BÖLÜM 10

YAKLAŞIKLIK YÖNTEMLERİ

Klasik "Cluster" açılımı:

N molekülü gaz V hacmine kapatılmış, ikişer ikişer etkileşiyorlar.

$$\mathcal{H} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i<j}^{N(N-1)/2} v_{ij}(|\vec r_i - \vec r_j|)$$

$$Q_N(V,T) = \frac{1}{N!\,h^{3N}} \int d^{3N}r \, d^{3N}p \, \exp\left\{-\beta \sum \frac{p_i^2}{2m} - \beta \sum_{i<j} v_{ij}\right\}$$

hesap edilmeli.

$$= \frac{1}{\lambda^{3N} N!} \underbrace{\int d^{3N}r \; e^{-\beta \sum v_{ij}}}_{Z_N}$$

$\lambda = \sqrt{2\pi\hbar^2/mkT}$ ısısal dalga boyu

bu integral konfigürasyonel integraldir.

$$e^{-\beta v_{ij}} - 1 = f_{ij} \qquad \text{Mayer fonk.}$$

└ yüksek sıcaklıklarda küçük değerler alır

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$$Z_N(V,T) \equiv \int d^3r_1 \ldots \int d^3r_N \, e^{-\beta \sum_{i<j} v_{ij}}$$

$$\prod_{i<j} e^{-\beta v_{ij}} \qquad 1+f_{ij}$$

$$\mathcal{Z}(z,V,T) = \sum_{N=0}^{\infty} z^N Q_N$$

$$Q_N = \frac{1}{N!\,\lambda^{3N}} Z_N(V,T)$$

$$\Rightarrow Z_N(V,T) = \int d^3r_1 \ldots d^3r_N \prod_{i<j} (1+f_{ij})$$

$$= \{ 1 + [f_{12} + f_{13} + \ldots]$$
$$+ [f_{12}f_{13} + f_{12}f_{14} + \ldots]$$
$$+ [f_{12}f_{13}f_{14} + \ldots] \ldots \}$$

Her bir terim bir grafik ile temsil edebiliriz

N parçacık grafiği herbiri $1, 2, \ldots, N$ ile numaralanmış çemberlerin bir topluluğu:

Çizgiler ile birleştirilmiş farklı çiftlerin sayısı $\alpha, \beta, \ldots, \gamma$ ise o zaman grafik $\int d^3r_1 \ldots d^3r_N \, f_\alpha f_\beta \ldots f_\gamma$ açılımındaki seçilen terimi temsil eder.

örn $N=3 \Rightarrow$

farklılar.

örn.

özdeş

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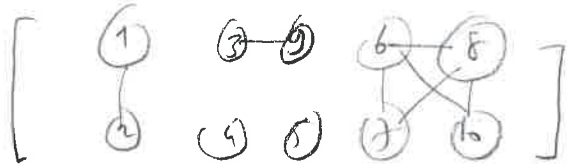
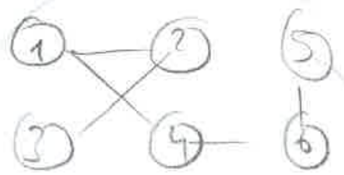
$N=10$

$$\int d^3r_1 \ldots d^3r_{10}\, f_{12}\, f_{39}\, f_{67}\, f_{68}\, f_{8,10}\, f_{6,10}\, f_{78} \equiv$$ 

Her bir çarpan bağlantılı bir grafiğe karşılık gelir.

Z_N N parçacık grafiklerinin toplamı.

l parçacık bağlantılı grafik ile l-küme tanımları. Örneğin

 $= \int d^3r_1 \ldots d^3r_6\, f_{12} f_{23} f_{14} f_{46} f_{56}$

6 küme

bir küme integrali $:= b_l(V,T) = \dfrac{1}{l!\,\lambda^{3(l-1)}V}$ (tüm mümkün l-klasterlerin toplamı

Normalizasyon çarpanı (i) b_l boyutsuz (ii) $V\to\infty$ iken $\lim_{V\to\infty} b_l(V,T)$

$\longrightarrow \bar{b}_l(T)$ sonlu.

olacak şekilde seçilir. (ii) özelliği f_{ij} nin sonlu menzilli olduğunu söyler. Öyleki, l kümede, sadece bir V çarpanına yol açan integrasyon l-parçacığın "ağırlık merkezi" üzerinden integrasyondur.

Bazı klaster integralleri

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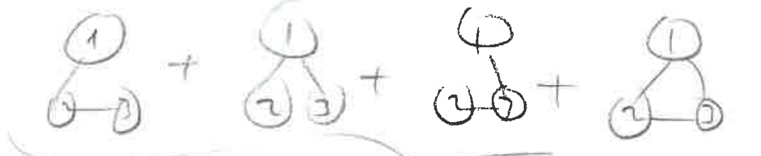
$$b_1 = \frac{1}{V}\,[\,①\,] = \frac{1}{V}\int d^3r_1 = 1$$

$$b_2 = \frac{1}{2!\,\lambda^3 V}\,[\,①—②\,] = \frac{1}{\lambda^3 2V}\int d^3r_1\, d^3r_2\, f_{12} = \frac{1}{2\lambda^3}\int d^3r_{12}\, f_{12}$$

$$b_3 = \frac{1}{3!\,\cancel{\lambda^6}\, V}\,\Big[$$



$$\Big]$$

$$\int d^3r_1\, d^3r_2\, d^3r_3\,[\,f_{12} f_{23} + \cdots\,]$$

$$= \frac{1}{6\cancel{V}\lambda^6}\left[3\cancel{V}\int d^3r_{12}\, d^3r_{13}\, f_{12} f_{13} + \cancel{V}\int d^3r_{12}\, d^3r_{13}\, d^3r_{23}\, f_{12} f_{13} f_{23}\right]$$

$$= 2\,b_2^2 + \frac{1}{6\lambda^6}\int d^3r_{12}\, d^3r_{13}\, d^3r_{23} \cdots$$

m_l tane l klaster var $\ni \displaystyle\sum_{l=1}^{N} l\, m_l = N$

$m_1 = 2 \qquad m_2 = 2 \qquad m_4 = 1$

$2\times 1 + 2\times 2 + 4\times 1 = 10$

$\{m_1, m_2, m_4\}$ ya da $\{Z_1, Z_2, Z_4\}$

$\downarrow$

$\{m_l\}$

$$Z_N = \sum_{\{m_l\}} S\{m_l\}$$

$$= \sum_{P} [○]^{m_1}\,[○–○]^{m_2}\,[\,\cdots + \cdots\,]^{m_3} \cdots$$

$$\frac{N!}{\prod_l (l!)^{m_l}}\;\frac{1}{\prod_l (m_l)!}\;\times\;(l!\,\lambda^{3l-3}\, V b_l)^{m_l}$$

