# Homework3— Free System

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**Problem 1.** : For a many particles system with Hamiltonian,

$$H = \sum_{i=1}^{N} \varepsilon s_i \qquad s_i = -1, 0, 1$$

(a) Calculate the partition function for classical case

$$Z = \sum_{s_i = -1, 0, 1} e^{-\beta \varepsilon s_i}$$

(b) From the partition function $Z$, calculate the total energy $E$, heat capacity $C$, entropy $S$ of this system.

**Solve**:

(a)

$$Z = \sum_{s_i=-1,0,1} e^{-\beta\varepsilon s_i} = e^{-\beta\varepsilon} + e^{\beta\varepsilon} + e^0 = 2\cosh\beta\varepsilon + 1$$

(b)

$$\begin{aligned} n_{s_i} &= e^{-\alpha-\beta\varepsilon s_i} \\ N &= \sum_{s_i} n_{s_i} = e^{-\alpha} Z \end{aligned}$$

$$\Longrightarrow$$

$$\begin{aligned}
E &= -n_{-1}\varepsilon + n_0 \times (0\times\varepsilon) + n_1\varepsilon \\
&= -\varepsilon e^{-\alpha+\beta\varepsilon} + \varepsilon e^{-\alpha-\beta\varepsilon} \\
&= \frac{N}{Z}(-\varepsilon e^{\beta\varepsilon} + \varepsilon e^{-\beta\varepsilon}) \\
&= \frac{-2N\varepsilon\sinh\beta\varepsilon}{2\cosh\beta\varepsilon + 1} \\
C &= \frac{dE}{dT} = \frac{d}{dT}\left(\frac{N\varepsilon}{2\cosh\beta\varepsilon + 1}(-\varepsilon e^{\beta\varepsilon} + \varepsilon e^{-\beta\varepsilon})\right) \\
&= -N\varepsilon\frac{d}{dT}\left(\frac{2\sinh\beta\varepsilon}{2\cosh\beta\varepsilon + 1}\right) \\
&= -N\varepsilon\frac{2\cosh\beta\varepsilon(2\cosh\beta\varepsilon+1) - 2\sinh\beta\varepsilon * 2\sinh\beta\varepsilon}{(2\cosh\beta\varepsilon+1)^2}\frac{-\varepsilon}{\kappa_{\mathrm{B}}T^2} \\
&= N\varepsilon\frac{4\sinh^2\beta\varepsilon - 4\cosh^2\beta\varepsilon - 2\cosh\beta\varepsilon}{(2\cosh\beta\varepsilon+1)^2}\frac{-\varepsilon}{\kappa_{\mathrm{B}}T^2} \\
&= N\varepsilon\frac{4+2\cosh\beta\varepsilon}{(2\cosh\beta\varepsilon+1)^2}\frac{\varepsilon}{\kappa_{\mathrm{B}}T^2} \\
&= N\kappa_{\mathrm{B}}\left(\frac{\varepsilon}{\kappa_{\mathrm{B}}T}\right)^2\frac{4+2\cosh\beta\varepsilon}{(2\cosh\beta\varepsilon+1)^2} \\
S &= -N\kappa_{\mathrm{B}}\left(\frac{e^{\beta\varepsilon}}{Z}\mathrm{In}\frac{e^{\beta\varepsilon}}{Z} + \frac{e^0}{Z}\mathrm{In}\frac{e^0}{Z} + \frac{e^{-\beta\varepsilon}}{Z}\mathrm{In}\frac{e^{-\beta\varepsilon}}{Z}\right. \\
&= -N\kappa_{\mathrm{B}}\left(\frac{e^{\beta\varepsilon}}{Z}\beta\varepsilon - \frac{e^{\beta\varepsilon}}{Z}\mathrm{In}\,Z - \frac{1}{Z}\mathrm{In}\,Z - \beta\varepsilon\frac{e^{-\beta\varepsilon}}{Z} - \frac{e^{-\beta\varepsilon}}{Z}\mathrm{In}\,Z\right) \\
&= -N\kappa_{\mathrm{B}}\left[\frac{\beta\varepsilon}{Z}(e^{\beta\varepsilon} - e^{-\beta\varepsilon}) - \frac{\mathrm{In}\,Z}{Z}(e^{\beta\varepsilon} + 1 + e^{-\beta\varepsilon})\right] \\
&= -N\kappa_{\mathrm{B}}\left[\frac{\beta\varepsilon\, 2\sinh\beta\varepsilon}{2\cosh\beta\varepsilon+1} - \frac{\mathrm{In}(2\cosh\beta\varepsilon+1)}{2\cosh\beta\varepsilon+1}(\cosh\beta\varepsilon+1)\right] \\
&= -\frac{1}{T}\frac{N\varepsilon\, 2\sinh\beta\varepsilon}{2\cosh\beta\varepsilon+1} + N\kappa_{\mathrm{B}}\frac{\mathrm{In}(2\cosh\beta\varepsilon+1)}{2\cosh\beta\varepsilon+1}(\cosh\beta\varepsilon+1)
\end{aligned}$$

