物理学演習第 3 レポート

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(1)

　全粒子数を N, 準位 ν に存在する粒子の個数を n_ν, その準位のエネルギーを ε_ν とすると, 大分配関数 Ξ は

$$
\begin{aligned}
\Xi &= \sum_{N=0}^{\infty} \sum_{N=\sum n_\nu} \prod_{\nu} \mathrm{e}^{-\beta(\epsilon_\nu-\mu)n_\nu} \\
&= \prod_{\nu} \sum_{n_\nu=0}^{\infty} \mathrm{e}^{-\beta(\epsilon_\nu-\mu)n_\nu} \\
&= \prod_{\nu} \frac{1}{1-\mathrm{e}^{-\beta(\varepsilon_\nu-\mu)}}
\end{aligned} \tag{1}
$$

したがって熱力学ポテンシャルは

$$
\begin{aligned}
\Omega &= -k_B T \log \Xi \\
&= -k_B T \log \prod_{\nu} \frac{1}{1-\mathrm{e}^{-\beta(\varepsilon_\nu-\mu)}} \\
&= -k_B T \sum_{\nu} \log \frac{1}{1-\mathrm{e}^{-\beta(\varepsilon_\nu-\mu)}} \\
&= -k_B T \sum_{\nu} \log \frac{\mathrm{e}^{\beta(\varepsilon_\nu-\mu)}}{\mathrm{e}^{\beta(\varepsilon_\nu-\mu)}-1} \\
&= -k_B T \sum_{\nu} \log(1+f_{BE}(\varepsilon_\nu))
\end{aligned} \tag{2}
$$

(2)

　エントロピーは $S=-\partial\Omega/\partial T$ なので

$$
\begin{aligned}
S &= -\frac{\partial \Omega}{\partial T} \\
&= k_B \sum_{\nu} \log(1+f_{BE}(\varepsilon_\nu)) + k_B T \sum_{\nu} \frac{1}{1+f_{BE}(\varepsilon_\nu)} \frac{\partial f_{BE}(\varepsilon_\nu)}{\partial T}
\end{aligned} \tag{3}
$$

ここで

$$
\begin{aligned}
\frac{\partial f_{BE}(\varepsilon_\nu)}{\partial T} &= \frac{1}{\mathrm{e}^{\beta(\varepsilon_\nu-\mu)}-1}\frac{\mathrm{e}^{\beta(\varepsilon_\nu-\mu)}}{\mathrm{e}^{\beta(\varepsilon_\nu-\mu)}-1}\frac{\varepsilon_\nu-\mu}{k_BT^2} \\
&= f_{BE}(\varepsilon_\nu)(1+f_{BE}(\varepsilon_\nu))\frac{\varepsilon_\nu-\mu}{k_BT^2}
\end{aligned}
\tag{4}
$$

したがって

$$
S = k_B\sum_\nu \log(1+f_{BE}(\varepsilon_\nu)) + \frac{1}{T}\sum_\nu(\varepsilon_\nu-\mu)f_{BE}(\varepsilon_\nu) \tag{5}
$$

ここで

$$
\beta(\epsilon_\nu-\mu) = \log\mathrm{e}^{\beta(\epsilon_\nu-\mu)} = \log(1+f_{BE}(\varepsilon_\nu)) - \log f_{BE}(\varepsilon_\nu) \tag{6}
$$

より

$$
\begin{aligned}
S &= k_B\sum_\nu \log(1+f_{BE}(\varepsilon_\nu)) + k_B\sum_\nu\left(\log(1+f_{BE}(\varepsilon_\nu)) - \log f_{BE}(\varepsilon_\nu)\right)f_{BE}(\varepsilon_\nu) \\
&= k_B\sum_\nu\left((1+f_{BE}(\varepsilon_\nu))\log(1+f_{BE}(\varepsilon_\nu)) - f_{BE}(\varepsilon_\nu)\log f_{BE}(\varepsilon_\nu)\right)
\end{aligned}
\tag{7}
$$