$N!$

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$$\frac{pv}{kT} = \frac{\sum z^l b_l}{\sum l z^l b_l}$$

$$\sum a_l(T) \left(\frac{\lambda^3}{v} \right)^{l-1} = \frac{\sum z^l b_l}{\sum l z^l b_l}$$

$$\sum_{l=1}^{\infty} a_l(T) \left(\sum_{n=1}^{\infty} n b_n z^n \right)^{l-1} \sum l z^l b_l = \sum z^l b_l$$

$$\left(a_1 + a_2 (b_1 z + 2 b_2 z^2 + \cdots) + a_3 (b_1 z + 2 b_2 z^2 + \cdots)^2 + \cdots \right)$$

$$\times \left(b_1 z + b_2 z^2 + \cdots \right) = b_1 z + b_2 z^2 + \cdots$$

z : $\quad a_1 b_1 = b_1 \qquad a_1 = 1$

z^2 : $\quad a_1 2 b_2 + a_2 b_1^2 = b_2 \qquad a_2 = - b_2$

$$a_3 = 4 b_2^2 - 2 b_3$$

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$$= \prod_{\ell} \underbrace{\sum_{m_\ell} \frac{1}{m_\ell!} \left(\frac{V z^\ell b_\ell}{\lambda^3} \right)^{m_\ell}}_{\exp\left(\frac{V z^\ell b_\ell}{\lambda^3} \right)}$$

$$\mathcal{Z}(z, V, T) = \prod_{\ell} \exp\left(\frac{V z^\ell b_\ell}{\lambda^3} \right)$$

$$= \exp\left[\frac{V}{\lambda^3} \sum z^\ell b_\ell \right]$$

$$\frac{1}{V} \ln \mathcal{Z} = \frac{1}{\lambda^3} \sum z^\ell b_\ell$$

$$\frac{P}{kT} = \frac{1}{\lambda^3} \sum_{\ell=1}^{\infty} z^\ell b_\ell$$

$$\frac{1}{v} = \frac{1}{\lambda^3} \sum_{\ell=1}^{\infty} \ell z^\ell b_\ell$$

$V \to \infty$ limitinde

$$\frac{P}{kT} = \frac{1}{\lambda^3} \sum_{\ell} z^\ell \bar{b}_\ell(T)$$

$$\frac{1}{v} = \frac{1}{\lambda^3} \sum \ell \bar{b}_\ell(T) z^\ell$$

$$\frac{Pv}{kT} = \sum_{\ell=1}^{\infty} a_\ell(T) \left(\frac{\lambda^3}{v} \right)^{\ell-1}$$

Virial kats.

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$$S\{m_\ell\} = N! \prod_\ell \frac{(V\lambda^{3\ell-3} b_\ell)^{m_\ell}}{m_\ell!}$$

$\lambda^{3\ell m_\ell}$ λ

$$\prod_\ell (\lambda^{3\ell-3})^{m_\ell} = \frac{1}{\lambda^3} \prod \lambda^{3\ell m_\ell}$$

$$\lambda^{3\sum \ell m_\ell} = \prod_\ell \lambda^{3\ell m_\ell}$$

$$? = N! \lambda^{3N} \prod_\ell \frac{1}{m_\ell!} \left(\frac{V b_\ell}{\lambda^3}\right)^{m_\ell}$$

$$Q_N(V,T) = \sum_{\{m_\ell\}} \prod_\ell \frac{1}{m_\ell!} \left(\frac{V b_\ell}{\lambda^3}\right)^{m_\ell}$$

? $\sum \ell m_\ell = N$ bundan dolayı Q_N 'i hesaplayamayız.

$$\mathcal{L}(z,V,T) = \sum z^N Q_N$$

$$z^N = z^{\sum \ell m_\ell} = \prod_\ell z^{\ell m_\ell} = \prod_\ell (z^\ell)^{m_\ell}$$

$$= \sum_N \sum_{(m_\ell)} \prod_\ell \frac{1}{m_\ell!} \left(\frac{z^\ell V b_\ell}{\lambda^3}\right)^{m_\ell}$$

$$\sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \cdots \sum_{m_\ell=0}^{\infty}$$

$$= \sum_{m_1, m_2, \ldots, m_\ell} \prod_\ell \frac{1}{m_\ell!} \left(\frac{V z^\ell b_\ell}{\lambda^3}\right)^{m_\ell}$$

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$\vec r_1, \dots, \vec r_N$ koordinatlarını

A ← → B iki gruba ayıralım.

$\vec r_A$ $\vec r_B$

$\vec r_i$ $\vec r_j$

bu farklı gruplara ait $\vec r_i$, $\vec r_j$ koordinatları

$$|\vec r_i - \vec r_j| \gg r_0$$

$$|\vec r_i - \vec r_j| \gg \lambda$$

kopyalama sağlanırlar: $W_N(1\dots N) = W_A(\vec r_A)\, W_B(\vec r_B)$

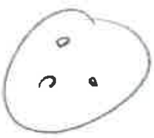
$N = 2$ $W_2(1,2) \to W_1(1)\, W_2(2)$ $|\vec r_1 - \vec r_2| \to \infty$ iken.

$W_2(1,2) = W_1(1)\, W_2(2) + U_2(1,2)$ tanımlayalım.

$$\left.\begin{matrix} U_2(1,2) \\ |\vec r_1 - \vec r_2| \to \infty \end{matrix}\right\} \to 0 \text{ olsun.}$$

bunun integrali ($\vec r_1, \vec r_2$ üzerinden) → klasikteki 2 klaster'ın anlamı.

