7/1

量子ボース気体

大分配関数

$$\Xi_{BE} = \prod_{k} \frac{1}{1-e^{-\beta(E_k-\mu)}} \quad (\mu < E_k)$$

$$\langle n_k \rangle = \frac{e^{-\beta(E_k-\mu)}}{1-e^{-\beta(E_k-\mu)}} = \frac{1}{e^{\beta(E_k-\mu)}-1}$$

$$N = \sum_k \langle n_k \rangle$$

$$= \left(\frac{L}{2\pi}\right)^3 \int_0^\infty 4\pi k^2 dk \frac{1}{e^{\beta(E_k-\mu)}-1}$$

$$\downarrow \; \varepsilon = \frac{\hbar^2}{2m}k^2$$

$$= \int_0^\infty \frac{D(\varepsilon)}{e^{\beta(\varepsilon-\mu)}-1} d\varepsilon$$

$$\left(D(\varepsilon) = \frac{V}{(2\pi)^3} \frac{4\pi m}{\hbar^3} \sqrt{2m\varepsilon} \right)$$

$$= \frac{V}{(2\pi)^3} \frac{4\pi m\sqrt{2m}}{\hbar^3} \int_0^\infty \frac{\sqrt{\varepsilon}\, d\varepsilon}{e^{\beta(\varepsilon-\mu)}-1}$$

$$\downarrow \; x = \beta\varepsilon$$

$$= \frac{V}{(2\pi)^3} \frac{4\pi m\sqrt{2m}}{\hbar^3} (k_B T)^{\frac{3}{2}} \int_0^\infty \frac{\sqrt{x}\, dx}{e^{x-\beta\mu}-1}$$

↳ 逆に解くと $\mu = \mu(N)$

(変形されたツェータ関数

$$\phi(z,s) = \frac{1}{\Gamma(z)} \int_0^\infty \frac{t^{z-1}}{\frac{e^t}{s}-1} dt$$
)

$$= \frac{V}{(2\pi)^3} \frac{4\pi m\sqrt{2m}}{\hbar^3 \beta^{\frac{3}{2}}} \Gamma\left(\frac{3}{2}\right) \phi\left(\frac{3}{2}, e^{\beta\mu}\right)$$

$\mu < \varepsilon$, $\varepsilon_{min} = 0$ より $\mu_{max} = 0$

$\phi(z, s)$ は $s \to 1$ で単調増加

$$N \leq N_{max} \equiv 2\pi V \left(\frac{2 \cdot k_B T}{h^2} \right)^{\frac{3}{2}} \Gamma\left(\tfrac{3}{2}\right) \phi\left(\tfrac{3}{2}, 1\right) < \infty$$

$$\left(\phi\left(\tfrac{3}{2}, 1\right) = \frac{1}{\Gamma\left(\frac{3}{2}\right)} \int_0^\infty \frac{\sqrt{t}\, dt}{e^t - 1} = 2.612 \right)$$

