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Statistikus fizika ⟷ Termodinamika

makroszkópikus leírás

Nagy részecskeszám

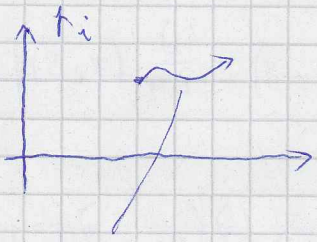
pl.: $N \sim 10^{23}$

kétállapotú r. $2^{10^{23}}$

mikroszkópikus leírás

klasszikus kvantumos

pl.: N db klasszikus részecske



fázistér: 6N dim

$H(p,q) = E = \text{const}$

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}$$

$$\dot{q}_i = \frac{\partial H}{\partial p_i}$$

trajektóriák:

- nem metszik egymást
- önmagukat nem

Gibbs-halmaz

$\rho(p,q)$ valószínűség-eloszlás

Liouville - tétel

$$\frac{dg}{dt}$$

All.: $$\frac{\partial g}{\partial t} + \sum_i \left(\frac{\partial g}{\partial r_i} \dot{r}_i + \frac{\partial g}{\partial q_i} \cdot \dot{q}_i \right) = 0$$

Biz.: $$\underline{v} = (\dot{r}_i, \dot{q}_i)$$

$$-\frac{d}{dt} \int dV \cdot g = \int d\underline{F} \cdot \underline{v}\, g$$

$$\int_V dV \left(\frac{\partial g}{\partial t} + \operatorname{div}(g \underline{v}) \right) = 0$$

$$\downarrow$$

$$\frac{\partial}{\partial r_i}, \frac{\partial}{\partial q_i}$$

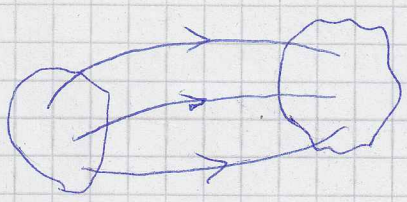
$$\frac{\partial g}{\partial t} + \operatorname{div}(g \cdot \underline{v}) = \frac{\partial g}{\partial t} + \sum_i \left(\frac{\partial}{\partial r_i}(\dot{r}_i g) + \frac{\partial}{\partial q_i}(\dot{q}_i g) \right) =$$

$$= \frac{\partial g}{\partial t} + \sum_i \left(\frac{\partial g}{\partial r_i} \cdot \dot{r}_i + \frac{\partial g}{\partial q_i} \cdot \dot{q}_i \right) + \sum_i \left(\frac{\partial \dot{r}_i}{\partial r_i} + \frac{\partial \dot{q}_i}{\partial q_i} \right) g$$

$$\downarrow$$

$$-\frac{\partial^2 H}{\partial r_i \partial q_i} + \frac{\partial^2 H}{\partial q_i \partial r_i} = 0$$

□



$$\int dV\, g = \int d\dot{V} \cdot \dot{g}$$

$$0 = \frac{dg}{dt} = \frac{\partial g}{\partial t} + \sum_i \left(\frac{\partial H}{\partial r_i} \cdot \frac{\partial g}{\partial q_i} - \frac{\partial g}{\partial r_i} \cdot \frac{\partial H}{\partial q_i} \right) = \frac{\partial g}{\partial t} + \{H, g\}$$

Egyensúlyban $\frac{\partial \varrho}{\partial t} = 0 \Rightarrow \{H, \varrho\} = 0$

Gibbs-sokaság $\varrho(\Gamma, q)$

$X(\Gamma, q)$ fizikai mennyiség

időátlag / sokaságátlag

$$\frac{1}{T}\int_0^T X \, dt \qquad \langle X \rangle = \int X(\Gamma, q)\, \varrho(\Gamma, q) \cdot d\Gamma$$

ergodikus-tétel

$$d\Gamma = \frac{d^{(3N)}\Gamma \cdot d^{(3N)}q}{N! \cdot h^{3N}}$$

↓

Gibbs-paradoxon

$\varrho = ?$

$$H(\Gamma, q) = \sum_{i=1}^{3N} \frac{\Gamma_i^2}{2m} + \sum U(q_i) + \frac{1}{2}\sum_{i,j} V(q_i, q_j)$$

↑ falak

↓ kh.

ténfogatfüggés

Nem ismerjük a rendszer állapotát!

Esetleg ismerünk néhány makroszkópikus mennyiséget, pl. E, V, N

Kitérő: Shannon-féle információs entrópia

$\{\uparrow_k\}_{k=1}^{\uparrow}$ $\qquad \sum_k \uparrow_k = 1$

Def.: $S = -\sum_k \uparrow_k \log_2 \uparrow_k = -\langle \log_2 \uparrow \rangle$

információ, bit

Fej / írás

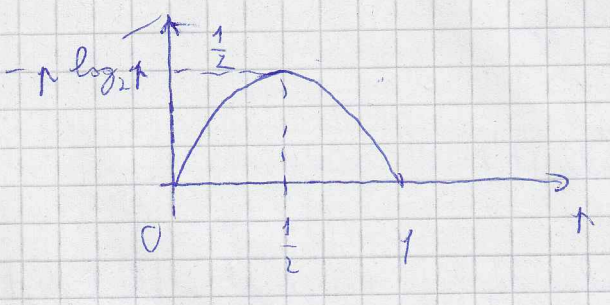
$$S = \left(-\frac{1}{2}\log_2\frac{1}{2}\right) + \left(-\frac{1}{2}\log_2\frac{1}{2}\right) = -\log_2\frac{1}{2} = \log_2 2 = 1$$

S tulajdonságai

1) $S = 0$, ha $\uparrow_i = \begin{cases} 1 & i = k \\ 0 & i \neq k \end{cases}$

biztos információ

2) $S = \max$, ha $\uparrow_i = \uparrow$ $\forall i$-re



egyenletes eloszlás (min. információ) max entrópia tartozik

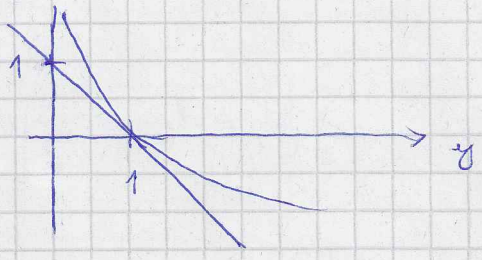
$$S = -\lambda \sum_i \uparrow_i \ln \uparrow_i \qquad \lambda = \frac{1}{\ln 2}$$

Biz.: Segédtétel:

$$\sum_i q_i \left(\ln \frac{q_i}{\tau_i} \right) \geq 0 \qquad \text{tetsz. } \{\tau_i\} \quad \{q_i\}$$

ha $\tau_i = q_i$ / egyenlőség van

Biz.: $-\ln y \geq 1 - y$



$$y = \frac{\tau_i}{q_i} \qquad -\ln \frac{\tau_i}{q_i} \geq 1 - \frac{\tau_i}{q_i}$$

$$\ln \frac{q_i}{\tau_i} \geq 1 - \frac{\tau_i}{q_i}$$

$$q_i \ln \frac{q_i}{\tau_i} \geq q_i - \tau_i \qquad / \sum_i$$

$$\sum_i q_i \ln \frac{q_i}{\tau_i} \geq \sum_i (q_i - \tau_i) = 0$$

áll.: $S\{\tau\} \geq S\{q\}$, ahol $\tau_i = \tau \ \forall i \qquad \tau = \frac{1}{n}$

q_i tetszőleges

$$-\lambda \sum_i \tau_i \ln \tau_i \geq -\lambda \sum_i q_i \ln q_i$$

$$-\lambda \cdot n \cdot \frac{1}{n} \ln \tau \geq -\lambda \sum_i q_i \ln q_i$$

$$\sum_i q_i \ln q_i \geq \ln \tau$$

$$0 \le \sum_i q_i \ln q_i - \ln \underbrace{\left(\sum_i q_i \right)}_{1} \quad \leftarrow \text{bizonyítandó}$$

$$0 \le \sum_i q_i \left(\ln q_i - \ln p_i \right) = \sum_i q_i \ln \left(\frac{q_i}{p_i} \right) \ge 0$$

3) tulajdonság

Ha $p_{ik} = u_i \cdot v_k \qquad \sum_i u_i = 1 \qquad \sum_k v_k = 1$

Ill: $S\{p\} = S\{u\} + S\{v\}$

Biz:

$$S\{p\} = -\lambda \sum_{i,k} p_{ik} \ln p_{ik} =$$

$$= -\lambda \sum_{i,k} u_i \cdot v_k \ln (u_i \cdot v_k) =$$

$$= -\lambda \sum_{i,k} u_i \cdot v_k \ln u_i - \lambda \sum_{i,k} u_i \cdot v_k \ln v_k =$$

$$= -\lambda \sum_i u_i \ln u_i - \lambda \sum_k v_k \ln v_k =$$

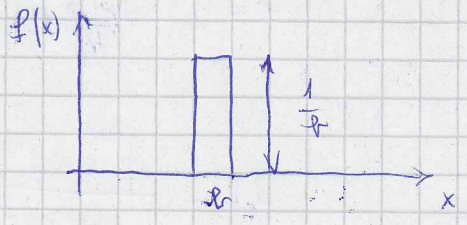
$$= S(\{u\}) + S(\{v\})$$

Folytonos eloszlás

$$S = -\lambda \int_{-a}^{+a} f(x) \ln f(x) \, dx$$

2) és 3) tulajdonság teljesül

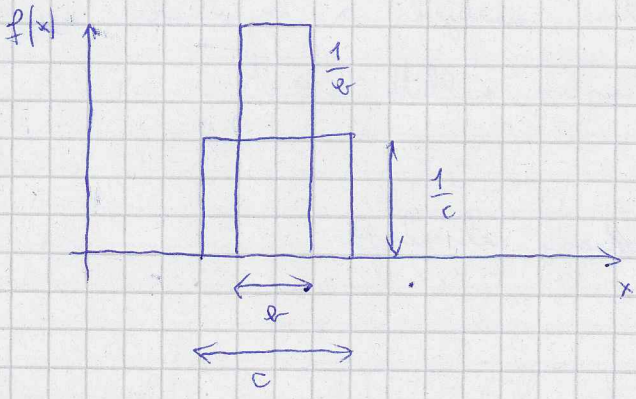
1) tul. em triv



$\varepsilon \to 0$

$\delta(x)$

$$S = -\lambda \int f(x) \ln f(x)\, dx = -\lambda \frac{1}{\varepsilon} \cdot \ln\left(\frac{1}{\varepsilon}\right) \cdot \varepsilon = \lambda \ln \varepsilon \xrightarrow{\varepsilon \to 0} -\infty$$



$\varepsilon \le c$

$\ln \varepsilon \le \ln c$

$S_\varepsilon \le S_c$

Statisztikus fizika:

$$S = -k_B \int \rho \ln \rho \cdot d\Gamma = -k_B \langle \ln \rho \rangle$$

$$[k_B] = \frac{J}{K}$$

$S\{\rho\}$ funkcionál

<u>tkp - posztulátum</u>: Olyan ρ-t kell választani, amelyik S-t maximálissá teszi, a (~~maradéknak~~) rendszerről rendelkezésre álló információ mellett

$$S = -\lambda \sum_i p_i \ln p_i \quad \longleftrightarrow \quad S = -\lambda \int f(x) \ln f(x)\, dx$$

Stat. fiz. $\quad S = -k \int \varrho \ln \varrho \, d\Gamma \qquad k = 1{,}380 \cdot 10^{-23} \frac{J}{K}$

(ha a részecskeszám is változhat:

$$S = -k \sum_N \int \varrho_N \ln \varrho_N \, d\Gamma_N \quad)$$

$$d\Gamma = \frac{d^{(3N)} \cdot d^{(3N)} \cdot dt}{N! \cdot h^{3N}}$$

klasszikus postulátum:

Olyan ϱ-t kell választani, amelyik a rendszerről rendelkezésre álló információ mellett S-et maximálissá teszi

$\varrho \equiv$ egyensúlyi sokaság eloszlásfv.