$\Downarrow$



$$W_1(1) = 1$$

$$W_2(1,2) = U_1(1)\, U_1(2) + U_2(1,2)$$

$$W_3(1,2,3) = U_1(1)\, U_1(2)\, U_1(3) + U_1(1)\, U_2(2,3)$$
$$+\, U_1(2)\, U_2(3,1) + U_1(3)\, U_2(1,2) + U_3(1,2,3)$$

$\vdots$

$$W_N(1,\dots,N) = \sum_{\{m_l\}} \sum_P \Big[\underbrace{U_1(\ )\dots U_1(\ )}_{m_1 \text{ faktör}}\Big]\Big[\underbrace{U_2(\ ,\ )\dots U_2(\ ,\ )}_{m_2}\Big]\dots\Big[\underbrace{U_N(\ ,\ ,\dots,\ )}_{m_N}\Big]$$

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10.2 Kuantum Cluster Açılımı

N özdeş parçacık V hacminde bulunsun. Sistemin Hamilton fonk.u;

$$\mathcal{H} = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \sum_{i<j} v_{ij}$$

$$Q_N(V,T) = \mathrm{Tr}\,(e^{-\beta\mathcal{H}})$$

$$= \int d^{3N}\vec{r} \sum_\alpha \psi_\alpha^*(1,2,\ldots,N)\, e^{-\beta\mathcal{H}}\, \psi_\alpha(1,2,\ldots,N)$$

$\{\psi_\alpha\}$ ort. DF nın tam kümü.

tanım:

$$W_N(1,\ldots,N) \equiv N!\,\lambda^{3N} \sum_\alpha \psi_\alpha^*(1\ldots N)\, e^{-\beta\mathcal{H}}\, \psi_\alpha(1,\ldots,N)$$

$$\Rightarrow Q_N(V,T) = \frac{1}{N!\,\lambda^{3N}} \int d^{3N}r\, W_N(1,\ldots,N)$$

[yüksek sıcaklıkta → klasik limit

$$\hat{W} \equiv N!\,\lambda^{3N}\, e^{-\beta\mathcal{H}}$$ olasılık yoğ. op.

$$\langle 1\ldots N|\hat{W}|1\ldots N\rangle = W$$]

W özellikleri:

a) $W_1(1) = 1$ proof: $\left(= W_1(\vec{r}_1) = \frac{\lambda^3}{V}\sum_p \cancel{e^{-i\vec{p}\cdot\vec{r}_1/\hbar}}\, e^{-\beta\hbar^2\nabla^2/2m}\, \cancel{e^{i\vec{p}\cdot\vec{r}_1/\hbar}} \right.$

$$\left. = (\lambda/\hbar)^3 \int d^3p\, e^{-\beta p^2/2m} = 1 \right)$$

b) $W_N(1\ldots N)$ sym.

c) W_N invar. Uniter dön. altında

proof: → var.

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$$\sum_l l\, m_l = N$$

$U_l \to W_N{}'$ $\quad N' \leq l$

l kılastır $b_l(V,T)$ integrali

$$b_l(V,T) \equiv \frac{1}{l!\,\lambda^{3l-3} V} \int d^3r_1 \ldots d^3r_l\, U_l(1,\ldots,l)$$

$$\lim_{V\to\infty} b_l(V,T) = b_l(T)$$

Şimdi BE nin kılastır integralleri cinsinden yazılabileceğini göstereceğiz

$$\frac{1}{\lambda^{3N}} = \prod \frac{1}{\lambda^{3 l m_l}}$$

$$\int d^3r\, W_N(1,\ldots N) = \sum_{\{m_l\}} \frac{N!}{(1!)^{m_1}(2!)^{m_2}\ldots \times m_1!\ldots} \int d^{3N}r\, [(U_1\ldots U_1)(U_2\ldots)\ldots]$$

$$= N! \sum_{\{m_l\}} \frac{1}{m_1!}\left[\frac{1}{1!}\int d^3r_1\, U_1(1)\right]^{m_1} \frac{1}{m_2!}\left[\frac{1}{2!}\int d^3r_1 d^3r_2\, U_2(1,2)\right]^{m_2}\cdots$$

$$= N! \sum_{\{m_l\}} \prod_{l=1}^{N} \frac{(V\lambda^{3l-3} b_l)^{m_l}}{m_l!} = N!\,\lambda^{3N} \sum_{\{m_l\}} \prod_{l=1}^{N} \frac{1}{m_l!}\left(\frac{V}{\lambda^3} b_l\right)^{m_l}$$

$$Q_N(V,T) = \frac{1}{\lambda^{3N}} \sum_{m_l} \prod_l \frac{1}{m_l!}[V\lambda^{3l-3} b_l]^{m_l}$$

$$= \sum_{m_l} \prod_l \frac{1}{m_l!}\left(\frac{V b_l}{\lambda^3}\right)^{m_l}$$

$$b_l^{(0)} = \begin{cases} l^{-5/2} & (BE) \\ (-1)^{l+1} l^{-5/2} & (FD) \end{cases}$$

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$$b_2 - b_2^{(0)} = \frac{1}{2\lambda^3 V} \int d^3R\, d^3r \left[W_2(1,2) - W_2^{(0)}(1,2) \right]$$

$$= 2\sqrt{2} \int d^3r \sum_n \left[|\psi_n(r)|^2 e^{-\beta \epsilon_n} - |\psi_n^{(0)}(r)|^2 e^{-\beta \epsilon_n^0} \right]$$

$$= 2\sqrt{2} \sum_n \left(e^{-\beta \epsilon_n} - e^{-\beta \epsilon_n^0} \right)$$

$$b_2^{(0)} = \begin{cases} 2^{-5/2} & \text{Bose gaz} \\ -2^{-5/2} & \text{Fermi gaz} \end{cases} \qquad \epsilon_n^{0} = \frac{\hbar^2 k^2}{m}$$

$$\epsilon_n = \frac{\hbar^2 k^2}{m} + \epsilon_B$$ iki parçacık bağlı durumu.

$g(k)\,dk$: $k - k+dk$ aralığındaki dalga sayısının durumlar sayısı olsun.

$g^{(0)}(k)\,dk$: etkileşmeyenlerinki olsun.

$$b_2 - b_2^{(0)} = 2^{3/2} \left\{ \sum_B e^{-\beta \epsilon_B} + \int_0^\infty dk \left[g(k) - g^{0}(k) \right] e^{-\beta \hbar^2 k^2/m} \right\}$$

$(\lambda / \lambda_{cm})^{3/2}$

bağıl dalga boyu KM ninkini

Faz kayması

$$g(k) - g^{(0)}(k) = \frac{1}{\pi} \sum_l{}' (2l+1) \frac{\partial \eta_l(k)}{\partial k} \qquad l = \begin{cases} 0, 2, \ldots & \text{BE} \\ 1, 3, 5, \ldots & \text{FD} \end{cases}$$

ispatı var!

$$= 2^{3/2} \left\{ \sum_B e^{-\beta \epsilon_B} + \frac{\lambda^2}{\pi^2} \sum_l{}' (2l+1) \int dk\, k\, \eta_l(k)\, e^{-\beta \hbar k^2/m} \right\}$$

<u>İspat</u>:

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10.3. $2^{\underline{nd}}$ Virial Katsayı

b_2 için $W_2(1,2)$ hesaplanacak.

