東工大　令和2年度　午後

【アインシュタインモデル】

2

$$H=\sum_{i=1}^{N}\left(\frac{p_i^2}{2m}+\frac{1}{2}m\omega^2 r_i^2\right)$$

$$r_i=(x_i, y_i, z_i)$$

$$p_i=(p_{x_i}, p_{y_i}, p_{z_i})$$

(1) 分配関数を求めよ.　$Z=\iint_{-\infty}^{\infty}\frac{dq\,dp}{h^{3N}}e^{-\beta E(q,p)}$

1粒子の分配関数 z

$$z=\frac{1}{h^3}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{-\frac{\beta}{2m}(p_x^2+p_y^2+p_z^2)}dp_x\,dp_y\,dp_z$$

$$\times\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{-\frac{\beta}{2}m\omega^2(x^2+y^2+z^2)}dx\,dy\,dz$$

$$=\frac{1}{h^3}\times\left(\sqrt{\frac{2m\pi}{\beta}}\right)^3\times\left(\sqrt{\frac{2\pi}{\beta m\omega^2}}\right)^3$$

$$=\frac{1}{h^3}\left(\sqrt{\frac{4\pi^2}{\beta^2\omega^2}}\right)^3$$

$$=\left(\frac{1}{h\beta\omega}\right)^3\times(2\pi)^3\qquad h=2\pi\hbar \text{ より}$$

$$=\left(\frac{1}{\hbar\beta\omega}\right)^3$$

これが N こあるので

$$Z=\left(\frac{1}{\hbar\beta\omega}\right)^{3N}$$

(2)　p98 まとめ

$\langle E\rangle=-\frac{d}{d\beta}(\log Z)$ を用いる

$$E=-\frac{\partial}{\partial\beta}\log Z$$

$$=-\frac{\partial}{\partial\beta}\log\left(\frac{1}{\hbar\omega\beta}\right)^{3N}$$

$$=3N\frac{\partial}{\partial\beta}\log(\hbar\omega\beta)$$

$$=3N\frac{1}{\hbar\omega\beta}\cdot\hbar\omega$$

$$=3N\frac{1}{\beta}$$

$$=3Nk_BT$$

$$C_{cl}=\frac{\partial E}{\partial T}$$

$$=3Nk_B$$

(3)　$E_n=(n+\frac{1}{2})\hbar\omega$

$$Z=\sum_{n_x n_y n_z}e^{-\beta E_{n_x},E_{n_y},E_{n_z}}$$

$$=\sum_{n_x=0}^{\infty}e^{-\beta(n_x+\frac{1}{2})\hbar\omega}\sum_{n_y=0}^{\infty}e^{-\beta(n_y+\frac{1}{2})\hbar\omega}\sum_{n_z=0}^{\infty}e^{-\beta(n_z+\frac{1}{2})\hbar\omega}$$

$$=e^{-\frac{\beta}{2}\hbar\omega}\left(\sum_{n_x=0}^{\infty}e^{-\beta n_x\hbar\omega}\sum_{n_y=0}^{\infty}e^{-\beta n_y\hbar\omega}\sum_{n_z=0}^{\infty}e^{-\beta n_z\hbar\omega}\right)$$

$$\sum_{n=1}^{\infty}a_n=\frac{a_1}{1-r}$$

$$=e^{-\frac{\beta}{2}\hbar\omega\,3}\left(\frac{1}{1-e^{-\beta\hbar\omega}}\cdot\frac{1}{1-e^{-\beta\hbar\omega}}\cdot\frac{1}{1-e^{-\beta\hbar\omega}}\right)$$

$$=\left(\frac{e^{-\frac{\beta}{2}\hbar\omega}}{1-e^{-\beta\hbar\omega}}\right)^3$$

$$=\left(\frac{1}{e^{\frac{\beta}{2}\hbar\omega}-e^{-\frac{\beta}{2}\hbar\omega}}\right)^3=\left(\frac{1}{2\sinh\left(\frac{\beta\hbar\omega}{2}\right)}\right)^3$$

$$\therefore Z = z^N$$

$$= \left(\frac{1}{2\sinh\left(\frac{\beta\hbar\omega}{2}\right)} \right)^{3N}$$

(4)

$$E = -\frac{\partial}{\partial\beta} \log Z$$

$(\sinh x)' = \cosh x$

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$(\tanh x)' = \frac{1}{\cosh^2 x} = 1 - \tanh^2 x$

$$= 3N \frac{\partial}{\partial\beta} \log\left(2\sinh\left(\frac{\beta\hbar\omega}{2}\right)\right)$$

$$= 3N \frac{1}{2\sinh\left(\frac{\beta\hbar\omega}{2}\right)} \times 2\cosh\left(\frac{\beta\hbar\omega}{2}\right) \times \frac{\hbar\omega}{2}$$