1) Mikrokanonikus sokaság

zárt rendszer E, N, V

$$E < \mathcal{H}(p,q) < E + \delta E$$

(E, δE: adott)

$$S\{\varrho\} = -k \int_{E<\mathcal{H}<E+\delta E} \varrho \ln \varrho \cdot d\Gamma \quad \text{és} \quad \int_{E<\mathcal{H}<E+\delta E} \varrho \, d\Gamma = 1 \quad \text{mellékfeltétel}$$

$$\delta \left\{ -k \int \varrho \ln \varrho \, d\Gamma + k\lambda \left(\int \varrho \, d\Gamma - 1 \right) \right\} = 0$$

$$\delta S = -k \int \left(\delta \varrho \ln \varrho + \varrho \cdot \frac{1}{\varrho} \cdot \delta \varrho + \lambda \delta \varrho \right) d\Gamma = 0$$

$$= -k \cdot \int \left(\ln \varrho + 1 + \lambda \right) \delta \varrho \, d\Gamma = 0$$

$$\Rightarrow \ln \varrho = \text{konst}$$

$$\Omega = \int_{E < \mathcal{H} < E + \delta E} d\Gamma$$

$$\varrho = \begin{cases} \frac{1}{\Omega} & , \text{ha } E < \mathcal{H}(r, p) < E + \delta E \\ 0 & , \text{különben} \end{cases}$$

$$\boxed{S = -k \int \varrho \ln \varrho \, d\Gamma} = -k \int \frac{1}{\Omega} \ln \frac{1}{\Omega} \, d\Gamma =$$

$$= -k \ln \frac{1}{\Omega} = \boxed{k \cdot \ln \Omega}$$

$\Omega(E, N, V)$

δE - től ki fog derülni, hogy lényegtelen

Tömegdefektus

$^2H \rightarrow 0{,}1\%$

$^4He \rightarrow 0{,}7\%$

$Fe \rightarrow 0{,}8\% - 0{,}9\%$

Ionizációs energia 13,5 eV $\rightarrow 10^{-8}$ tömegtelen.

2) Kanonikus sokaság, eloszlás

adott $\langle \mathcal{H} \rangle$, N, V, energia fluktuál

Lagrange-multiplikátor

$S\{\varrho\} = \max$, ha $\int \varrho \, d\Gamma = 1$ $\quad (-k\lambda)$

$\int \mathcal{H} \varrho \, d\Gamma = \langle \mathcal{H} \rangle$ rögzített $\quad (-k\beta)$

$$\delta S = -k \int \left[\ln \varrho + 1 + \lambda + \beta \mathcal{H} \right] \delta \varrho \, d\Gamma = 0$$

$$\varrho = e^{-1-\lambda-\beta\mathcal{H}}$$

$$1 = \int \varrho \, d\Gamma = e^{-1-\lambda} \underbrace{\int e^{-\beta\mathcal{H}} \, d\Gamma}_{Z} \Rightarrow e^{-1-\lambda} = Z^{-1}$$

kanonikus állapotösszeg

$$\varrho = \frac{1}{Z} e^{-\beta\mathcal{H}}$$

$\varrho' \rightarrow \int \varrho' \mathcal{H} \, d\Gamma = \langle \mathcal{H} \rangle$ tetszőleges rögzített eloszlás

$$\int \varrho' \, d\Gamma = 1$$

$$S' = -k \int \varrho' \ln \varrho' \, d\Gamma \leq -k \int \varrho' \ln \varrho \, d\Gamma$$

Segédtétel: $\sum_i q_i \ln \frac{q_i}{r_i} \geq 0$

$$-\sum_i q_i \ln q_i \leq -\sum_i q_i \ln r_i$$

→ folytonos változóra általánosítjuk

$$S' \leq -k \int \dot{\varrho} \ln \varrho \, d\Gamma = -k \int \dot{\varrho} (-\beta \mathcal{H} - \ln Z) \, d\Gamma =$$

$$= k \ln Z + k\beta \langle \mathcal{H} \rangle = S$$

$$S = -k \int \varrho \ln \varrho \, d\Gamma = -k \int \varrho (-\beta \mathcal{H} - \ln Z) \, d\Gamma =$$

$$= k\beta \langle \mathcal{H} \rangle + k \ln Z$$

□

3) Nagykanonikus sokaság

kitartály és részecske-reservoire

adott V, $\langle \mathcal{H} \rangle$, $\langle N \rangle$

$$\sum_N \int \varrho_N \, d\Gamma_N = 1 \qquad \rightarrow -k\lambda$$

$$\sum_N \int \mathcal{H} \varrho_N \, d\Gamma_N = \langle \mathcal{H} \rangle \rightarrow -k\beta$$

$$\sum_N \int N \varrho_N \, d\Gamma_N = \langle N \rangle \rightarrow -k\alpha$$

$$S = -k \sum_N \int \left\{ \rho_N \ln \rho_N + (\lambda \rho_N - 1) + (\beta \mathcal{H} \rho_N - 1) + (\alpha N \rho_N - 1) \right\} d\Gamma_N$$

$$= \max$$

$$\delta S = -k \sum_N \int \left\{ \ln \rho_N + 1 + \lambda + \beta \mathcal{H} + \alpha N \right\} \delta \rho_N \, d\Gamma_N = 0$$

$$\rho_N = e^{-1-\lambda-\beta\mathcal{H}-\alpha N}$$

$$1 = \sum_N \int \rho_N \, d\Gamma_N = e^{-1-\lambda} \sum_N \int e^{-\beta\mathcal{H}-\alpha N} \, d\Gamma_N$$

$$e^{1+\lambda} = \sum_N \int e^{-\beta\mathcal{H}-\alpha N} \, d\Gamma_N = Q$$

$$\rho_N = \frac{1}{Q} e^{-\beta\mathcal{H}-\alpha N}$$

$$S = -k \sum_N \int \rho_N \ln \rho_N \, d\Gamma_N = -k \sum_N \int \rho_N \left[-\ln Q - \beta\mathcal{H} - \alpha N \right] d\Gamma_N =$$

$$= k \ln Q + k\beta \langle \mathcal{H} \rangle + k\alpha \langle N \rangle$$

$$\left.\frac{\partial S}{\partial \langle \mathcal{H} \rangle}\right|_{\langle N \rangle, V} = k \left.\frac{\partial \ln Q}{\partial \langle \mathcal{H} \rangle}\right|_{\langle N \rangle, V} + k\beta + k\langle N \rangle \cdot \left.\frac{\partial \alpha}{\partial \langle \mathcal{H} \rangle}\right|_{\langle N \rangle, N} + k\langle \mathcal{H} \rangle \left.\frac{\partial \beta}{\partial \langle \mathcal{H} \rangle}\right|_{\langle N \rangle, V}$$

$$= k \cdot \frac{1}{Q} \left.\frac{\partial Q}{\partial \langle \mathcal{H} \rangle}\right|_{\langle N \rangle, V} = k \cdot \frac{1}{Q} \sum_N \int d\Gamma_N \, e^{-\beta\mathcal{H}-\alpha N} \cdot$$

$$\cdot \left[(-\mathcal{H}) \left.\frac{\partial \beta}{\partial \langle \mathcal{H} \rangle}\right|_{\langle N \rangle, V} + (-N) \left.\frac{\partial \alpha}{\partial \langle \mathcal{H} \rangle}\right|_{\langle N \rangle, V} \right]$$

$$= -k \langle \mathcal{H} \rangle \left.\frac{\partial \beta}{\partial \langle \mathcal{H} \rangle}\right|_{\langle N \rangle, V} - k \langle N \rangle \left.\frac{\partial \alpha}{\partial \langle \mathcal{H} \rangle}\right|_{\langle N \rangle, V}$$

$$\left.\frac{\partial S}{\partial \langle \mathcal{H} \rangle}\right|_{\langle N \rangle, V} = k\beta = \frac{1}{T} \quad \text{def.} \qquad \beta = \frac{1}{kT}$$

$$\left.\frac{\partial S}{\partial \langle N \rangle}\right|_{\langle \mathcal{H} \rangle, V} = \dots = k \cdot \alpha = -\frac{\mu}{T} \quad \Rightarrow \quad \alpha = -\beta\mu$$

$$\rho_N = \frac{1}{Q} e^{-\beta \mathcal{H} - \alpha N} = \frac{1}{Q} e^{-\beta(\mathcal{H} - \mu N)}$$

helstlstó: $S = \max$

$V = \text{áll.}$ $\qquad dS = \frac{1}{T} dE - \frac{\mu}{T} dN$

$$\Downarrow$$

$$dE = T\,dS + \mu\,dN$$

<u>Mikrokanonikus</u> $\qquad E, V, N$

$$\Omega(E, V, N) = \int d\Gamma$$

$$E < \mathcal{H}(p, q) < E + \Delta E$$

$$S = k \ln \Omega$$

Kanonikus

$\langle \mathcal{H} \rangle, N, V$

$$\varrho = \frac{1}{Z} e^{-\beta \mathcal{H}}, \quad Z = \int e^{-\beta \mathcal{H}} \, d\Gamma$$

$$S = k\beta \langle \mathcal{H} \rangle + k \ln Z \quad \Rightarrow \quad T \cdot S = \langle \mathcal{H} \rangle + kT \ln Z$$

$$F = \langle \mathcal{H} \rangle - TS = -kT \ln Z$$

Nagykanonikus

$\langle \mathcal{H} \rangle, \langle N \rangle, V$

$$\varrho_N = \frac{1}{Q} e^{-\beta(\mathcal{H} - \mu N)}$$

$$Q = \sum_N \int e^{-\beta(\mathcal{H} - \mu N)} \, d\Gamma_N$$

$$T \cdot S = kT \cdot \ln Q + \langle \mathcal{H} \rangle - \mu N$$

$$\Phi(T, \mu, N) = \langle \mathcal{H} \rangle - TS - \mu N = -kT \ln Q$$

$$S = k \cdot \ln Q + k\beta \langle \mathcal{H} \rangle - \frac{\mu}{T} \langle N \rangle$$

$$T \cdot S = kT \ln Q + \langle \mathcal{H} \rangle - \mu \langle N \rangle$$

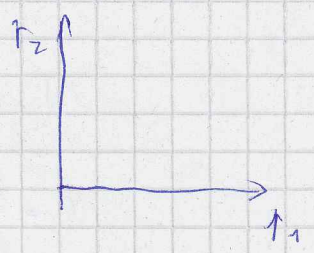
} kondíciót finomít

Példa: Ω-ra:

$$\Omega = \frac{1}{N! \cdot h^{3N}} \int_{E < \mathcal{H}(r,q) < E + \delta E} d^{3N} r \, d^{3N} q$$

legyen $\mathcal{H}(p,q) = \sum_{i=1}^{3N} \frac{p_i^2}{2m}$

$$\Omega(E,V,N) = \frac{V^N}{N! \cdot h^{3N}} \int_{E<\mathcal{H}<E+\delta E} d^{3N}p$$