$$\mathcal{H} = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) + v(|\bar{r}_1 - \bar{r}_2|)$$

$$\mathcal{H}\psi_\alpha(1,2) = E_\alpha \psi_\alpha(1,2)$$

$$\vec{R} = \frac{1}{2}(\bar{r}_1 + \bar{r}_2) \qquad \vec{r} = (\bar{r}_2 - \bar{r}_1) \Big\} \quad \psi_\alpha(1,2) = \frac{1}{\sqrt{V}} e^{i\vec{P}\cdot\vec{R}} \psi_n(\bar{r})$$

$$E_\alpha = \frac{P^2}{2M} + \epsilon_n \qquad \alpha \equiv (\vec{P}, n)$$

<u>rel. mot</u> : $\left(-\frac{\hbar^2}{m}\nabla^2 + v(r)\right)\psi_n(r) = \epsilon_n \psi_n(r)$

$$\int d^3\bar{r}\, |\psi_n(\bar{r})|^2 = 1$$

$$W_2(1,2) = 2\lambda^6 \sum_\alpha |\psi_\alpha(1,2)|^2 e^{-\beta E_\alpha}$$

$$= \frac{2\lambda^6}{V} \sum_{\vec{P},n} |\psi_n(r)|^2 e^{-\beta\frac{P^2}{4m}} e^{-\beta\epsilon_n}$$

$$\frac{1}{V}\sum_P e^{-\beta P^2/4m} \rightarrow \int dP\, P^2 e^{-\beta P^2/4m} = \frac{2^{3/2}}{\lambda^3}$$

$$= 2^{5/3}\lambda^3 \sum_n |\psi_n(r)|^2 e^{-\beta\epsilon_n}$$

$$W_2^{(0)}(1,2) = 2^{5/2}\sum_n |\psi_n^{(0)}(r)|^2 e^{-\beta\epsilon_n}$$ etkileşmeyen parçacıklar

10.49 – 10.47 $\quad b_2 = \frac{1}{2\lambda^3 V}\int d^3r_1\, d^3r_2\, U_2(1,2)$

$$= \frac{1}{2\lambda^3 V}\int d^3\bar{R}\, d^3\bar{r}\,[W_2(1,2) - 1]$$

BS K

$$\psi_{klm} = A_{klm}\, Y_l^m\, \frac{u_{kl}(r)}{r}$$

$$\psi^{(0)}_{klm} = A^{(0)}_{klm}\, Y_l^m\, \frac{u^{(0)}_{kl}(r)}{r}$$

$\psi(\vec r) = \psi(-\vec r)$ (BE) $\qquad \psi(\vec r) = -\psi(\vec r)$ FD

$u_{kl}(R) = u^{(0)}_{kl}(R) = 0$ für certain vereich

$$u_{kl}(r) \xrightarrow[r\to\infty]{} \sin\left(kr + \frac{l\pi}{2} + \eta_l(k)\right)$$

$$u^{0}_{kl}(r) \xrightarrow[r\to\infty]{} \sin\left(kr + \frac{l\pi}{2}\right)$$

$kR + \frac{l\pi}{2} + \eta_l(k) = n\pi$ (int.)

$kR + \frac{l\pi}{2} = n\pi$ (non-int) $\qquad n = 0, 1, 2, \ldots$

l'ye bağlı m'ye değil $(2l+1)$ katlı dejenere.

$$\Delta k = \frac{\pi}{R + \frac{\partial \eta_l}{\partial k}}$$

$$\Delta k^0 = \frac{\pi}{R}$$

$$(k+\Delta k)R + \frac{l\pi}{2} + \eta_l(k+\Delta k) = (n+1)\pi$$

$$kR + \frac{l\pi}{2} + \eta_l = n\pi$$

$$\Delta k R + \underbrace{\eta_l(k+\Delta k) - \eta(k)}_{\Delta k \frac{\partial \eta}{\partial k}} = \pi$$

$$g_l(k)\,\Delta k = 2l+1$$

$$g_l^0(k)\,\Delta k = (2l+1)$$

$$\Rightarrow \quad g_l(k) - g_l^0(k) = \frac{2l+1}{\pi}\,\frac{\partial \eta_l(k)}{\partial k}$$

BS K

10.4. Varyasyon Methodu

<u>Gibbs yöntemi</u> : ρ normalize yoğ. fonk. u (klasik ya da QM sel topluluk için)

reel ve poz. (klasik)

pozitif özdeğerli termalsel QM

$$\mathrm{Tr}\,\rho = 1 \qquad (\#)$$

Klasik durumda $\Rightarrow$ $\mathrm{Tr} \to \int dp\, dq$

$$\psi(\rho) \equiv \mathrm{Tr}(\mathcal{H}\rho) + \frac{1}{\beta}\mathrm{Tr}(\rho \ln \rho)$$ tanımlayalım.

(a) $\psi(\rho)$ yu min. yapan (# koşulu altında) bir varyasyon.

$\psi(\rho)$ yu ext yapan $\bar{\rho}$ (kT ye ait yoğ. fonk. u)

(b) Helmholtz serb. enerji $A = \psi(\bar{\rho})$ olacaktır.

Lagrange çarpanı

$$\delta\psi(\rho) + \lambda\,\delta\,\mathrm{Tr}(\rho) = 0 \qquad \delta^2\psi(\rho) \geq 0 \text{ olmalı.}$$

$$\mathrm{Tr}\left(\mathcal{H}\,\delta\rho + \frac{1}{\beta}(1+\ln\rho)\,\delta\rho + \lambda\,\delta\rho\right) = 0$$

$$\mathcal{H} + \frac{1}{\beta}(1+\ln\bar{\rho}) + \lambda = 0$$

$$\ln\bar{\rho} = -\beta\mathcal{H} - \beta\lambda - 1$$

$$\bar{\rho} = e^{-\beta\mathcal{H} - \beta\lambda - 1} \qquad \boxed{\bar{\rho} = e^{-\beta\mathcal{H}} \Big/ \mathrm{Tr}\, e^{-\beta\mathcal{H}}}$$

$$\psi(\bar{\rho}) = \mathrm{Tr}\left\{\mathcal{H}\,\cancel{\frac{e^{-\beta\mathcal{H}}}{\mathrm{Tr}\,e^{-\beta\mathcal{H}}}} + \frac{1}{\cancel{\beta}}\,\cancel{\frac{e^{-\beta\mathcal{H}}}{\mathrm{Tr}\,e^{-\beta\mathcal{H}}}}\left(-\cancel{\beta\mathcal{H}} - \ln\mathrm{Tr}\,e^{-\beta\mathcal{H}}\right)\right\}$$

