi_q$$
$$- ku_N\left(\alpha e^{iq(N+1)} + \beta e^{-iq(N+1)}\right) - (\alpha+\beta)ku_1$$

$$\alpha+\beta=0 \;;\; \alpha e^{iq(N+1)}+\beta e^{-iq(N+1)}=0$$

$\beta=-\alpha$として，$e^{iq(N+1)}-e^{-iq(N+1)}=0$となるような$q$をとる。

$$2i\sin[q(N+1)]=0 \qquad q(N+1)=\pi n,\; n=1,2,\dots,N.$$

$$q=\frac{\pi n}{N+1}$$

$$\Rightarrow m\ddot{\xi}_q=-2k(1-\cos q)\xi_q$$

$$\ddot{\xi}_q=-2\frac{k}{m}(1-\cos q)\xi_q \equiv -\omega^2(q)\xi_q$$

分散関係 … $\omega(q)=\sqrt{2\frac{k}{m}(1-\cos q)} \overset{q\sim 0}{\sim} \sqrt{\frac{2k}{m}}|q|$