**Problem 2.** : For a 2D many particles system with Hamiltonian,

$$H = \sum_{i=1}^{N} c|\vec{p}_i|$$

(a) Calculate the partition function for classical case

$$Z = \int \frac{d^2\vec{q}\, d^2\vec{p}}{h^2} e^{-\beta c|\vec{p}|}$$

(b) From the partition function $Z$, calculate the energy $E$, heat capacity $C$, entropy $S$ and pressure $P$ of this system.

**Solve**:

(a)

$$
\begin{aligned}
Z &= \int \frac{d^2\vec{q}\, d^2\vec{p}}{h^2} e^{-\beta c|\vec{p}|} = \frac{1}{h^2}\int d^2\vec{q} \int e^{-\beta c|\vec{p}|} d^2\vec{p} \\
&= \frac{1}{h^2}\int d^2\vec{q} \iint e^{-\beta c\sqrt{p_x^2+p_y^2}} dp_x dp_y \\
&= \frac{1}{h^2}\int d^2\vec{q} \int_0^{+\infty}\int_0^{2\pi} e^{-\beta c\sqrt{r^2}} r\, d\theta dr \qquad (r \geqslant 0) \\
&= \frac{1}{h^2}\int d^2\vec{q}\, 2\pi \int_0^{+\infty} r e^{-\beta c r} dr \\
&= \frac{1}{h^2}\int d^2\vec{q}\, \frac{2\pi}{\beta c} e^{-\beta c r}|_0^{+\infty} = \frac{2\pi}{h^2\beta c}\int d^2\vec{q} = \frac{2\pi A}{h^2\beta c} \qquad \left(A = \int d^2\vec{q}\right)
\end{aligned}
$$

(b)

$$
\begin{aligned}
E &= -N\frac{\partial \mathrm{In}\, Z}{\partial \beta} = -N\frac{\partial}{\partial \beta}\left(\frac{2\pi A}{h^2\beta c}\right) \\
&= N\frac{2\pi A}{h^2 c\beta^2} \\
C &= \frac{dE}{dT} = \frac{d}{dT}\left(N\frac{2\pi A}{h^2 c}\kappa_{\mathrm{B}}^2 T^2\right) \\
&= -N\kappa_{\mathrm{B}}^2\frac{4\pi A}{h^2 c} T
\end{aligned}
$$

$$
\mathcal{F} = -\kappa_{\mathrm{B}} T\, \mathrm{In}\left(\frac{2\pi A}{h^2\beta c}\right)
$$

$$
\begin{aligned}
S &= -N\frac{\partial \mathcal{F}}{\partial T} = N\kappa_{\mathrm{B}}\frac{\partial}{\partial T}\left(T\, \mathrm{In}\frac{2\pi a\kappa_{\mathrm{B}} T}{h^2 c}\right) \\
&= N\kappa_{\mathrm{B}}\left(\mathrm{In}\frac{2\pi A\kappa_{\mathrm{B}} T}{h^2 c} + \frac{h^2 c}{2\pi A\kappa_{\mathrm{B}}}\right) \\
P &= -\frac{\partial \mathcal{F}}{\partial A} = \kappa_B T\frac{h^2\beta c}{2\pi A}
\end{aligned}
$$