$1/\beta$

$$= -kT \ln Q_N$$

BS K

Pierles Prensibi: $Q = \mathrm{Tr}\, e^{-\beta H}$

$$Q \geq \sum_n e^{-\beta(\phi_n, H\phi_n)}$$

(tst, ilah heyfi bir DF u)

H nin öz fonk. u ⇒ (=) geçerli. $f(x)$ konveks bir fonk. olsun

($f''(x) > 0$ olsun.) $\overline{f(x)} \equiv \sum C_n f(x_n)$: $\{x_n\}$ keyfi reel sayılar kümesi

$C_n \geq 0 \quad \sum C_n = 1$

$$f(x) = f(\bar{x}) + \frac{1}{2}(x-\bar{x})^2 f''(\bar{x}) + \dots$$ ort. değ. teoremi.

$$\overline{f} = \overline{f(\bar{x})} + \frac{1}{2}\overline{(x-\bar{x})^2 f''(\bar{x})} + \dots$$

$$\overline{f}(x) \geq \overline{f(\bar{x})}$$

Φ_n tam küme; [H özfonk larına $\{f_n\}$]

$$\Phi_n = \sum_m S_{nm} f_m \qquad \sum_m |S_{nm}|^2 = 1$$

$$(\Phi_n, H\Phi_n) = \sum_m |S_{nm}|^2 E_m$$

$\sum_n e^{-\beta E_n}$

$$Q = \sum_n (\Phi_n, e^{-\beta H}\Phi_n) = \sum_{n,m} |S_{nm}|^2 e^{-\beta E_m}$$

$$q = \sum_n e^{-\beta(\Phi_n, H\Phi_n)} = \sum_n e^{-\beta \sum_m |S_{nm}|^2 E_m}$$

$f(x) = e^{-\beta x}$ olsun.

BS K

$$\bar{E}_n = \sum_m |S_{nm}|^2 E_m$$

$$\overline{f(E)}_n = \sum_m |S_{nm}|^2 f(E_m)$$

$$Q - q = \sum_n [\overline{f(E)}_n - f(\bar{E}_n)] \geq 0 \quad **$$

Teorem gibi.

Pseudopot. yöntemi: Seyreltik bir gaz, bunu oluşturan moleküller bağlı durum oluşturacak şekilde etkileşmiyorlar. iki parçacık arası etk. sonlu potansiyellerle daech.

1. λ termal DB $\sim \frac{1}{T}$; $T \to 0$ $\lambda \to \infty$
2. $v^{1/3}$ ort. parçacıklar arası uzaklık
3. a saçılma uzunluğu

parçacığın λ dalga boyu içerisinde 2. bir parçacığın bulunma olasılığı yok.

(a) bir parçacık tarafından hissedilen etkin etkileşme küçük

(b) pot. in ayrıntıları önemsiz.

$\frac{a}{\lambda}$, $\frac{v^{1/3}}{\lambda}$ mertebesinde işlem yapıyoruz.

İki parçacık için:

$$\mathcal{H} = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) + u(r)$$

$$u(r) = \begin{cases} \infty & r > a \\ 0 & r < a \end{cases}$$ katı küre pot.

$H\Psi = E\Psi$ çözülecek $\Psi = \Psi(\bar{r}_1, \bar{r}_2)$

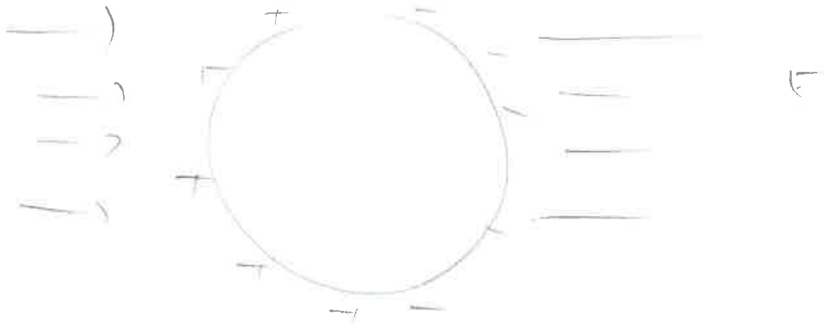
$$\Psi(\bar{r}_1, \bar{r}_2) = e^{i\vec{P}\cdot\vec{R}}\,\psi(r)$$

$$\bar{R} = \frac{\bar{r}_1 + \bar{r}_2}{2} \qquad \bar{r} = \bar{r}_1 - \bar{r}_2$$

$$(\nabla^2 + k^2)\, \psi(r) = 0 \qquad r > a$$

$$\psi(r) = 0 \qquad r \le a$$

$$E = \frac{\vec{P}^2}{2M} + \epsilon = \frac{\vec{P}^2}{2M} + \frac{\hbar^2 k^2}{2\mu}$$



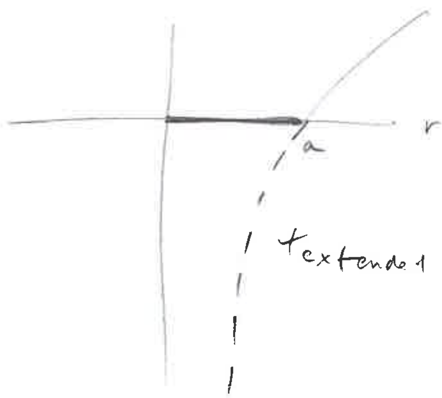
küresel simetrik s-dalga çözümü : düşük enerji $(k \to 0)$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{d\psi}{dr}\right) = 0 \qquad r > a$$

$$\psi(r) = 0 \qquad r \le a$$

$$r^2 \frac{d\psi}{dr} = B \qquad \psi = A + \frac{B}{r}$$

$$\psi = \begin{cases} \text{Sbt}\left(1 - \frac{a}{r}\right) & r > a \\ 0 & r \le a \end{cases}$$



$$(\nabla^2 + k^2)\, \psi_{ext}(r) = 0 \qquad r > a$$

$$\psi_{ext}(a) = 0 \qquad r = a$$

r = 0 da tanımlı değil.
sınır koşulu ile

$k \to 0$ için $\quad \psi_{ext} \xrightarrow[r \to 0]{} \left(1 - \frac{a}{r}\right)$ — r → ∞ daki koşulları sağlayacak şekilde sbt.