$2mE = \sum_i p_i^2 \rightarrow$ 3N dimenziós, $\underbrace{\sqrt{2mE}}_{R}$ sugarú gömb

gömb térfogata: $C(N) \cdot R^{3N}$

gömb felszíne: $\tilde{C}(N) \cdot R^{3N-1}$ $\qquad \tilde{C}(N) = 3N \cdot C(N)$

gömbhéj térf.: $\tilde{C}(N) R^{3N-1} \cdot \delta R$

$R = \sqrt{2mE}$

$\delta R = \sqrt{2m} \frac{1}{2\sqrt{E}} \delta E = \frac{\sqrt{2m}}{2} E^{-\frac{1}{2}} \cdot \delta E$

Pl.: $\Omega(E,N,V,\delta E)$ kiszámítása

a) H. g.

$$\Omega(E,V,N,\delta E) = \frac{1}{N! \cdot h^{3N}} \int_{E<\mathcal{H}<E+\delta E} d^{3N}p \; d^{3N}q$$

$$\mathcal{H}(p,q) = \sum_{i=1}^{3N} \frac{p_i^2}{2m} = E$$

$$\sum_{i=1}^{3N} r_i^2 = \underbrace{\left(\sqrt{2mE}\right)^2}_{R}$$

$3N$ dim gömb

$$R = \sqrt{2mE}$$

$$dR = \sqrt{2m} \cdot \frac{1}{2\sqrt{E}} \delta E = (2m)^{\frac{1}{2}} \cdot \frac{1}{2} \cdot E^{-\frac{1}{2}} \cdot \delta E$$

$3N$ dim gömb

térfogata $C(N) \cdot R^{3N}$

felülete $\tilde{C}(N) \cdot R^{3N-1}$

gömbhéja $\tilde{C}(N) \cdot R^{3N-1} \cdot dR$

$$\downarrow$$

$$\tilde{C}(N) \cdot (2mE)^{\frac{3N-1}{2}} \cdot (2m)^{\frac{1}{2}} \cdot \frac{1}{2} E^{-\frac{1}{2}} \cdot \delta E =$$

$$= \tilde{C}(N) \cdot (2m)^{\frac{3N}{2}} \cdot E^{\frac{3N}{2}-1} \cdot \frac{1}{2} \delta E$$

$$\Omega = \frac{V^N}{N! \cdot h^{3N}} \cdot \frac{\tilde{C}(N)}{2} \cdot (2m)^{\frac{3N}{2}} \cdot E^{\frac{3N}{2}-1} \cdot \delta E$$

$$S = k_B \ln \Omega = k_B \left[N \ln V + \underbrace{\left(\frac{3N}{2} - 1\right)}_{\approx} \ln E + \ln \delta E + \text{const}(N) \right]$$

a) $\frac{3N}{2}$

b) $\frac{3N}{2} \ln E \gg \ln \delta E$

$$S = k_B N \ln V + k_B \frac{3N}{2} \ln E + \widetilde{\text{const.}}(N)$$

b) Harmonic oscillator

$$\mathcal{H} = \sum_{i=1}^{3N} \left(\frac{p_i^2}{2m} + \frac{1}{2} m \omega^2 q_i^2 \right) = \sum_{i=1}^{6N} p_i^2 \to E$$

$$p_i^2 = \begin{cases} \frac{p_i^2}{2m} & i = 1, \dots, 3N \\ \frac{1}{2} m \omega^2 q_i^2 & i = 3N, \dots, 6N \end{cases}$$

$$\Omega = \frac{1}{h^{3N}} \int_{E < \mathcal{H} < E + \delta E} dP_i^{6N}$$

$$R = \sqrt{E} \to dR = \frac{1}{2\sqrt{E}} \delta E$$

n dim gömb felszíne: $2 \cdot \frac{\pi^{\frac{n}{2}}}{\Gamma(\frac{n}{2})} R^{n-1}$

$$\Omega = \frac{1}{h^{3N}} \cdot 2 \cdot \frac{\pi^{3N}}{\Gamma(3N)} \cdot E^{\frac{6N-1}{2}} \cdot \frac{1}{2\sqrt{E}} \delta E$$

$$\downarrow$$

$$E^{3N-1}$$

$$\ln \Gamma(3N) = \ln (3N-1)! \approx (3N-1) \ln (3N-1) - (3N-1)$$

$$\rightarrow S = k_B \left[(3N-1) \ln E + \text{const}(N) \right] \simeq k_B \cdot 3N \cdot \ln \frac{E}{\hbar\omega} + \tilde{\text{const}}(N)$$

k $\quad 3N$

$S(E, V, N)$

$$\frac{\partial S}{\partial E} = \frac{1}{T} \rightarrow \frac{1}{T} = 3N \cdot k_B \cdot \frac{1}{E} \Rightarrow E = 3N k T = 6N \cdot \frac{1}{2} k T$$

$$\left(\text{id. g.} \quad \frac{1}{T} = \frac{3N}{2} k_B \cdot \frac{1}{E} \Rightarrow E = 3N \cdot \frac{1}{2} k T \right)$$

<u>ttth'lan</u>: $\Omega \sim E^{af}$ $\quad C(n) = 1$

f: szb. fokok száma

$$S = k \ln \Omega = k af \ln E + \ldots$$

$\ln(\beta E)$

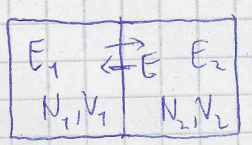
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id. g. $\quad S = k_B N \ln V + k_B \frac{3N}{2} \ln E + \text{const}(N)$

ossz.: $\quad S = 3N k \ln \frac{E}{\hbar\omega} + S_0 \qquad S_0 = k \ln 2 - 3Nk (\ln 3N - 1)$

<u>Egensúly feltétele</u>

zárt



$E = E_1 + E_2$

$N = N_1 + N_2$

$V = V_1 + V_2$

Tfh. 2. részrendszer független

a kk. ~ felülettel, rövid hatótávolságú erők

$$S = S_1 + S_2$$

$$S = S(E_1, E_1) = S_1(E_1) + S_2(E - E_1)$$

egyensúly: S max E-ben

$$0 = \left.\frac{\partial S}{\partial E_1}\right|_{\substack{N_1,V_1\\N_2,V_2}} = \left.\frac{\partial S_1}{\partial E_1}\right| + \left.\frac{\partial S_2}{\partial E_1}\right| = \frac{\partial S_1}{\partial E_1} + \frac{\partial S_2(E-E_1)}{\partial E_1} =$$

$$= \frac{\partial S_1}{\partial E_1} \cdot + \frac{\partial S_2}{\partial E_2}(-1) = \frac{\partial S_1}{\partial E_1} - \frac{\partial S_2}{\partial E_2} = 0$$

Def.: $\left.\frac{\partial S}{\partial E}\right|_{N,V} = \frac{1}{T}$ dimenzója ol

$$[ST] = 1 = [E]$$

id. g. $\left.\frac{\partial S}{\partial E}\right|_{N,V} = k \cdot \frac{3N}{2} \cdot \frac{1}{E} \rightarrow E = k\frac{3N}{2} T = 3N \cdot \frac{1}{2} kT$

hőm. egy. $\left.\frac{\partial S}{\partial E}\right|_{N,V} = k \cdot 3N \cdot \frac{1}{E} \rightarrow E = k \cdot 3N \cdot T$

ált. $\Omega \sim E^{af}$ $S = k \cdot af \cdot \ln E \Rightarrow \frac{1}{T} = \left.\frac{\partial S}{\partial E}\right|_{N,V} = \frac{k \cdot af}{E}$

$$E = k \cdot a \cdot f \cdot T$$

fal mozgat

$$S(V_1) = S_1(V_1) + S_2(V - V_1)$$

$$0 = \left.\frac{\partial S}{\partial V_1}\right|_{\substack{E_1,N_1\\E_1,N_2}} = \left.\frac{\partial S_1}{\partial V_1}\right| + \left.\frac{\partial S_2(V-V_1)}{\partial V_1}\right| = \frac{\partial S_1}{\partial V_1} + \frac{\partial S_2}{\partial V_2}(-1)$$

Def.: $\left.\frac{\partial S}{\partial V}\right|_{E,N} = \frac{p}{T}$

egyensúly feltétele:

$\frac{p_1}{T_1} = \frac{p_2}{T_2}$ $\xrightarrow[\text{energiacsere}]{\text{hő is}}$ $p_1 = p_2$

id. g. $\left.\frac{\partial S}{\partial V}\right|_{E,N} = \frac{p}{T} = k_B \cdot N \cdot \frac{1}{V} \Rightarrow$ $\boxed{pV = k_B N \cdot T}$

ideális gáz állapotegyenlete

kísérletileg: $k_B = (1{,}38044 \pm 0{,}00007) \cdot 10^{-23} \cdot \frac{J}{K}$

$R = k_B \cdot N_A = (8{,}31696 \pm 0{,}00034) \cdot 10^{-16} \frac{J}{K} = 2\ cal/fok$

$1\ cal = 4{,}187 \cdot 10^{-16}\ J$

→ definíció T-t

részrendszer mennyiség a falon

$S(N, N_1) = S_1(N_1) + S_2(N - N_1)$

$0 = \left.\frac{\partial S}{\partial N_1}\right|_{\substack{E_1 V_1 \\ E_2 V_2}} = \left.\frac{\partial S_1}{\partial N_1}\right| + \left.\frac{\partial S_2(N-N_1)}{\partial N_1}\right| = \frac{\partial S_1}{\partial N_1} - \frac{\partial S_2}{\partial N_2}$

def.: $\left.\frac{\partial S}{\partial N}\right|_{E,V} = -\frac{\mu}{T}$ → kémiai potenciál → dimenziója ?