(3)

$\boldsymbol{k}$ が密に存在し, その間隔が $\Delta k_x = \Delta k_y = \Delta k_z = 2\pi/L$ であるならば

$$
\begin{aligned}
\sum_{\boldsymbol{k}} &= \frac{1}{\Delta k_x\Delta k_y\Delta k_z}\sum \Delta k_x\Delta k_y\Delta k_z \\
&= \left(\frac{L}{2\pi}\right)^3\int \mathrm{d}\boldsymbol{k}
\end{aligned}
\tag{8}
$$

という置換ができるので, 熱力学ポテンシャルは

$$
\begin{aligned}
\Omega &= k_BT\sum_{\boldsymbol{k}=0}^{\infty}\log\left(1-\mathrm{e}^{-\beta(\varepsilon_k-\mu)}\right) \\
&= k_BT\frac{V}{8\pi^3}\int \mathrm{d}\boldsymbol{k}\log\left(1-\mathrm{e}^{-\beta(\varepsilon_k-\mu)}\right)
\end{aligned}
\tag{9}
$$

被積分項は k にしか依らないので, 角度方向の積分を実行して

$$
\Omega = k_BT\frac{V}{8\pi^3}\int \mathrm{d}k\ 4\pi k^2\log\left(1-\mathrm{e}^{-\beta(\varepsilon_k-\mu)}\right) \tag{10}
$$

ここで $\mathrm{d}\varepsilon/\mathrm{d}k = \hbar^2k/m$, $k=\sqrt{2m\varepsilon}/\hbar$ なので

$$
\Omega = k_BT\frac{V}{2\pi^2}\frac{m\sqrt{2m}}{\hbar^3}\int_0^\infty \mathrm{d}\varepsilon\sqrt{\varepsilon}\log\left(1-\mathrm{e}^{-\beta(\varepsilon-\mu)}\right) \tag{11}
$$

ここで部分積分を行うと

$$
\begin{aligned}
&\int_0^\infty \mathrm{d}\epsilon \sqrt{\varepsilon} \log\left(1-\mathrm{e}^{-\beta(\varepsilon-\mu)}\right) \\
&= \left[\frac{2}{3}\varepsilon\sqrt{\varepsilon}\log\left(1-\mathrm{e}^{-\beta(\varepsilon-\mu)}\right)\right]_0^\infty - \int_0^\infty \mathrm{d}\varepsilon \frac{2}{3}\varepsilon\sqrt{\varepsilon}\frac{-\mathrm{e}^{-\beta(\varepsilon-\mu)}(-\beta)}{1-\mathrm{e}^{-\beta(\varepsilon-\mu)}} \\
&= -\frac{2\beta}{3}\int_0^\infty \mathrm{d}\varepsilon\sqrt{\varepsilon} f_{BE}(\varepsilon)\varepsilon
\end{aligned}
\tag{12}
$$

なので

$$
\Omega = -\frac{2}{3}\frac{V}{2\pi^2}\frac{m\sqrt{2m}}{\hbar^3}\int_0^\infty \mathrm{d}\varepsilon\sqrt{\varepsilon} f_{BE}(\varepsilon)\varepsilon \tag{13}
$$

ここで積分を再び級数に戻すと

$$
\Omega = -\frac{2}{3}\sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} f_{BE}(\varepsilon_{\boldsymbol{k}}) = -\frac{2}{3}E \tag{14}
$$

$\Omega = -pV$ なので

$$
pV = \frac{2}{3}E \tag{15}
$$

(4)

(11) 式をマクローリン展開し,2 次までを拾うと

$$
\begin{aligned}
\Omega &= -k_B T\frac{V}{2\pi^2}\frac{m\sqrt{2m}}{\hbar^3}\int_0^\infty \mathrm{d}\varepsilon\sqrt{\varepsilon}\sum_{n=1}^\infty \frac{1}{n}\mathrm{e}^{-n\beta(\varepsilon-\mu)} \\
&= -k_B T\frac{V}{2\pi^2}\frac{m\sqrt{2m}}{\hbar^3}\left(\int_0^\infty \mathrm{d}\varepsilon\sqrt{\varepsilon}\mathrm{e}^{-\beta(\varepsilon-\mu)} + \frac{1}{2}\int_0^\infty \mathrm{d}\varepsilon\sqrt{\varepsilon}\mathrm{e}^{-2\beta(\varepsilon-\mu)}\right)
\end{aligned}
\tag{16}
$$