BS K

$$\frac{\partial}{\partial r}\left(r\psi_{ext}\right)\Big|_{r\to 0} \cancel{=}$$

0 değil

$$\nabla^2 \psi_{ext}(r) \xrightarrow[r\to 0]{} 4\pi a\, \delta(r) \cancel{}$$

hayır

$$\to 4\pi a \delta(r) \frac{\partial}{\partial r}\left(r\psi_{ext}\right)$$

$$(\nabla^2 + k^2)\, \psi_{ext}(r) = \underbrace{4\pi a\, \delta(r) \frac{\partial}{\partial r}}\left(r\psi_{ext}\right)$$

$v(r)$'i $r=0$ da geçerli olan pseudopot.

(a)

tam çözüm yapılmış olsaydı. $-\frac{4\pi}{k\cot\eta_0}\,\delta(r)\,\frac{\partial}{\partial r}r$

$$-\frac{1}{k\cot\eta_0} = \frac{\tan ka}{k} = a\left[1+\frac{1}{3}(ka)^2+\cdots\right]$$

(b) ℓ dalga pseudopot. için

$a^{2\ell+1}$ ile orantılı bir terim bulunur.

$$\frac{\hbar^2}{\gamma}(\nabla^2+k^2)\,\psi(r) = v(r)\,\psi(r)$$

düşük enerjilerde, s-dalgası çözümleri $\psi(r) \equiv \frac{u(r)}{r}$

$$u'' + k^2 u = \frac{\gamma}{\hbar^2}\, v(r)\, u(r)$$

$r\to 0$ için $u(r)$ çözümleri asimptotik

$$u_\infty(r) = r\psi_\infty(r) = \text{sbt}\,(\sin kr + \tan\eta_0 \cos kr)$$

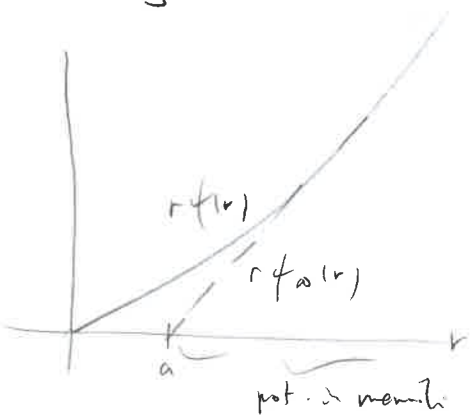
$$\psi_\infty(r) \xrightarrow[r\to 0]{} \text{sbt}\left(1+\frac{\tan\eta_0}{kr}\right)$$

$$k\cot\eta_0 = -\frac{1}{a} + \frac{1}{2}k^2 r_0$$

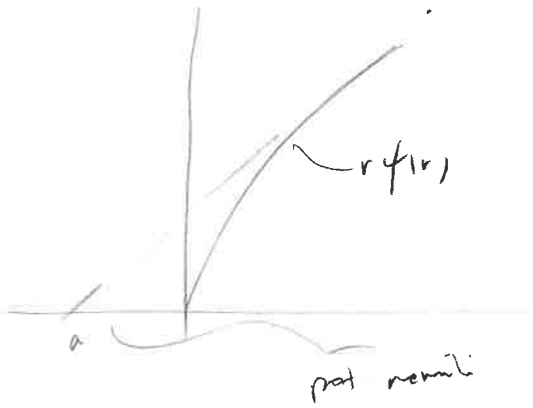
a : saçılma uzunluğu, r_0 : etkin menzil.

$$r_0 = \frac{2a}{3}$$

itici pot.

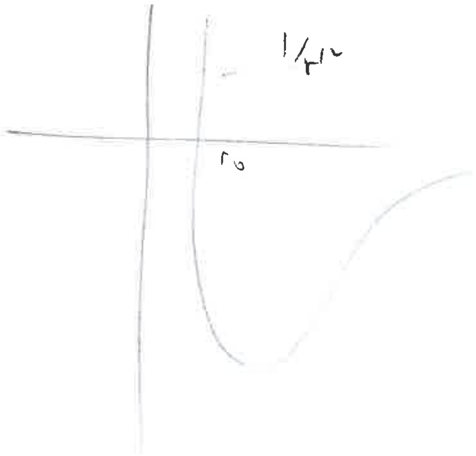


çekici pot



BS K

$$u(r) = \frac{A}{r^{12}} - \frac{B}{r^{6}}$$



$$u(r) = \begin{cases} +\infty & r < r_0 \\ -u_0 \left(\frac{r_0}{r}\right)^6 & r > r_0 \end{cases}$$

$$a_2 = -b_2 = \frac{2\pi}{\lambda^3} \int_0^\infty \left(1 - e^{-u/kT}\right) r^2 \, dr$$

$u_0/kT \ll 1$

$\Rightarrow 1 - e^{-u/kT}$

$\rightarrow -\frac{u_0}{kT}\left(\frac{r_0}{r}\right)^6$

$$a_2 = \frac{2\pi}{\lambda^3}\left(\frac{r_0^3}{3}\right)\left(1 - \frac{u_0}{kT}\right)$$

$$\frac{Pv}{kT} = \sum_{l=1}^{\infty} a_l(T) \left(\frac{\lambda^3}{v}\right)^{l-1}$$

$$= 1 + \frac{2\pi}{\cancel{\lambda^3}} \frac{r_0^3}{3} \left(1 - \frac{u_0}{kT}\right) \frac{\cancel{\lambda^3}}{v}$$

$$P = \frac{kT}{v}\left(1 + \frac{B_2(T)}{v}\right) \qquad \underbrace{B_2(T)}_{\text{2. virial kats.}} = a_2 \lambda^3 = \frac{2\pi r_0^3}{3}\left(1 - \frac{u_0}{kT}\right)$$

$$= \frac{kT}{v}\left\{1 + \frac{1}{v}\frac{2\pi r_0^3}{3}\left(1 - \frac{u_0}{kT}\right)\right\}$$

$$P + \frac{kT}{v^2}\frac{2\pi r_0^3}{3kT} u_0 = \frac{kT}{v}\left\{1 - \frac{1}{v}\frac{2\pi r_0^3}{3}\right\}^{-1}$$

$$\left(P + \underbrace{\frac{2\pi r_0^3 u_0}{3v^2}}_{a}\right)\left(v - \underbrace{\frac{2\pi r_0^3}{3}}_{b}\right) = kT$$

BS K

10.1.