→ 粒子数に上限があるのはおかしい

怪しい所

$$N = \sum_{k} \langle n_{k} \rangle$$

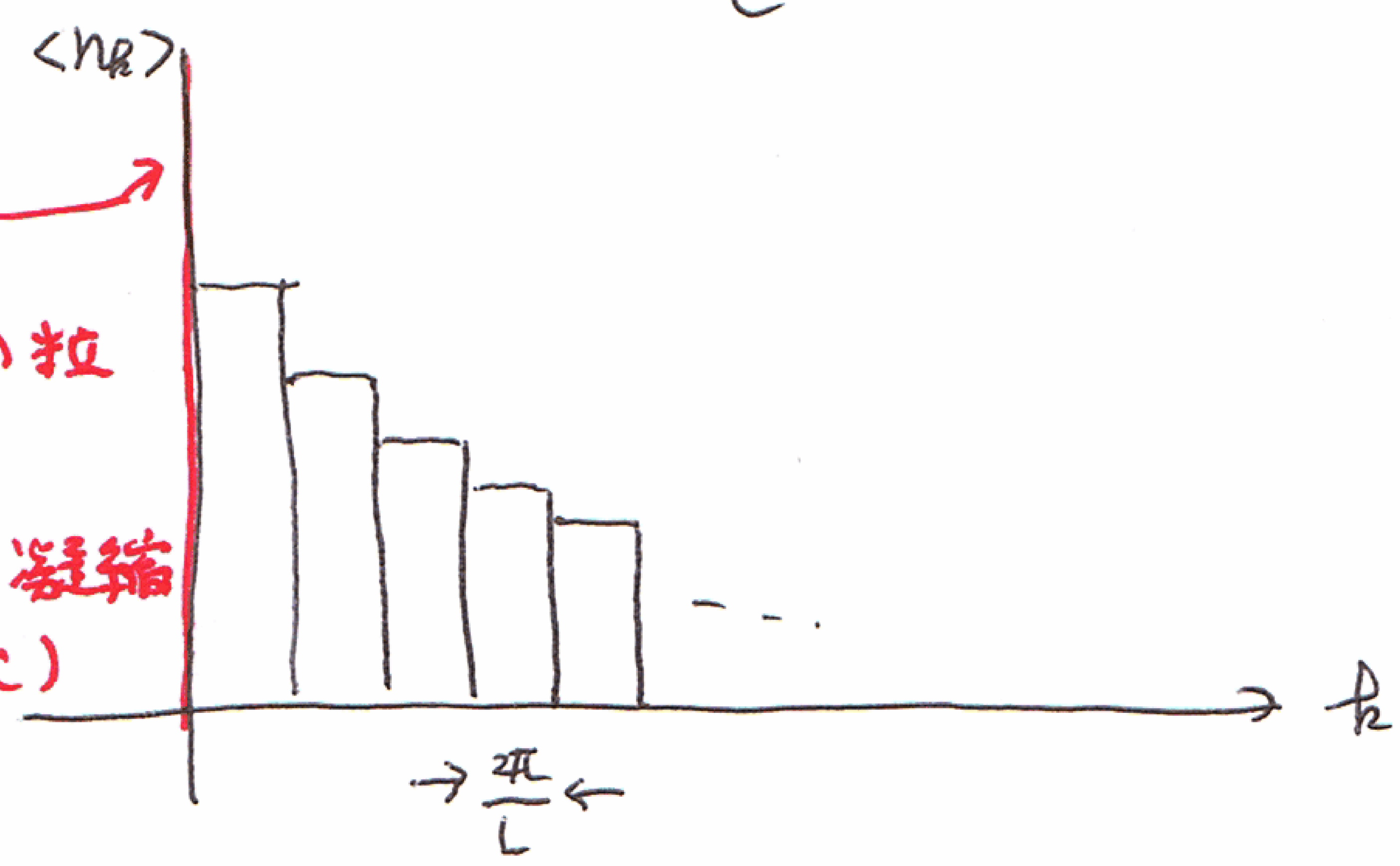
$$= \left(\frac{L}{2\pi} \right)^3 \int_0^\infty (4\pi k^2) \frac{dk}{e^{\beta(E_k - \mu)} - 1}$$

↓ ?