ここで

$$
\int_0^\infty \mathrm{d}x\sqrt{x}\mathrm{e}^{-a(x-b)} = \mathrm{e}^{ab}\frac{1}{a}\int_0^\infty \mathrm{d}y\sqrt{\frac{y}{a}}\mathrm{e}^{-y} = \frac{\mathrm{e}^{ab}}{a\sqrt{a}}\Gamma\left(\frac{3}{2}\right) = \frac{\mathrm{e}^{ab}}{a\sqrt{a}}\frac{\sqrt{\pi}}{2} \tag{17}
$$

を用いれば

$$
\begin{aligned}
\Omega &= -k_B T\frac{V}{2\pi^2}\frac{m\sqrt{2m}}{\hbar^3}\frac{\mathrm{e}^{\beta\mu}}{\beta\sqrt{\beta}}\frac{\sqrt{\pi}}{2}\left(1+\frac{\mathrm{e}^{\beta\mu}}{4\sqrt{2}}\right) \\
&= -(k_B T)^{5/2}\frac{m\sqrt{2m}}{4\pi^2\hbar^3}V\sqrt{\pi}\mathrm{e}^{\beta\mu}\left(1+\frac{1}{2^{5/2}}\mathrm{e}^{\beta\mu}\right)
\end{aligned}
\tag{18}
$$

となる. ここで $N = -\partial\Omega/\partial\mu$ なので

$$
\begin{aligned}
&N = (k_B T)^{5/2}\frac{m\sqrt{2m}}{4\pi^2\hbar^3}V\sqrt{\pi}\beta\mathrm{e}^{\beta\mu}\left(1+\frac{2}{2^{5/2}}\mathrm{e}^{\beta\mu}\right) \\
\therefore\quad &\mathrm{e}^{\beta\mu} = (k_B T)^{-5/2}\frac{4\pi^2\hbar^3}{m\sqrt{2m}}\frac{1}{V\sqrt{\pi}\beta}\left(1+\frac{2}{2^{5/2}}\mathrm{e}^{\beta\mu}\right)^{-1}N
\end{aligned}
\tag{19}
$$

したがって

$$\Omega = -Nk_BT\left(1+\frac{1}{2^{5/2}}\mathrm{e}^{\beta\mu}\right)\left(1+\frac{2}{2^{5/2}}\mathrm{e}^{\beta\mu}\right)^{-1} \tag{20}$$

ここで $\mathrm{e}^{\beta\mu} \ll 1$ から

$$\begin{aligned}\Omega &\simeq -Nk_BT\left(1+\frac{1}{2^{5/2}}\mathrm{e}^{\beta\mu}\right)\left(1-\frac{2}{2^{5/2}}\mathrm{e}^{\beta\mu}\right) \\ &\simeq -Nk_BT\left(1-\frac{1}{2^{5/2}}\mathrm{e}^{\beta\mu}\right)\end{aligned} \tag{21}$$

ここに再び (19) 式を代入して $\mathrm{e}^{\beta\mu}$ の 2 次以降を無視すると

$$\begin{aligned}\Omega &= -Nk_BT\left(1-\frac{1}{2^{5/2}}(k_BT)^{-5/2}\frac{4\pi^2\hbar^3}{m\sqrt{2m}}\frac{1}{V\sqrt{\pi}\beta}\left(1+\frac{2}{2^{5/2}}\mathrm{e}^{\beta\mu}\right)^{-1}N\right) \\ &\simeq -Nk_BT\left(1-\frac{\pi^{3/2}N}{2V}\left(\frac{\hbar^2}{mk_BT}\right)^{3/2}\right)\end{aligned} \tag{22}$$