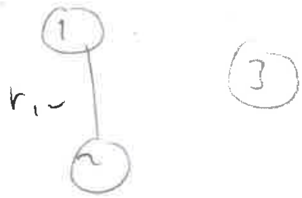
$$v(r) = \begin{cases} \infty & r \le r_0 \\ 0 & r > r_0 \end{cases}$$

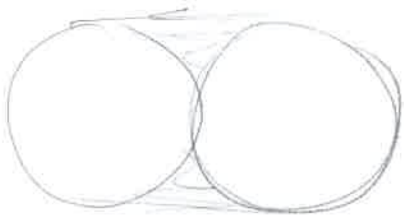
$$f(r) = e^{-\beta v(r)} - 1 = \begin{cases} -1 & r \le r_0 \\ 0 & r > r_0 \end{cases}$$

$$a_2 = -b_2 = \frac{1}{2\lambda^3}\int d^3 r_{12}\, f_{12} = \frac{1}{2\lambda^3}\int_0^{r_0} 4\pi r^2\, dr = \frac{2\pi}{\lambda^3}\frac{r_0^3}{3}$$

$$a_3 = -\frac{1}{3\lambda^6}\iiint f_{12} f_{13} f_{23}\, d^3 r_{12}\, d^3 r_{13}$$

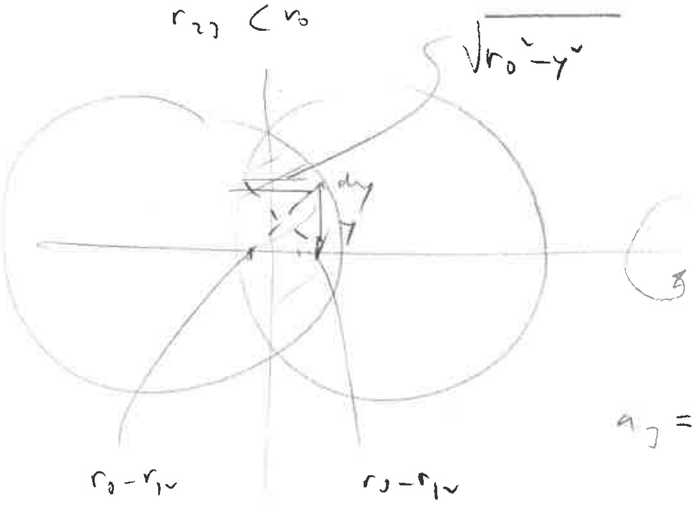
$$= \frac{1}{3\lambda^6}\int_0^{r_0}\left(\int d^3 r_{13}\right) d^3 r_{12}$$





$r_{13} < r_0$

$r_{23} < r_0$



$$2\sqrt{r_0^2-y^2}-r_{12}$$

$$\int d^3 r_{13} = \int_0^{[r_0^2-(\frac{r_{12}}{2})^2]^{1/2}} \left\{ 2(r_0^2-y^2)^{1/2} - r_{12} \right\} 2\pi y\, dy$$

$$= \frac{4\pi}{3}\left\{ r_0^3 - \frac{3 r_0^2 r_{12}}{4} + \frac{r_{12}^3}{16} \right\}$$

$$a_3 = \frac{1}{3\lambda^6}\int_0^{r_0} \left\{ \quad \right\} d^3 r_{12} = \frac{5\pi^2 r_0^6}{18\lambda^6}$$

BS K

2.

$$F_2 - F_2^0 = 2^{3/2}\left[\sum_\ell (2\ell+1)\int_0^\infty dk\, k\,\eta_\ell(k)\, e^{-\beta\hbar^2k^2/m}\right]$$

hard sphere $\tan\eta_\ell(ka) = \frac{j_\ell(ka)}{n_\ell(ka)}$

$j_0(ka) = \frac{\sin ka}{ka}$ $\quad n_0(ka) = -\frac{\cos ka}{ka}$

yerine koy ve integrali al!

$\eta_0(ka) = -ka$

3. $Q \geq \sum_n e^{-\beta(\phi_n, H, \phi_n)}$

$$H = -\epsilon\sum_{\langle ij\rangle}\bar\sigma_i\cdot\bar\sigma_j - \mu\sum_{i=1}^{N}\bar\sigma_i\cdot\bar H \quad \text{Heisenberg}$$

$$= -\epsilon\sum_{\langle ij\rangle} s_i s_j - \mu\sum_{i=1}^{N} s_i H \quad \text{Ising}$$

$H = H_0\hat z$

$\langle\alpha_i\alpha_j|H|\alpha_i\alpha_j\rangle_{\uparrow\uparrow} = -\epsilon\gamma$

$\langle\alpha_i\alpha_j|H|\alpha_i\alpha_j\rangle_{\downarrow\downarrow} =$

$$Q \geq e^{-\beta\langle H\rangle_{\uparrow\uparrow}} + e^{-\beta\langle H\rangle_{\downarrow\downarrow}}$$

$$\geq e^{\beta\left(\frac{\epsilon N\gamma}{4}+N\mu H_0\right)} + e^{-\beta\langle}$$

BS K

$$Q_N = \frac{1}{N!}\left(e^{-\beta\epsilon_0} + e^{-\beta\epsilon_1} + \cdots\right)^N$$

$$\sum_{\bar p} e^{-\beta\epsilon_{\bar p}} = V\left(\frac{mkT}{2\pi\hbar^2}\right)^{3/2} \Rightarrow \frac{V}{h^3}\int_0^\infty dp\, 4\pi p^2 e^{-\beta p^2/2m}$$

BKT $$\mathcal{Z}(z,V,T) = \prod_{\bar p} \frac{1}{1-ze^{-\beta\epsilon_p}}$$ Bose

$$\left(\prod_{\bar p}\left(1+ze^{-\beta\epsilon_p}\right)\right)$$ Ferm

$N = \sum_{\bar p} n_{\bar p}$ den dolayı kolayca hesaplanamaz.

$$\frac{PV}{kT} = \ln\mathcal{Z}(z,V,T) = \begin{cases} -\sum_{\bar p}\ln\left(1-ze^{-\beta\epsilon_p}\right) & BE \\ \sum_{\bar p}\ln\left(1+ze^{-\beta\epsilon_p}\right) & FD \end{cases}$$

$$N = z\partial_z \ln\mathcal{Z}(z,V,T) = \begin{cases} \sum_{\bar p}\dfrac{ze^{-\beta\epsilon_p}}{1-ze^{-\beta\epsilon_p}} & BE \\ \sum_{\bar p}\dfrac{ze^{-\beta\epsilon_p}}{1+ze^{-\beta\epsilon_{\bar p}}} & FD \end{cases}$$

$$\langle n_{\bar p}\rangle = \frac{1}{\mathcal{Z}}\sum_{N=0} z^N \sum_{\substack{\{n_p\} \\ N=\sum_p n_p}} n_{\bar p}\, e^{-\beta\sum_p \epsilon_{\bar p} n_{\bar p}} = -\frac{1}{\beta}\partial_{\epsilon_{\bar p}}\ln\mathcal{Z}$$

$$= \frac{ze^{-\beta\epsilon_p}}{1\mp ze^{-\beta\epsilon_p}}$$ BE & FD

BS K

Ideal Fermi D.