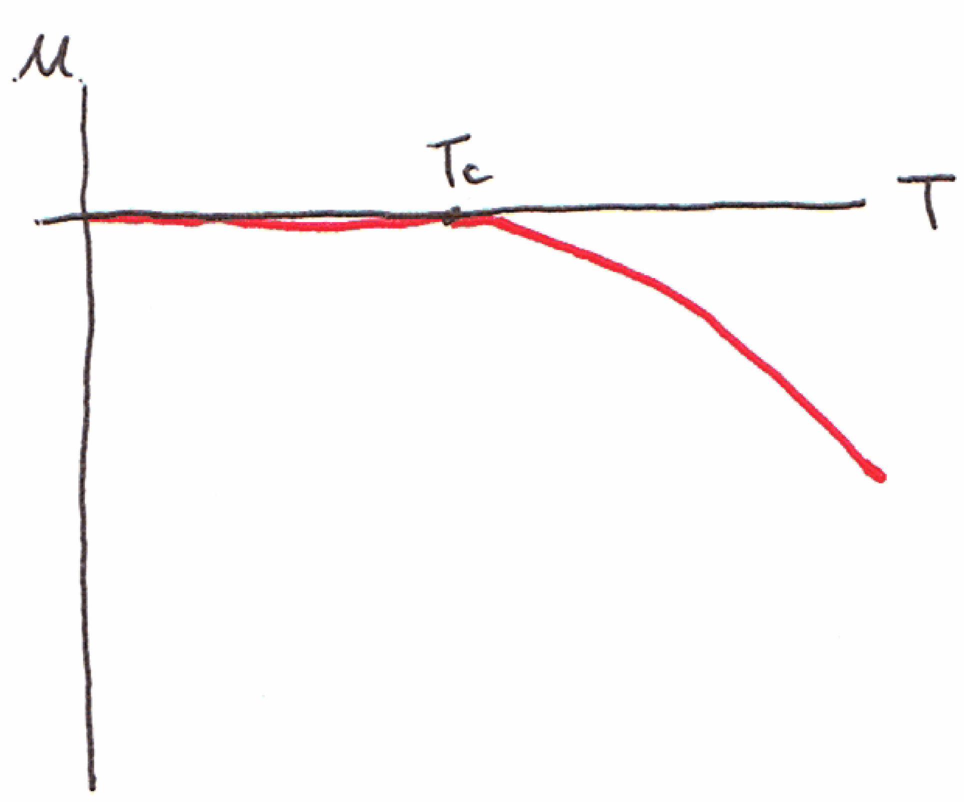
不定

$\Delta N = N - N_{max}$ の粒子が入っている

→ Bose Einstein 凝縮 (BEC)



$k=0$ の時 $\mu \to 0^-$ とすると被積分関数が発散するため、デルタ関数の不定性が生じる



$$N = 2\pi V \left(\frac{2m k_B T_c}{h^2} \right)^{\frac{3}{2}} \Gamma\left(\tfrac{3}{2}\right) \phi\left(\tfrac{3}{2}, 1\right)$$

$$\Leftrightarrow \boxed{T_c = \frac{h^2}{2m k_B} \left[\frac{N}{V} \frac{1}{2\pi \Gamma\left(\frac{3}{2}\right) \phi\left(\frac{3}{2}, 1\right)} \right]^{\frac{2}{3}}}$$

内部エネルギー $(T<T_c)$

$$\langle E\rangle = \int_0^\infty \frac{\varepsilon D(\varepsilon)\,d\varepsilon}{e^{\beta(\varepsilon-\mu)}-1}$$

$$\Big\downarrow \mu=0$$

$$= 2\pi V\left(\frac{2mk_BT}{h^2}\right)^{\frac{3}{2}} k_BT\int_0^\infty \frac{x^{\frac{3}{2}}}{e^x-1}dx$$

$$= 2\pi V\left(\frac{2mk_BT}{h^2}\right)^{\frac{3}{2}} k_BT\,\phi\left(\frac{5}{2},1\right) \propto T^{\frac{5}{2}}$$

圧力

$$\frac{PV}{k_BT} = \ln \Xi = -\sum_{\vec{k}} \ln\left(1-e^{-\beta(E_{\vec{k}}-\mu)}\right)$$

$$= -\frac{V}{(2\pi)^3}\int_0^\infty 4\pi k^2 \ln\left(1-e^{-\beta\left(\frac{\hbar^2k^2}{2m}-\mu\right)}\right)dk$$

$$= -\frac{V}{(2\pi)^3}\frac{4\pi k^3}{3}\ln\left(1-e^{-\beta\left(\frac{\hbar^2k^2}{2m}-\mu\right)}\right)\Bigg|_0^\infty + \frac{V}{(2\pi)^3}\int_0^\infty \frac{4\pi k^2}{3}\,\frac{\frac{\beta\hbar^2}{2m}2k\,e^{-\beta\left(\frac{\hbar^2k^2}{2m}-\mu\right)}}{1-e^{-\beta\left(\frac{\hbar^2k^2}{2m}-\mu\right)}}dk$$