egyensúly feltétele:

$$\frac{\mu_1}{T_1} = \frac{\mu_2}{T_2} \xrightarrow[\text{fősere}]{\text{van}} \mu_1 = \mu_2$$

↓ diatermikus a fal

Fundamentális - egyenlet

izolált r. $S = S(E,V,N) \longleftrightarrow E(S,V,N)$

↘ természetes változók

$E = k \cdot \frac{3N}{2} \cdot T$ nem fundamentális egyenlet

$$dS = \underbrace{\left.\frac{\partial S}{\partial E}\right|_{V,N}}_{\frac{1}{T}} dE + \underbrace{\left.\frac{\partial S}{\partial V}\right|_{E,N}}_{\frac{p}{T}} \cdot dV + \underbrace{\left.\frac{\partial S}{\partial N}\right|_{E,V}}_{-\frac{\mu}{T}} \cdot dN$$

I. főtétel ↓

$$dS = \frac{dE + p\,dV - \mu\,dN}{T} \Rightarrow dE = \underbrace{T\,dS}_{\delta Q} \underbrace{- p\,dV + \mu\,dN}_{\delta W}$$

↓ ↓

függnek az úttól

Legendre - transzformáció

$$E(S,V,N) \xrightarrow{S \leftrightarrow T} F(T,V,N) = E - \left.\frac{\partial E}{\partial S}\right|_{V,N} \cdot S = E - T \cdot S$$

$$dF = dE - T\,dS - S\,dT = \cancel{T\,dS} - p\,dV + \mu\,dN - \cancel{T\,dS} - S\,dT =$$

$$= -S\,dT - p\,dV + \mu\,dN$$

$$E(S,V,N) \longrightarrow H(S,p,N) = E - \left.\frac{\partial E}{\partial V}\right|_{S,N} \cdot V = E + pV$$

$$dH = \ldots = T\,dS + V\,dp + \mu\,dN$$

(↑ I. főtétel)

$$G(T,p,N) = E - \left.\frac{\partial E}{\partial S}\right|_{V,N} \cdot dS - \left.\frac{\partial E}{\partial V}\right|_{S,N} \cdot V = E - T \cdot S + pV$$

$$dG = -S\,dT + V\,dp + \mu\,dN$$

Euler-összefüggés

$E(S,V,N)$ → itt V mennyiség extenzív

$$\lambda E = E(\lambda S, \lambda V, \lambda N) \qquad / \frac{\partial}{\partial \lambda}$$

$$E = \left.\frac{\partial E}{\partial(\lambda S)}\right|_{V,N} \cdot S + \left.\frac{\partial E}{\partial(\lambda V)}\right|_{S,N} \cdot V + \left.\frac{\partial E}{\partial(\lambda N)}\right|_{S,V} \cdot N \qquad \lambda := 1$$

$$E = \left.\frac{\partial E}{\partial S}\right|_{V,N} \cdot S + \left.\frac{\partial E}{\partial V}\right|_{S,N} \cdot V + \left.\frac{\partial E}{\partial N}\right|_{S,V} \cdot N$$

$$\boxed{E = T \cdot S - p \cdot V + \mu N}$$

$$S = -k \int \rho \ln \rho \, d\Gamma$$

$$d\Gamma = \frac{d^{(3N)} \uparrow \, d^{(3N)} q}{h^{3N} \cdot N!}$$

Mikro

$$\rho = \frac{1}{\Omega}$$

$$\Omega = \int d\Gamma$$

$$E < \mathcal{H}(\uparrow, q) < E + \delta E$$

$$S = k \cdot \ln \Omega$$

$$\left.\frac{\partial S}{\partial E}\right|_{V,N} = \frac{1}{T}$$

Kanonikus

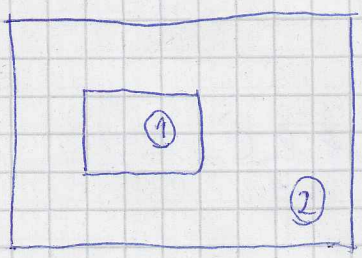
$$\rho = \frac{1}{Z} e^{-\beta \mathcal{H}}$$

$$Z = \int d\Gamma \cdot e^{-\beta \mathcal{H}(\uparrow, q)}$$

$$S = -k \int \frac{e^{-\beta \mathcal{H}}}{Z} \left[-\beta \mathcal{H} + \ln Z \right] d\Gamma$$

$$= k \beta \langle \mathcal{H} \rangle + k \ln Z$$

$$\langle O \rangle = \int O \rho \, d\Gamma$$



① : E_1, N_1 részrendszer $\uparrow_1, q_1$

② : E_2, N_2 környezet $\uparrow_2, q_2$

① + ② : zárt $\Rightarrow$ $E_1 + E_2 = E$

$N_1 + N_2 = N$

② $\gg$ ① $\Rightarrow$ $E_2 \gg E_1$ $N_2 \gg N_1$

① + ② zárt $\rho = \text{const} = \frac{1}{\Omega}$

$$\Omega = \frac{1}{h^{3N} \cdot N!} \int d^{(3N_1)} \uparrow_1 \, d^{(3N_1)} q_1 \, d^{(3N)} \uparrow_2 \, d^{(3N)} q_2$$

$$\varrho_1(r_1, q_1) = C \int \varrho(r_1, q_1, r_2, q_2)\, d r_2\, d q_2 =$$

↑

(biztosítja, hogy ϱ_1 normált

$$= \frac{C'}{\Omega} \frac{1}{h^{3N_2} N_2!} \int d^{(3N_2)} r_2 \, d^{(3N_2)} q_2 =$$

$$E - \mathcal{H}_1 < \mathcal{H}_2 < E - \mathcal{H}_1 + \delta E$$

$$= \frac{C'}{e^{\frac{S(E)}{k}}} \cdot \Omega_2(E - \mathcal{H}_1) = C' \cdot \frac{e^{\frac{S_2(E-\mathcal{H}_1)}{k}}}{e^{\frac{S(E)}{k}}}$$

$$\Rightarrow k \cdot \ln \varrho_1 = S_2(E - \mathcal{H}_1) - S(E) + k \cdot \ln C'$$

$E \gg \mathcal{H}_1$, S_2 sorfejtés

$$k \cdot \ln \varrho_1 \simeq S_2(E) - \frac{\partial S_2}{\partial E} \cdot \mathcal{H} - S(E) + k \cdot \ln C'$$

$$\varrho_1 \simeq \text{const} \cdot e^{-\frac{1}{k} \frac{\partial S_2}{\partial E} \mathcal{H}_1} \qquad \frac{\partial S_2}{\partial E} = \frac{1}{T_2}$$

kanonikus eloszlás adódik el $\beta = \frac{1}{k T_2}$

T_2 hőtartály hőmérséklete

Gibbs-tétele

A rendszer hő mennyiségi fokú is lehet, akkor a hőmérsékletet definiálja az entrópia-ban rejlő összefüggést.

hőtartály

$$S = k\beta\langle\mathcal{H}\rangle + k \ln Z$$

$$\frac{\partial S}{\partial\langle\mathcal{H}\rangle} = \frac{\partial(k\beta)}{\partial\langle\mathcal{H}\rangle}\langle\mathcal{H}\rangle + k\beta + k\frac{\partial \ln Z}{\partial\langle\mathcal{H}\rangle} = k\frac{\partial\beta}{\partial\langle\mathcal{H}\rangle}\cdot\langle\mathcal{H}\rangle + k\beta +$$

$$+ k\cdot\frac{1}{Z}\cdot\frac{\partial Z}{\partial\langle\mathcal{H}\rangle} =$$

$$= k\cdot\frac{\partial\beta}{\partial\langle\mathcal{H}\rangle}\cdot\langle\mathcal{H}\rangle + k\beta + k\cdot\underbrace{\frac{1}{Z}\frac{\partial Z}{\partial(-\beta)}}_{\langle\mathcal{H}\rangle}\cdot\frac{\partial(-\beta)}{\partial\langle\mathcal{H}\rangle} = k\beta$$

$$Z = \int e^{-\beta\mathcal{H}}\, d\Gamma$$

$$\frac{1}{Z}\frac{\partial Z}{\partial(-\beta)} = \frac{1}{Z}\int \mathcal{H}\cdot e^{-\beta\mathcal{H}}\, d\Gamma = \langle\mathcal{H}\rangle$$

Kanonikus: $\left.\frac{\partial S}{\partial\langle\mathcal{H}\rangle}\right|_{V,N} = k\cdot\beta$

Mikrokanonikus: $\left.\frac{\partial S}{\partial E}\right|_{V,N} = \frac{1}{T} = k\beta$

$$Z = \int e^{-\beta\mathcal{H}}\, d\Gamma$$



$\mathcal{H}(p,q) = E$

$$Z = \int e^{-\beta E}\, \omega(E)\, dE$$

↑ állapotsűrűség

$$d\Gamma_0(E) = \omega(E)\, dE$$

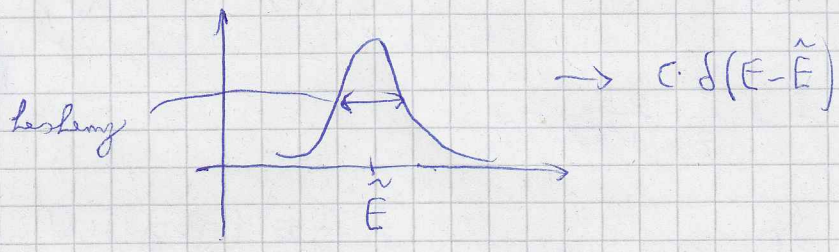
↘ E-nél kisebb energiájú állapotok száma

$$\Gamma \sim E^{af}$$

$$\omega \sim E^{af}$$

$$\int e^{-\beta E} \cdot E^{af}\, dE$$

↓

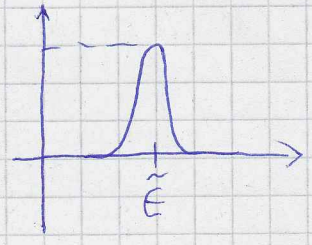


$$\rightarrow C \cdot \delta(E - \tilde{E})$$

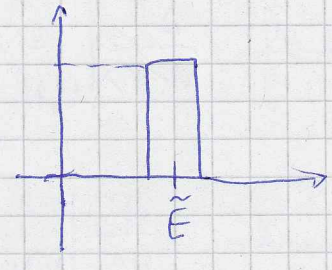
$$\langle \mathcal{H} \rangle = \int \mathcal{H}\, \varrho\, d\Gamma = \int \mathcal{H} \cdot \frac{1}{Z} e^{-\beta \mathcal{H}}\, d\Gamma = \frac{1}{Z} \int E \cdot e^{-\beta E}\, \omega(E)\, dE$$

$$= \frac{1}{Z} \int E \cdot \underbrace{e^{-\beta E} \cdot E^{af}}_{C\,\delta(E-\tilde{E})}\, dE = \frac{1}{Z} C \tilde{E} = \tilde{E}$$

Kanonikus



Mikrokanonikus



Nagy szabadsági fok esetén minden ≈ Dirac-delta

A mikrokanonikus és kanonikus eloszlás ekvivalens.