$$= 3N \frac{1}{\tanh\left(\frac{\beta\hbar\omega}{2}\right)} \cdot \frac{\hbar\omega}{2}$$

$$C = \frac{\partial E}{\partial T} \qquad \beta = \frac{1}{k_B T}$$

$$= \frac{\partial}{\partial T}\left(\frac{3N}{2}\hbar\omega \frac{1}{\tanh\left(\frac{\hbar\omega}{2k_B}\frac{1}{T}\right)} \right)$$

$$= \frac{3}{2}N\hbar\omega \frac{\partial}{\partial T}\left(\tanh^{-1}\left(\frac{\hbar\omega}{2k_B}\frac{1}{T}\right) \right)$$

$$= \frac{3}{2}N\hbar\omega \; -\tanh^{-2}\left(\frac{\hbar\omega}{2k_B}\frac{1}{T}\right) \times \frac{1}{\cosh^2\left(\frac{\hbar\omega}{2k_B}\frac{1}{T}\right)} \times \frac{\hbar\omega}{2k_B} \; -T^{-2}$$

$$= 3N\left(\frac{\beta\hbar\omega}{2}\right)^2 k_B \cdot \frac{1}{\sinh^2\left(\frac{\beta\hbar\omega}{2}\right)}$$

(5)

$$\boxed{\begin{aligned} \sinh x &= \frac{e^x - e^{-x}}{2} = x + \frac{x^3}{3!} + \cdots \\ &\propto \begin{cases} e^x & (x \to \infty) \\ x & (x \to 0) \end{cases} \\ \lim_{x\to 0}\left(\frac{x}{\sinh x}\right)^2 &= \lim_{x\to 0} \frac{(x^2)'}{(\sinh^2 x)'} \\ &= \lim_{x\to 0} \frac{2x}{2\sinh x \cosh x} \\ &= \frac{2x}{2\cdot x \cdot 1} \\ &= 1 \end{aligned}}$$

$T \to 0$

$\beta \to \infty$ a z ?

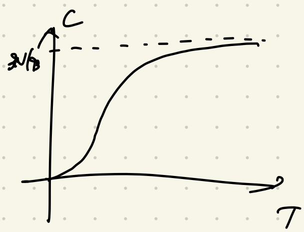
$$C \to 3Nk_B\left(\frac{\beta\hbar\omega}{2}\right)^2 e^{-\frac{\beta\hbar\omega}{\cancel{2}}\cdot\cancel{2}}$$

$T \to \infty$

$\beta \to 0$

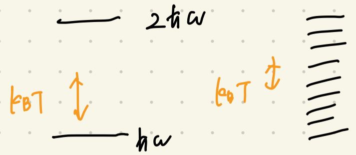
$$C \to 3Nk_B \cancel{x^2} \cdot \frac{1}{\cancel{x^2}}$$

$$= C_{cl}$$



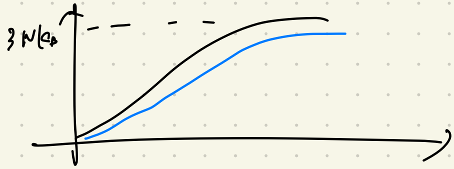
(6)

Tが低温の時　　　　Tが高温の時



エネルギー等分配則

この様な違いから
低温でのふるまいが異なる



(7) この系にz方向の異方性を加える.

$$H' = \sum_{i=1}^{N} \left[\frac{p_i^2}{2m} + \frac{1}{2} m\omega^2 (x_i^2 + y_i^2) + \frac{1}{2} m\Omega^2 z_i^2 \right]$$

$$\Omega \gg \omega$$

$$E_x = E_y = \left(n + \frac{1}{2}\right)\hbar\omega$$

$$E_z = \left(n + \frac{1}{2}\right)\hbar\Omega$$

$$C = 3N\left(\frac{\beta\hbar\omega}{2}\right)^2 k_B \cdot \frac{1}{\sinh^2\left(\frac{\beta\hbar\omega}{2}\right)}$$ より

$$C = Nk_B\left[2\left(\frac{\beta\hbar\omega}{2}\right)^2 \frac{1}{\sinh^2\left(\frac{\beta\hbar\omega}{2}\right)} + \underbrace{\left(\frac{\beta\hbar\Omega}{2}\right)^2 \frac{1}{\sinh^2\left(\frac{\beta\hbar\Omega}{2}\right)}}\right]$$

$$\frac{\hbar\Omega}{k_B} = T_E \qquad = \frac{1}{4}\left(\frac{T_E}{T}\right)^2 \cdot \frac{1}{\sinh^2\left(\frac{T_E}{2T}\right)}$$