4-10

(1)

$$\begin{aligned}N &= \sum_{N=0}^{\infty}\sum_{\nu}\frac{1}{\mathrm{e}^{\beta(\varepsilon_\nu-\mu)}-1} \\ &= \sum_{n_x}\sum_{n_y}\sum_{n_z}\frac{1}{\mathrm{e}^{\beta(\varepsilon_{\boldsymbol{n}}-\mu)}-1} \\ &= \int_0^\infty \mathrm{d}n_x\int_0^\infty \mathrm{d}n_y\int_0^\infty \mathrm{d}n_z\frac{1}{\mathrm{e}^{\beta(\varepsilon_{\boldsymbol{n}}-\mu)}-1}\end{aligned} \tag{23}$$

ここで $\varepsilon_{\boldsymbol{n}} = \hbar\omega(n_x+n_y+n_z)$ である.(定数部分は省略した)

(2)

(23) 式において $i = \beta\hbar\omega n_i$ $(i = x, y, z)$ すれば

$$N = \left(\frac{k_BT}{\hbar\omega}\right)^3\int_0^\infty \mathrm{d}x\int_0^\infty \mathrm{d}y\int_0^\infty \mathrm{d}z\frac{1}{\mathrm{e}^{-\beta\mu}\mathrm{e}^{x+y+z}-1} \tag{24}$$

また

$$
\begin{aligned}
\int_0^\infty \frac{x^{n-1}}{z^{-1}\mathrm{e}^x - 1}\mathrm{d}x &= \int_0^\infty \frac{x^{n-1}z\mathrm{e}^{-x}}{1 - z\mathrm{e}^{-x}} \\
&= \int_0^\infty x^{n-1}z\mathrm{e}^{-x}\sum_{k=0}^{\infty} z\mathrm{e}^{-x^k}\mathrm{d}x \\
&= \sum_{k=0}^{\infty}\int_0^\infty t^{n-1}\mathrm{e}^{-t}\mathrm{d}t\frac{z^{k+1}}{(k+1)^n} \\
&= \Gamma(n)\sum_{k=1}^{\infty}\frac{z^k}{k^n}
\end{aligned}
\tag{25}
$$

を用いれば

$$
\begin{aligned}
N &= \left(\frac{k_B T_c}{\hbar\omega}\right)^3 \int_0^\infty \mathrm{d}x \int_0^\infty \mathrm{d}y\ \Gamma(1)\sum_{k=1}^{\infty}\frac{\mathrm{e}^{-k(x+y-\beta\mu)}}{k} \\
&= \left(\frac{k_B T_c}{\hbar\omega}\right)^3 \int_0^\infty \mathrm{d}x\ \sum_{k=1}^{\infty}\frac{\mathrm{e}^{-k(x-\beta\mu)}}{k^2} \\
&= \left(\frac{k_B T_c}{\hbar\omega}\right)^3 \sum_{k=1}^{\infty}\frac{\mathrm{e}^{k\beta\mu}}{k^3}
\end{aligned}
\tag{26}
$$

また $T \leq T_c$ において $\mu = 0$ なので

$$
N = \left(\frac{k_B T}{\hbar\omega}\right)^3 \zeta(3) \tag{27}
$$

したがって

$$
T_c = \frac{\hbar\omega}{k_B}\left(\frac{N}{\zeta(3)}\right)^{1/3} \tag{28}
$$

(3)

(27) 式は凝縮していない粒子の数なので, 凝縮した粒子の数を $N_0(T)$ とすると

$$
N_0(T) = N - \left(\frac{k_B T}{\hbar\omega}\right)^3 \zeta(3) \tag{29}
$$

(28) 式から $(k_B/\hbar\omega)^3\zeta(3) = N/T_c^3$ なので

$$
N_0(T) = N\left(1 - \left(\frac{T}{T_c}\right)^3\right) \tag{30}
$$