Mennyi az energia szórása? $\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2 = ?$

$$\frac{\partial (\ln Z)}{\partial (-\beta)} = \frac{1}{Z} \frac{\partial Z}{\partial (-\beta)} = \frac{1}{Z} \int \mathcal{H} e^{-\beta \mathcal{H}} \, d\Gamma = \langle \mathcal{H} \rangle$$

$$\frac{\partial^2 (\ln Z)}{\partial (-\beta)^2} = \frac{\partial \langle \mathcal{H} \rangle}{\partial (-\beta)} = \frac{\partial}{\partial (-\beta)} \int \mathcal{H} \cdot \frac{e^{-\beta \mathcal{H}}}{Z} \, d\Gamma =$$

$$= \frac{1}{Z^2} \left(\int \mathcal{H}^2 \cdot e^{-\beta \mathcal{H}} \cdot Z \cdot d\Gamma - \int \mathcal{H} \cdot e^{-\beta \mathcal{H}} \frac{\partial Z}{\partial (-\beta)} \, d\Gamma \right)$$

$$= \underbrace{\frac{1}{Z} \int \mathcal{H}^2 \cdot e^{-\beta \mathcal{H}} \, d\Gamma}_{\langle \mathcal{H}^2 \rangle} - \underbrace{\frac{1}{Z} \frac{\partial Z}{\partial (-\beta)}}_{\langle \mathcal{H} \rangle} \cdot \underbrace{\int \mathcal{H} \cdot \frac{e^{-\beta \mathcal{H}}}{Z} \, d\Gamma}_{\langle \mathcal{H} \rangle} =$$

$$= \langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2$$

$S = k \cdot \beta \cdot \langle \mathcal{H} \rangle + k \cdot \ln Z$

$$\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2 = \frac{\partial \langle \mathcal{H} \rangle}{\partial (-\beta)} = - \frac{\partial \langle \mathcal{H} \rangle}{\partial \left(\frac{1}{kT} \right)} = - \frac{\partial \langle \mathcal{H} \rangle}{\partial (kT)} \cdot \frac{\partial (kT)}{\partial \left(\frac{1}{kT} \right)} =$$

$\langle \mathcal{H} \rangle = E$ belső energia

$\beta = \frac{1}{kT}$

$$= - \frac{\partial E}{\partial (kT)} \cdot \left(- \frac{1}{(kT)^2} \right)^{-1}$$

$$\frac{1}{\frac{\partial \left(\frac{1}{kT} \right)}{\partial (kT)}} = \left(- \frac{1}{(kT)^2} \right)^{-1}$$

$$\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2 = \frac{1}{Z} \cdot \frac{\partial E}{\partial T} \cdot (kT)^2 = C_V \cdot k \cdot T^2$$

↓ exterior $\sim N$

$\langle \mathcal{H} \rangle \sim N$

$$\boxed{\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2 = C_V \cdot k \cdot T^2} \sim N$$

$\Rightarrow$ relative errors $\sim \frac{1}{\sqrt{N}}$

$$S = k \beta \langle \mathcal{H} \rangle + k \ln Z$$

$$S \cdot T = k \cdot \frac{1}{kT} T \langle \mathcal{H} \rangle + kT \ln Z$$

$$\Rightarrow \boxed{\underbrace{-kT \ln Z}_{F} = \underbrace{\langle \mathcal{H} \rangle}_{E} - T \cdot S = F(T, V, N)}$$

$$\left.\frac{\partial F}{\partial T}\right|_{V,N} = -k \ln Z - kT \cdot \left.\frac{\partial (\ln Z)}{\partial T}\right|_{V,N} =$$

$$= -k \ln Z - k^2 T \cdot \left.\frac{\partial (\ln Z)}{\partial (kT)}\right|_{V,N} = -k \ln Z - k^2 T \cdot \frac{\partial (\ln Z)}{\partial \left(\frac{1}{kT}\right)} \cdot \frac{\partial \left(\frac{1}{kT}\right)}{\partial (kT)}$$

$$= -k \ln Z - k^2 T \cdot \frac{\partial (\ln Z)}{\partial \beta} \left(-\frac{1}{(kT)^2}\right) =$$

$$= -k \ln Z - \underbrace{\frac{1}{T}}_{k\beta} \cdot \underbrace{\frac{\partial (\ln Z)}{\partial (-\beta)}}_{\langle \mathcal{H} \rangle} = -k \ln Z - k\beta \langle \mathcal{H} \rangle = -S$$

Mikro

zárt r.

E, V, N rögz

$$\varrho = \frac{1}{\Omega} \qquad \Omega = \int d\Gamma$$

$$E < \mathcal{H}(r,q) < E + \delta E$$

$$d\Gamma = \frac{1}{h^{3N} \cdot N!} \int d^{(3N)} r \; d^{(3N)} q$$

$$S(E,V,N) = k \cdot \ln \Omega$$

$$\left.\frac{\partial S}{\partial E}\right|_{V,N} = \frac{1}{T} \qquad \left.\frac{\partial S}{\partial V}\right|_{E,N} = \frac{p}{T}$$

$$\left.\frac{\partial S}{\partial N}\right|_{E,V} = -\frac{\mu}{T}$$

Kanonikus

kötött T

T, V, N rögz

$$Z = \int e^{-\beta \mathcal{H}} \, d\Gamma$$

$$\varrho = \frac{e^{-\beta \mathcal{H}}}{Z}$$

$$F(T,V,N) = -k T \ln Z$$

$$S = -\left.\frac{\partial F}{\partial T}\right|_{V,N} \qquad dF = -S\,dT - p\,dV + \mu\,dN$$

$$E = \langle \mathcal{H} \rangle = \frac{\partial \ln Z}{\partial(-\beta)}$$

$$p = -\left.\frac{\partial F}{\partial V}\right|_{T,N} \qquad \mu = \left.\frac{\partial F}{\partial N}\right|_{T,V}$$

Pl.: ideális gáz (kanonikus)

$$\mathcal{H} = \sum_{i=1}^{3N} \frac{p_i^2}{2m}$$

$$Z = \frac{1}{h^{3N} \cdot N!} \int d^{(3N)} r \; d^{(3N)} q \cdot e^{-\beta \sum_{i=1}^{3N} \frac{p_i^2}{2m}} =$$

$$= \frac{V^N}{h^{3N} \cdot N!} \cdot \prod_{i=1}^{3N} \int_{-\infty}^{+\infty} dp_i \cdot e^{-\beta \frac{p_i^2}{2m}} = \frac{V^N}{h^{3N} \cdot N!} \cdot \left(\sqrt{\frac{\pi}{\frac{1}{2m}\beta}}\right)^{3N} = \frac{V^N}{h^{3N} \cdot N!} \cdot \left(\pi \, 2m \, \beta\right)^{\frac{3N}{2}}$$

$$F = -kT \ln Z \qquad E = \frac{\partial(\ln Z)}{\partial(-\beta)} = -\frac{\partial(\ln Z)}{\partial \beta}$$

$$\ln Z = \text{const} - \frac{3N}{2} \ln \beta$$

$$E = -\frac{\partial(\ln Z)}{\partial \beta} = \frac{3N}{2} \cdot \frac{1}{\beta} = \frac{3N}{2} \cdot kT$$

$$p = -\left.\frac{\partial F}{\partial V}\right|_{T,N} = kT \frac{\partial(\ln Z)}{\partial V} = kT \cdot \frac{\partial(N \ln V)}{\partial V} = k \cdot T \cdot N \cdot \frac{1}{V}$$

$$p = \frac{N \cdot kT}{V}$$

$$F = -kT\left[N \ln V - 3N \ln k - \underbrace{\ln N!}_{-(N \ln N - N)} + \frac{3N}{2} \ln\left(\frac{2\pi m}{\beta}\right)\right]$$

$$\mu = \left.\frac{\partial F}{\partial N}\right|_{T,V} = -kT\left[\ln V - 3 \ln k - \left(\ln N + N \cdot \frac{1}{N} - 1\right) + \underbrace{\frac{3}{2} \ln\left(\frac{2\pi m}{\beta}\right)}_{\ln\left(\frac{2\pi m}{\beta}\right)^{\frac{3}{2}}}\right]$$

$$= -kT\left[\ln \frac{V}{N} + \ln\left(\frac{2\pi m}{\beta}\right)^{\frac{3}{2}} \cdot \frac{1}{k^3}\right]$$

$$S = -\lambda \int f(x) \ln f(x)\, dx$$

Gauss $\quad f(x) = \frac{1}{a\sqrt{\pi}} \cdot e^{-\frac{x^2}{a^2}}$

$$S = -\lambda \int_{-\infty}^{+\infty} \frac{1}{a\sqrt{\pi}} e^{-\frac{x^2}{a^2}} \left[-\ln a\sqrt{\pi} - \frac{x^2}{a^2} \right] dx$$

$$= +\lambda \frac{\ln(a\sqrt{\pi})}{a\sqrt{\pi}} \cdot \sqrt{\frac{\pi}{\frac{1}{a^2}}} + \lambda \int_{-\infty}^{+\infty} \frac{1}{a\sqrt{\pi}} \cdot \frac{x^2}{a^2} \cdot e^{-\frac{x^2}{a^2}} dx =$$

$$\int_{-\infty}^{+\infty} t^2 \cdot e^{-at^2} dt = -\frac{\partial}{\partial a} \int_{-\infty}^{+\infty} e^{-at^2} dt = -\frac{\partial}{\partial a} \sqrt{\frac{\pi}{a}} = \frac{1}{2} a^{-\frac{3}{2}} \cdot \sqrt{\pi}$$

$$a = 1 : \quad \int_{-\infty}^{+\infty} t^2 e^{-t^2} dt = \frac{\sqrt{\pi}}{2}$$

$a = \sqrt{2}\sigma$

$$= \ldots = \frac{\lambda}{2} \left(\ln\left(a\sqrt{\pi}\right) + \frac{1}{2} \right) = \frac{\lambda}{2} \left(\ln\left(2\pi\sigma^2\right) + 1 \right)$$

1.d.g $\quad F = -kTN \cdot \ln\left[\frac{V}{N} e \left(\frac{2\pi m k T}{h^2} \right)^{\frac{3}{2}} \right]$

↑ l'athstom extenir

$N!$ ← $d\Gamma = \frac{1}{N! h^{3N}} \int d_{\uparrow}^{(3N)} d_{\downarrow}^{(3N)}$