$$\begin{cases} P/kT = \dfrac{4\pi}{h^3} \displaystyle\int_0^\infty dp\, p^2 \ln\left(1 + z e^{-\beta p^2/2m}\right) \\[2ex] \dfrac{1}{v} = \dfrac{4\pi}{h^3} \displaystyle\int_0^\infty dp\, p^2 \dfrac{1}{z^{-1} e^{\beta p^2/2m} + 1} \end{cases}$$

$$\frac{V}{N} \qquad z\partial_z \ln \mathcal{Z}$$

$$\begin{cases} P/kT = \dfrac{1}{\lambda^3} f_{5/2}(z) \\[2ex] 1/v = \dfrac{1}{\lambda^3} f_{3/2}(z) \end{cases} \qquad \lambda = \sqrt{2\pi\hbar^2/mkT}$$

$$f_{5/2}(z) = \frac{4}{\sqrt{\pi}} \int_0^\infty dx\, x^2 \ln\left(1 + z e^{-x^2}\right) = \sum_{\ell=1}^{\infty} \frac{(-1)^{\ell+1} z^\ell}{\ell^{5/2}}$$

$$f_{3/2}(z) \equiv z\, \partial_z f_{5/2}(z) = \sum_{\ell=1}^{\infty} \frac{(-1)^{\ell+1} z^\ell}{\ell^{3/2}}$$

Ideal Bose E

$$P/kT = -\frac{4\pi}{h^3} \int dp\, p^2 \ln\left(1 - z e^{-\beta p^2/2m}\right) - \frac{1}{V} \ln(1-z)$$

$p=0$ a hozzá[illegible] [illegible]

$$\frac{1}{v} = \frac{4\pi}{h^3} \int_0^\infty dp\, p^2 \frac{1}{z^{-1} e^{\beta p^2/2m} - 1} + \frac{1}{V} \frac{z}{1-z} \quad \langle n_0 \rangle$$

$z \to 1$ a gázokban Bose E. kondenzáció v.v. [illegible] egy Tabon [illegible] [illegible].

BS K

$$P/kT = \frac{1}{\lambda^3} g_{5/2}(z) - \frac{1}{V} \ln(1-z)$$

$$1/v = \frac{1}{\lambda^3} g_{3/2}(z) + \frac{1}{V} \frac{z}{1-z}$$

$$g_{5/2}(z) = -\frac{4}{\sqrt{\pi}} \int_0^\infty dx\, x^2 \ln(1 - z e^{-x^2}) = \sum_{\ell=1}^{\infty} \frac{z^\ell}{\ell^{5/2}}$$

$$g_{3/2}(z) \equiv z \partial_z g_{5/2}(z) = \sum_{\ell=1}^{\infty} \frac{z^\ell}{\ell^{3/2}}$$

$\langle n_0 \rangle / V \to$ [illegible]

BS K

BS K

1

$$\mathcal{L}(z,V,T) = \sum_{N=0}^{\infty} z^N Q_N(V,T) = \sum_{n_{\vec p}} g\{n_{\vec p}\}\, e^{-\beta E\{n_{\vec p}\}}$$

$$E\{n_{\vec p}\} = \sum_{\vec p} n_{\vec p}\, \epsilon_{\vec p}$$

$$g\{n_{\vec p}\} = \begin{cases} 1 & \text{FD - BE} \\ 1 \Big/ \prod_{\vec p} n_{\vec p}! & \text{Boltz.} \end{cases}$$

$$= \sum_N \sum_{\substack{\{n_{\vec p}\} \\ \sum n_{\vec p} = N}} z^N e^{-\beta \sum_{\vec p} \epsilon_{\vec p} n_{\vec p}}$$

$$= \sum_N \sum_{\{n_{\vec p}\}} \prod_{\vec p} \left(z e^{-\beta \epsilon_p}\right)^{n_{\vec p}}$$

$\underbrace{\sum n_{\vec p} = N}$

Çift top. her bir $n_{\vec p}$ yi ayrı ayrı bağımsız toplayacaksın demek

$$= \sum_{n_0} \sum_{n_1} \cdots \left[\left(z e^{-\beta \epsilon_0}\right)^{n_0} \left(z e^{-\beta \epsilon_1}\right)^{n_1} \cdots \right]$$

$$= \left(\sum_{n_0} \left(z e^{-\beta \epsilon_0}\right)^{n_0} \right) \left(\sum_{n_1} \left(z e^{-\beta \epsilon_1}\right)^{n_1} \right) \cdots$$

$$= \prod_{\vec p} \left[\sum_n \left(z e^{-\beta \epsilon_p}\right)^n \right]$$

$n = 0, 1, 2, \ldots$ BE

$= 0, 1$ FD

$$\sum_n x^n = \begin{cases} 1 + x & \text{FD} \\ \dfrac{1}{1-x} & \text{BE} \end{cases}$$

$$= \prod_{\vec p} \begin{cases} 1 + z e^{-\beta \epsilon_p} & \text{FD} \\ \dfrac{1}{1 - z e^{-\beta \epsilon_p}} & \text{BE} \end{cases}$$

BS K

$$\frac{PV}{kT} = \ln \mathcal{Z}(z, V, T) = \sum_{\vec{p}} \begin{cases} \ln\left(1 + z e^{-\beta \epsilon_p}\right) & \text{FD} \\ -\ln\left(1 - z e^{-\beta \epsilon_p}\right) & \text{BE} \end{cases}$$

$$N = z \partial_z \ln \mathcal{Z}(z, V, T) = \sum_{\vec{p}} \begin{cases} \dfrac{z e^{-\beta \epsilon_p}}{1 - z e^{-\beta \epsilon_p}} & \text{BE} \\ \dfrac{z e^{-\beta \epsilon_p}}{1 + z e^{-\beta \epsilon_p}} & \text{FD} \end{cases}$$

$$\langle n_{\vec{p}} \rangle \equiv \frac{1}{\mathcal{Z}} \sum_{N=0}^{\infty} z^N \sum_{n_{\vec{p}}} n_{\vec{p}}\, e^{-\beta \sum_{\vec{p}} \epsilon_{\vec{p}} n_{\vec{p}}} = -\left(1/\beta\right) \partial_{\epsilon_{\vec{p}}} \ln \mathcal{Z} = \frac{z e^{-\beta \epsilon_p}}{1 \mp z e^{-\beta \epsilon_p}}$$