$$= \frac{V}{(2\pi)^3}\int_0^\infty dk\,\frac{\frac{\beta\hbar^2}{2m}\frac{8\pi}{3}k^4}{e^{\beta\left(\frac{\hbar^2k^2}{2m}-\mu\right)}-1}$$

$$\Big\downarrow \varepsilon=\frac{\hbar^2k^2}{2m}$$

$$= \frac{V}{(2\pi)^3}\frac{\beta\hbar^2}{2m}\frac{8\pi}{3}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\frac{m}{\hbar^2}\underbrace{\int_0^\infty d\varepsilon\,\frac{\varepsilon^{\frac{3}{2}}}{e^{\beta(\varepsilon-\mu)}-1}}$$

$$\Big\downarrow x=\beta\varepsilon$$

$$= \beta^{\frac{5}{2}}\int_0^\infty dx\,\frac{x^{\frac{3}{2}}}{e^{x-\beta\mu}-1}$$

$$= \frac{V}{k_BT}\left(\frac{2\pi m}{h^2}\right)^{\frac{3}{2}}(k_BT)^{\frac{5}{2}}\phi\left(\frac{5}{2},e^{\beta\mu}\right) \quad \left(\Gamma\left(\frac{5}{2}\right)=\frac{3}{4}\sqrt{\pi}\right)$$

$$\Leftrightarrow \boxed{P=\left(\frac{2\pi m}{h^2}\right)^{\frac{3}{2}}(k_BT)^{\frac{5}{2}}\phi\left(\frac{5}{2},e^{\beta\mu}\right)=\frac{2}{3}\frac{\langle E\rangle}{V}}$$

$$P = -\left(\frac{\partial U}{\partial V}\right)_{S,N}$$

$$E_k = \frac{\hbar^2}{2m}k^2 \quad \left(\vec{k} = \frac{\pi}{L}(n_x, n_y, n_z)\right)$$

↓体積を変化させる

$$= \alpha L^{-2} = \alpha V^{-\frac{2}{3}} \quad (\alpha はkによらない)$$

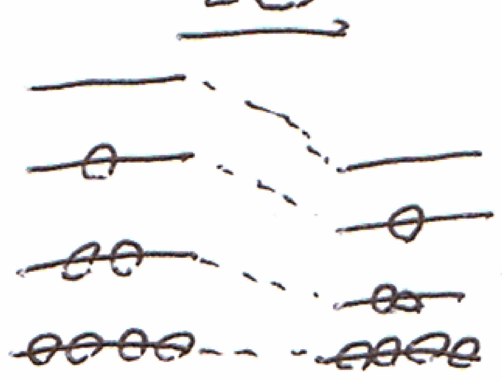
$$\left(\frac{\partial U}{\partial V}\right)_{S,N} = -\frac{2}{3}\alpha V^{-\frac{5}{3}} = -\frac{2}{3}\frac{U}{V} = -P$$

↑

断熱変化：エネルギー準位を占める粒子数が不変となるような変化（遷移しない）

→エントロピー不変に対応

L大



2次元以下でのBEC

$$N = \frac{L^2}{(2\pi)^2}\int_0^\infty 2\pi k\,dk\,\frac{1}{e^{\beta(\varepsilon-\mu)}-1} \quad \downarrow \varepsilon = \frac{\hbar^2 k^2}{2m}$$

$$= \int_0^\infty d\varepsilon\,\frac{D(\varepsilon)}{e^{\beta(\varepsilon-\mu)}-1} \quad \left(D(\varepsilon) = \frac{L^2}{2\pi}\frac{m}{\hbar^2} \cdots \varepsilon によらない\right)$$

$$\mu_{max} = 0$$

$$N_{max} \underset{\uparrow\, x=\beta\varepsilon}{=} \frac{L^2 m^2}{2\pi\hbar^2}k_B T\int_0^\infty \frac{dx}{e^x-1} = \infty$$

有限のNに対して $\mu < 0$

→ $\boxed{\text{2次元でBECは起こらない}}$