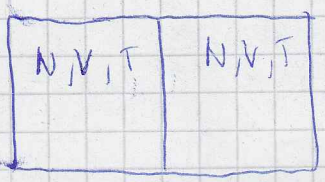
Gibbs - paradoxon

$F = E - T \cdot S \longrightarrow S = \ldots$

$$S = \frac{3kN}{2} - 3Nk \ln k + \frac{3Nk}{2} \ln(2\pi m k T) + kN \ln V$$

$$-N \ln N + N = \tilde{S} - N \ln N + N$$

$-\ln(N!)$ ↑ $N!$ -ből



Falat kivesszük:

$$\Delta S = -2S(N,V,T) + S(2N,2V,T) = 0$$

$$\Delta \tilde{S} = \tilde{S}(2N,2V,T) - 2\tilde{S}(N,V,T) =$$

$$= 2Nk\left(\ln(2V) - \ln V\right) = 2Nk \ln 2 = k \cdot \ln\left(2^{2N}\right)$$

↓ keveredési entrópia

Ekvipartíció - tétel:

$\mathcal{H} = ax^2 + \mathcal{H}'$; $\mathcal{H}'$ független x-től

$$? = \langle ax^2 \rangle = \frac{1}{Z} \int ax^2 e^{-\beta \mathcal{H}} d\Gamma$$

$$\rho = \frac{1}{Z} e^{-\beta \mathcal{H}}$$

$$Z = \int e^{-\beta \mathcal{H}} d\Gamma = \int e^{-\beta a x^2 - \beta \mathcal{H}'} dx\, d\Gamma' =$$

$$= Z' \int e^{-\beta a x^2} dx$$

$$\langle a x^2 \rangle = \frac{1}{Z} \cdot \frac{\int_{-\infty}^{+\infty} a x^2 e^{-\beta a x^2} dx \cdot Z}{\int_{-\infty}^{+\infty} e^{-\beta a x^2} dx} =$$

$$= \frac{\int_{-\infty}^{+\infty} a x^2 \cdot e^{-\beta a x^2} dx}{\int_{-\infty}^{+\infty} e^{-\beta a x^2} dx} = \frac{-\frac{\partial I}{\partial \beta}}{I} = -\frac{\partial}{\partial \beta}(\ln I)$$

$$I = \int_{-\infty}^{+\infty} e^{-\beta a x^2} dx = \sqrt{\frac{\pi}{\beta a}}$$

$$\frac{\partial I}{\partial(-\beta)} = \int a x^2 e^{-\beta a x^2} dx$$

$$\underline{\langle a x^2 \rangle} = -\frac{\partial}{\partial \beta}(\ln I) = -\frac{\partial}{\partial \beta} \ln \sqrt{\frac{\pi}{\beta a}} = -\frac{\partial}{\partial \beta}\left(-\frac{1}{2} \ln \beta\right) =$$

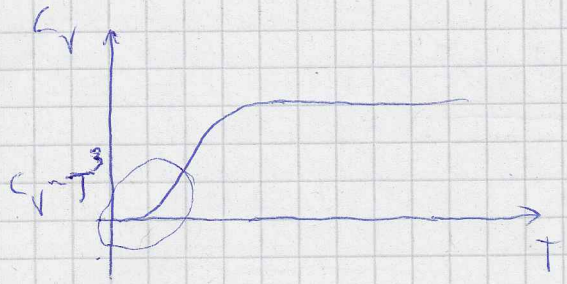
$$= \frac{1}{2} \cdot \frac{1}{\beta} = \underline{\frac{1}{2} k T} \quad \checkmark$$

Ha csak kvadratikus taglól áll, ránk f

$$\langle \mathcal{H} \rangle = f \cdot \frac{kT}{2}$$

pl.: $\mathcal{H} = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2$

$f = 6N \quad \langle \mathcal{H} \rangle = E = 6N \cdot \frac{kT}{2}$



Debye - Petit

Pl.: Harm. osc.

$$\mathcal{H}_1 = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 q^2 \qquad N \qquad f = 3N$$

$$Z_N = \frac{1}{N! \cdot h^{3N}} \int d^{(3N)}p \, d^{(3N)}q \cdot e^{-\beta \mathcal{H}} =$$

$$= \frac{1}{N!} \cdot Z_1^{3N}$$

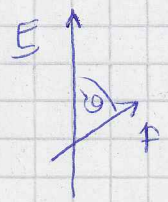
$$Z_1 = \frac{1}{h} \int_{-\infty}^{+\infty} e^{-\beta\left(\frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2\right)} dp \, dx = \sqrt{\frac{\pi}{\frac{\beta}{2m}}} \cdot \sqrt{\frac{\pi}{\frac{1}{2} m \omega^2}} \cdot \frac{1}{h} =$$

$$= \frac{2\pi}{\beta h \omega} = \frac{1}{\beta \hbar \omega}$$

$$F = -k_B T \cdot \ln Z \qquad E = -\frac{\partial}{\partial \beta}(\ln Z) =$$

$$= -\frac{\partial}{\partial \beta} \ln\left[\frac{1}{N!}\left(\frac{1}{\beta \hbar \omega}\right)^{3N}\right] = -\frac{\partial}{\partial \beta}\left[(-3N) \ln \beta\right] = \frac{3N}{\beta} = 3N k T$$

Elektromos (~~dipól~~) dipól



$$E_{\uparrow} = -E_{\updownarrow} = -E_{\uparrow}\cos\vartheta$$

$$\langle \uparrow \rangle = ?$$

$$f \cdot d\Omega = C \cdot e^{+\beta E_{\uparrow}\cos\vartheta} \cdot d\Omega$$

↑ tároljuk

$$\int f\, d\Omega = 1$$

$$\langle \uparrow_z \rangle = \int \uparrow \cos\vartheta \cdot f\, d\Omega = \uparrow \cdot \frac{\int \cos\vartheta \cdot e^{+\beta E_{\uparrow}\cos\vartheta} \cdot d\Omega}{\int e^{\beta E_{\uparrow}\cos\vartheta}\, d\Omega} =$$

$$\alpha = \beta E_{\uparrow} \qquad x = \cos\vartheta$$

$$\downarrow$$

$$dx = -\sin\vartheta\, d\vartheta$$

$$d\Omega = \sin\vartheta\, d\vartheta\, d\varphi = -dx \cdot d\varphi$$

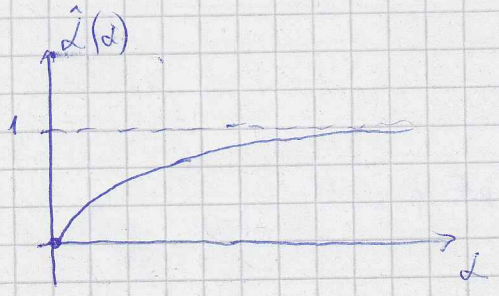
$$= \uparrow \cdot \frac{2\pi \int_{-1}^{+1} x\, e^{\alpha x}\, dx}{2\pi \int_{-1}^{+1} e^{\alpha x}\, dx} = \uparrow \frac{d}{d\alpha}\left(\ln \int_{-1}^{+1} e^{\alpha x}\, dx\right) =$$

$$= \uparrow \cdot \frac{d}{d\alpha}\left[\ln\left(\frac{e^{\alpha} - e^{-\alpha}}{\alpha}\right)\right] = \uparrow \frac{d}{d\alpha}\left(\ln \frac{2\sinh\alpha}{\alpha}\right) =$$

$$= \uparrow \frac{d}{d\alpha}\left(\ln \sinh\alpha - \ln\alpha\right) = \uparrow\left[\frac{1}{\sinh\alpha}\cosh\alpha - \frac{1}{\alpha}\right]$$

$$\langle \mu_z \rangle = \mu \cdot \left(\operatorname{cth} \alpha - \frac{1}{\alpha} \right) = \mu \cdot \mathcal{L}(\alpha)$$

↑ Langevin-fv.



$$\mathcal{L}(\alpha) = \frac{\alpha}{3} - \frac{\alpha^3}{45} + \dots$$

$T \to \infty$ $\qquad \alpha = \beta E_\mu = \frac{E \cdot \mu}{k \cdot T} \ll 1$, ha $kT \gg E_\mu$

$$\langle P_z \rangle = N \mu \cdot \mathcal{L}(\alpha) \xrightarrow[\alpha \to 0]{} N \cdot \mu \frac{\alpha}{3} = \frac{1}{3} \frac{N \mu^2 E}{kT}$$

↑ N db d. dipól

Maxwell-eloszlás

Keressük annak a valószínűségét, hogy id. g. egyik kiragadott molekulájának a sebesség abszolútértéke $(v, v + dv)$-be essen, tekintet nélkül v irányára és a többi molekulára.

$f(v)$ $\qquad \int f(v)\, dv = N$

↑ egyrészecskés eloszlás fv.

$$f(v)\, dv = N \int d\mu_x\, d\mu_y\, d\mu_z \int \dots \int d\Gamma' \cdot \frac{e^{-\beta \mathcal{H}}}{Z} =$$

tesszes

$$\mathcal{H} = \frac{\mu_x^2 + \mu_y^2 + \mu_z^2}{2m} + \mathcal{H}' = \frac{\mu^2}{2m} + \mathcal{H}'$$

$$= N \frac{4\pi p^2 \cdot dp \cdot e^{-\beta \cdot \frac{p^2}{2m}} \cdot \int d\Gamma' \cdot e^{-\beta \mathcal{H}'}}{\int 4\pi p^2 dp \cdot e^{-\beta \frac{p^2}{2m}} \int d\Gamma' \cdot e^{-\beta \mathcal{H}'}}$$

$$p = mv \qquad dp = m\,dv \qquad p^2 = (mv)^2$$

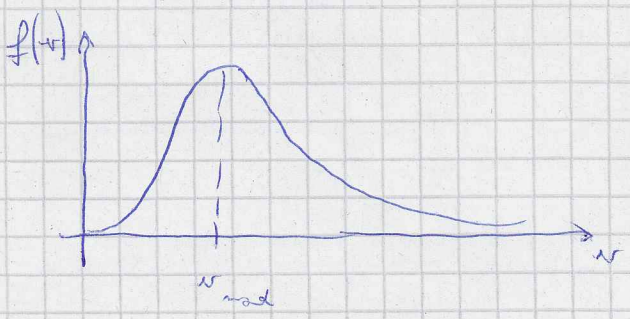
$$= N \cdot (mv)^2 \cdot m\,dv \cdot \frac{e^{-\beta \frac{mv^2}{2}}}{\int e^{-\beta \frac{p^2}{2m}} \cdot p^2 dp} =$$

$$= N \cdot m^3 \cdot v^2 \cdot e^{-\frac{mv^2}{2kT}} \cdot \frac{4}{\sqrt{\pi}} \cdot (2mkT)^{-\frac{3}{2}} \cdot dv$$

$$f(v) = N \cdot \sqrt{\frac{8m}{\pi kT}} \cdot \frac{mv^2}{2kT} \cdot e^{-\frac{mv^2}{2kT}}$$

$$\int_0^{+\infty} f(v)\,dv = N$$

Maxwell - elosclas



zon els fr.

$$\frac{m v_{mod}^2}{2} = kT \qquad \longrightarrow \quad v_{mod}^2 \neq \langle v^2 \rangle$$

equipart

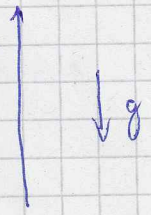
$$\longrightarrow \left\langle \frac{p^2}{2m} \right\rangle = \frac{1}{2} kT$$

$$\left\langle \frac{1}{2} m v^2 \right\rangle = \frac{1}{2} kT$$

$E = \frac{1}{2} m v^2$ $\quad f(E)\,dE = ?$

Kolloid részecskék negatív szintű elosztása?

Homogén gravitációs tér, z irányban:



$$\mathcal{H} = \sum_i \left(\frac{p_i^2}{2m} + m g z_i \right)$$

$f(z)\,dz$: $\forall$ koordinátán lévő, z koordinátán lévő részecske

$$\beta = \frac{e^{-\beta \mathcal{H}}}{z}$$

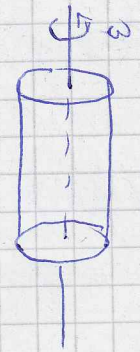
$$f(z)\,dz = C \cdot \frac{e^{-\beta m g z}\,dz}{\int_0^\infty e^{-\beta m g z}\,dz} = \tilde{C} \cdot e^{-\frac{mgz}{kT}}\,dz$$

$$f(z) = N_0 \cdot e^{-\frac{mgz}{kT}}, \quad \text{ahol} \quad N_0 = f(0)$$

↑

k mérendő

Példa: $\Rightarrow \langle m v^2 \rangle = \frac{kT}{m}$



Nagykanonikus sokaság (folyt.)

tudtuk V, $\langle \mathcal{H} \rangle$, $\langle N \rangle$

$S\{\varrho\} = \max$

([illegible]) $\qquad \varrho_N = \frac{1}{Q} \cdot e^{-\beta \mathcal{H} - \alpha N}$

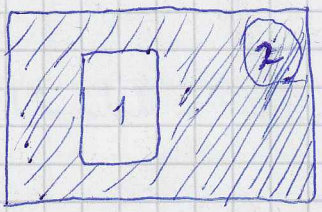
(α: Lagrange-multiplikátor)

$$Q = \sum_{N=0}^{\infty} \int d\Gamma_N \cdot e^{-\beta \mathcal{H} - \alpha N}$$

$$d\Gamma_N = \frac{1}{h^{3N} \cdot N!} \, d^{(3N)}_{\uparrow} \, d^{(3N)}_{q}$$

$$S = -k \sum_N \int \varrho_N \ln \varrho_N \, d\Gamma_N = -k \sum_N \int \varrho_N (-\beta \mathcal{H} - \alpha N - \ln Q) \, d\Gamma_N$$

$$= k \cdot \ln Q + k\beta \langle \mathcal{H} \rangle + k\alpha \cdot \langle N \rangle$$



$E = E_1 + E_2 \qquad E_1 \ll E_2$

$N = N_1 + N_2 \qquad N_1 \ll N_2$

$$\varrho_1(\mathcal{H}_1, N_1) = \frac{C}{h^{3N_2} \cdot N_2!} \int \varrho(q_1, \uparrow_1, q_2, \uparrow_2) \, dq_2 \, d\uparrow_2$$

$E - \mathcal{H}_1 < \mathcal{H}_2 < E - \mathcal{H}_1 + \delta E$

$$\varrho = \frac{1}{\Omega}$$

$$\varrho_1(\mathcal{H}_1, N_1) = C \cdot \frac{\Omega_2(E-\mathcal{H}_1, N-N_1)}{\Omega(E,N)}$$

$$k \ln \varrho_1 = k \ln C + k \ln \Omega_2 - k \ln \Omega =$$

$$= k \ln C + S_2(E-\mathcal{H}_1, N-N_1) - S(E,N)$$

konst

$$= k \ln C + S_2(E,N) - \frac{\partial S_2}{\partial E} \cdot \mathcal{H}_1 - \frac{\partial S_2}{\partial N} N_1 - S(E,N)$$

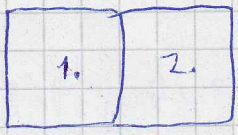
$$\frac{\partial S_2}{\partial E} \to \frac{1}{T_2} \qquad \frac{\partial S_2}{\partial N} \to -\frac{\mu_2}{T_2}$$

$$\varrho_1 = \text{konst} \cdot e^{-\frac{\mathcal{H}_1 - \mu_2 N_1}{k T_2}}$$

↑ normáló

$$\beta = \frac{1}{k T_2} \qquad k\alpha = -\frac{\mu_2}{T_2}$$

A hőmérsékletet állítja be a Lagrange-multiplikátorokat



2. makroszkopikus

ha 1. is makroszkopikus

$$\frac{\mu_1}{T_1} = \frac{\mu_2}{T_2} \quad , N \text{ változik}$$

$$T_1 = T_2 \quad , \text{ha is hőzsé}$$

$$\varrho = \text{konst.} \cdot e^{-\beta(\mathcal{H} - \mu N)}$$

β, μ a rendszer (1) paraméterei

$$S = k \ln Q + k\beta \langle \mathcal{H} \rangle + k\alpha \langle N \rangle$$

$$\left.\frac{\partial S}{\partial \langle \mathcal{H} \rangle}\right|_{\langle N \rangle, V} = k\beta = \frac{1}{T} \qquad \left.\frac{\partial S}{\partial \langle N \rangle}\right|_{\langle \mathcal{H} \rangle, V} = k\alpha = -\frac{\mu}{T}$$

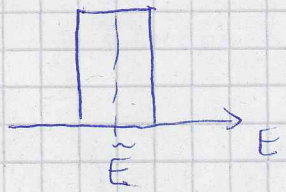
mikrokanonikus $\longrightarrow$ nagykanonikus

$E \longrightarrow \langle \mathcal{H} \rangle$

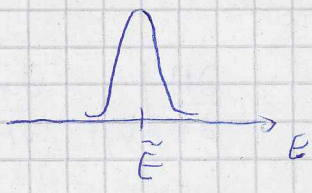
$N \longrightarrow \langle N \rangle$

Ingadozások:

mikrokanonikus



kanonikus



relatív szórás $\sim \frac{1}{\sqrt{N}}$

$$\frac{\partial (\ln Q)}{\partial (-\beta)} = \frac{1}{Q} \sum_{N=0}^{\infty} \int d\Gamma_N \, (\mathcal{H} - \mu N) \, e^{-\beta(\mathcal{H} - \mu N)} = \langle \mathcal{H} - \mu N \rangle$$

$$\frac{\partial^2 (\ln Q)}{\partial (-\beta)^2} = \ldots = \langle (\mathcal{H} - \mu N)^2 \rangle - \langle \mathcal{H} - \mu N \rangle^2 \quad \text{szórásnégyzet}$$

$\sim \langle N \rangle$

$$\frac{\partial(\ln \mathcal{G})}{\partial(-\alpha)} = \langle N \rangle$$

$$\frac{\partial^2(\ln \mathcal{G})}{\partial(-\alpha)} = \dots = \langle N^2 \rangle - \langle N \rangle^2 \sim \langle N \rangle$$

relatív szórás $\sim \frac{1}{\sqrt{\langle N \rangle}}$

másodrendű (~~fázisátalakulásnál~~) fázistalakulásnál

$\mathcal{H}$ és N fluktuációi divergálnak

$\Rightarrow$ ez egyes elsőtől nem elválasztanak.

$$\langle N^2 \rangle - \langle N \rangle^2 = \left.\frac{\partial N}{\partial(-\alpha)}\right|_{T,V} = \left.\frac{\partial N}{\partial \mu}\right|_{T,V} \cdot \left.\frac{\partial \mu}{\partial(-\alpha)}\right|_{T,V} = k \cdot T \cdot \left.\frac{\partial N}{\partial \mu}\right|_{T,V} = ?$$

láncszabály $\left.\frac{\partial x}{\partial y}\right|_z = -\frac{\left.\frac{\partial z}{\partial y}\right|_x}{\left.\frac{\partial z}{\partial x}\right|_y}$

$$\left.\frac{\partial N}{\partial \mu}\right|_{V,T} = \left.\frac{\partial N}{\partial \tau}\right|_{V,T} \cdot \left.\frac{\partial \tau}{\partial \mu}\right|_{V,T} =$$

$$= -\frac{\left.\frac{\partial V}{\partial \tau}\right|_{N,T}}{\left.\frac{\partial V}{\partial N}\right|_{\tau,T}} \cdot \left.\frac{\partial \tau}{\partial \mu}\right|_{V,T} = \frac{V \cdot \kappa_T}{\left.\frac{\partial V}{\partial N}\right|_{\tau,T}} \cdot \left.\frac{\partial \tau}{\partial \mu}\right|_{V,T}$$

$$\kappa_T = -\frac{1}{V} \cdot \left.\frac{\partial V}{\partial \tau}\right|_{T,N}$$

Maxwell rel.

$$\left.\frac{\partial V}{\partial N}\right|_{\tau,T} = \left.\frac{\partial \mu}{\partial \tau}\right|_{N,T}$$

$\uparrow$

$\mu\, dN + V\, d\tau$

$$G(T, p, N) = E - T \cdot S + p \cdot V = \mu \cdot N$$

T: $\uparrow$ S, p: $\uparrow$ V

Euler-összefüggés: $E = T \cdot S - p \cdot V + \mu \cdot N$

1. főtétel: $dE = T\,dS - p\,dV + \mu\,dN$

$$\left.\frac{\partial N}{\partial \mu}\right|_{V,T} = \frac{V \cdot K_T}{\left.\frac{\partial \mu}{\partial p}\right|_{N,T}} \cdot \left.\frac{\partial p}{\partial \mu}\right|_{V,T}$$

$dG = -S\,dT + V\,dp + \mu\,dN$

$$\left.\frac{\partial \mu}{\partial p}\right|_{N,T} = \frac{1}{N}\left.\frac{\partial G}{\partial p}\right|_{N,T} = \frac{V}{N}$$

$$\left(\left.\frac{\partial p}{\partial \mu}\right|_{V,T} = \frac{1}{\left.\frac{\partial \mu}{\partial p}\right|_{V,T}}\right) \leftarrow \text{nem kell}$$

$$\phi(T, V, \mu) = E - T \cdot S - \mu \cdot N = -p \cdot V$$

$$d\phi = -S\,dT - p\,dV - N\,d\mu$$

$$\left.\frac{\partial p}{\partial \mu}\right|_{V,T} = -\frac{1}{V} \cdot \left.\frac{\partial \phi}{\partial \mu}\right|_{V,T} = -\frac{1}{V} \cdot (-N) = \frac{N}{V}$$

$$\left.\frac{\partial N}{\partial p}\right|_{V,T} = \frac{V \cdot K_T}{\frac{V}{N}} \cdot \frac{N}{V} = \frac{N^2}{V} \cdot K_T$$

$$\Rightarrow \quad \langle N^2 \rangle - \langle N \rangle^2 = k_B T \cdot \frac{N^2}{V} \cdot \kappa_T$$

Kritikus opalescencia: kritikus pont

κ_T divergál $\Rightarrow$ nagy részecske-fluktuációk

$\Rightarrow$ nagyon szórja a fényt $\rightarrow$ fehéres, ködös lesz a gáz

$\Phi(T,V,\mu) = ?$

Láttuk: $S = k \ln Q + k\beta \underbrace{\langle \mathcal{H} \rangle}_{E} + k\alpha \cdot N$

$\frac{1}{kT}$ $\qquad$ $-\frac{\mu}{kT}$

$$-kT \ln Q = E - T \cdot S - \mu \cdot N = \Phi(T,V,\mu)$$

$$\boxed{\Phi(T,V,\mu) = -kT \ln Q} \qquad d\Phi = -S\,dT - p\,dV - N\,d\mu$$

$$\Phi = -pV$$

(kanonikus: $F(T,V,N) = -kT \ln Z$)

Pl.: id. g.

$$Q = \sum_{N=0}^{\infty} e^{-\alpha N} \underbrace{\int e^{-\beta \mathcal{H}} \, d\Gamma_N}_{Z_{\text{kanonikus}}} = \sum_{N=0}^{\infty} e^{-\alpha N} \cdot \frac{V^N}{h^{3N} \cdot N!} \cdot (2\pi m k T)^{\frac{3N}{2}}$$

$$= \sum_{N=0}^{\infty} \frac{1}{N!} \cdot \left(e^{-\alpha} \cdot \frac{V}{h^3} (2\pi m k T)^{\frac{3}{2}} \right)^N =$$

$$\uparrow \quad \sum_{N=0}^{\infty} \frac{1}{N!} \cdot x^N = e^x$$

$$= \exp\left(e^{-\alpha} \cdot \frac{V}{h^3} \cdot (2\pi m k T)^{\frac{3}{2}} \right)$$

$$\ln Q = e^{-\alpha} \cdot \frac{V}{h^3} \cdot (2\pi m k T)^{\frac{3}{2}}$$

$$\Phi = -kT \ln Q = -kT \cdot e^{-\alpha} \cdot \frac{V}{h^3} (2\pi m k T)^{\frac{3}{2}} =$$

$$= -kT\, e^{+\frac{\mu}{kT}} \cdot V \cdot \frac{(2\pi m k T)^{3/2}}{h^3}$$

$$N = -\left.\frac{\partial \Phi}{\partial \mu}\right|_{T,V} = +kT \cdot e^{\frac{\mu}{kT}} \cdot V \cdot \frac{(2\pi m k T)^{\frac{3}{2}}}{h^3} \cdot \frac{1}{kT} = \frac{-\Phi}{kT} = \frac{pV}{kT}$$

$\Phi = -pV$

$-\Phi$

$$\Downarrow$$

$$pV = NkT$$

$$Q = \exp\left\{ e^{-\alpha} \cdot \frac{V}{h^3} \int e^{-\beta \frac{p^2}{2m}} d^3p \right\} =$$

$$\Downarrow$$

Z_1

$$= \exp\left\{ \frac{V}{h^3} \int e^{-\beta\left(\frac{p^2}{2m} - \mu\right)} d^3p \right\}$$

$$\frac{\partial \ln Q}{\partial(-\alpha)} = \langle N \rangle = e^{-\alpha} \cdot \frac{V}{h^3} \int e^{-\beta \frac{p^2}{2m}} d^3p = \frac{V}{h^3} \int e^{-\beta\left(\frac{p^2}{2m} - \mu\right)} d^3p$$

$$\Downarrow$$

helyettesítsünk: $n_p = e^{-\beta(\varepsilon_p - \mu)}$

$$\varepsilon_p = \frac{p^2}{2m}$$

$$\frac{\partial \ln Q}{\partial(-\beta)} = \langle \mathcal{H} - \mu N \rangle = \frac{V}{h^3} \int \left(\frac{p^2}{2m} - \mu\right) e^{-\beta\left(\frac{p^2}{2m} - \mu\right)} d^3p =$$

$$= \frac{V}{h^3} \int (\varepsilon_\uparrow - \mu)\, e^{-\beta(\varepsilon_\uparrow - \mu)}\, d^3\uparrow = \frac{V}{h^3} \int (\varepsilon_\uparrow - \mu) \cdot n_\uparrow \cdot d^3\uparrow$$

$$\Rightarrow (\mathcal{H}) = \frac{V}{h^3} \int \varepsilon_\uparrow \cdot n_\uparrow \cdot d^3\uparrow$$

$$N = V \cdot \frac{(2\pi m kT)^{\frac{3}{2}}}{h^3}\, e^{\frac{\mu}{kT}}$$

$$e^{\frac{\mu}{kT}} = \frac{N}{V} \cdot \left(\frac{h^2}{2\pi m kT}\right)^{\frac{3}{2}}$$

$$\lambda = \sqrt{\frac{h^2}{2\pi m kT}} \qquad r_0 = \left(\frac{V}{N}\right)^{\frac{1}{3}}$$

termikus de Broigle hullámhossz

$$e^{\frac{\mu}{kT}} = \left(\frac{\lambda}{r_0}\right)^3$$

Ha a gáz elég ritka, elég nagy hőmérsékletű

$$e^{\frac{\mu}{kT}} << 1 \Rightarrow \frac{\mu}{kT} < 0 \text{ és } \left|\frac{\mu}{kT}\right| >> 1$$

klasszikus gázra

sokszögek: $T \rightarrow$ hasonlóság

$T/\mu \rightarrow$ nagyhasonlóság

$T, \uparrow \rightarrow T, \uparrow$ sokszög

T, p Ensemble

$$Y = \int e^{-\beta(\mathcal{H}(V) - (-p)V)} \, d\Gamma \, dV$$

$$\downarrow$$

$$G(T, p, N) = -k_B T \cdot \ln Y$$

$$G = E - T \cdot S + p \cdot V = \mu \cdot N$$

$$dG = -S \, dT + V \, dp + \mu \, dN$$

Mikrokanonisches

Zust. E, V, N

$$\Omega(E, V, N, \delta E) = \int_{E < \mathcal{H}(r,q) < E + \delta E} d\Gamma$$

$$\updownarrow$$

$$\Omega_0 = \int_{\mathcal{H}(r,q) < E} d\Gamma \qquad \Omega = \frac{\partial \Omega_0}{\partial E} \cdot \delta E$$

$$S = k \cdot \ln \Omega$$

$$\left.\frac{\partial S}{\partial E}\right|_{V,N} = \frac{1}{T} \qquad \left.\frac{\partial S}{\partial N}\right|_{E,V} = -\frac{\mu}{T}$$

$$C_V = \left.\frac{\partial E}{\partial T}\right|_V = T \cdot \left.\frac{\partial S}{\partial T}\right|_V$$

Kanonikus

kötött sly

$$Z = \int e^{-\beta \mathcal{H}(r,q)} \, d\Gamma$$

$$F(T,V,N) = -kT \ln Z$$

$$E = -\frac{\partial(\ln Z)}{\partial \beta}$$

$$dF = -S\,dT - p\,dV + \mu\,dN$$

$$S = -\left.\frac{\partial F}{\partial T}\right|_{V,N} \quad \text{----}$$

$$C_V = T \cdot \left.\frac{\partial S}{\partial T}\right|_V$$

Nagykanonikus

kötött sly, részecskeszám sly

$$Q = \sum_{N=0}^{\infty} \int e^{-\beta(\mathcal{H}_N(r,q) - \mu N)} \, d\Gamma_N$$

$$\Phi(T,V,\mu) = -pV = -kT \ln Q$$

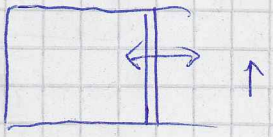
$$d\Phi = -S\,dT - p\,dV - N\,d\mu$$

$$N = -\left.\frac{\partial \Phi}{\partial \mu}\right|_{T,V} \qquad S = -\left.\frac{\partial \Phi}{\partial T}\right|_{V,\mu}$$

$$C_V = T \cdot \left.\frac{\partial S}{\partial T}\right|_V$$

T – p sokaság

T, p



$$Y = \int e^{-\beta(\mathcal{H}_V - (-p)V)} \, d\Gamma \, dV$$

$$G(T, p, N) = -kT \ln Y$$

$$dG = -S\,dT + V\,dp + \mu\,dN$$

Kvantum statisztikus fizika

Sűrűségmátrix

t részben p_k valószínűséggel a Ψ_k-val jellemzett állapotban van.

$$\langle A \rangle := \sum_k p_k \langle \Psi_k | \hat{A} | \Psi_k \rangle$$

$$|\Psi\rangle = \sum_k c_k |\Psi_k\rangle \qquad p_k = |c_k|^2$$

nem egyenlő: interferenciatagok a előbbiben nincsenek

Bázistranszformáció: $|\Psi_k\rangle = \sum_i a_{ki} |\varphi_i\rangle$

$$\langle A \rangle = \sum_k \uparrow_k \langle \Psi_k | \hat{A} | \Psi_k \rangle = \sum_{e,m} \underbrace{\sum_k \uparrow_k a^*_{ke} a_{km}}_{(\rho)_{me}} \cdot \underbrace{\langle \varphi_e | \hat{A} | \varphi_m \rangle}_{A_{em}}$$

$$= S_\uparrow (\rho \cdot A)$$

$$\sum_k \uparrow_k = 1 \quad \Rightarrow \quad S_\uparrow \rho = 1$$

Def.: $$S = -k_B \sum_e \uparrow_e \ln \uparrow_e = -k_B S_\uparrow (\rho \ln \rho) = -k_B \langle \ln \rho \rangle$$

Zárt rendszer, E adott

$|\Psi_k\rangle$ legyen olyan az adott E-hez tartozó állapotok

$$E = \sum_k n_k \varepsilon_k$$

ε_k: egyrészecske energiaszintek

n_k: betöltési számok

$\Omega(E)$: degeneráció foka az E energiánál

$$\uparrow_e = \uparrow = \Omega^{-1}$$

egyenlő eloszlás maximalizálja S-t

$$S = -k_B \sum_e \uparrow_e \ln \uparrow_e = -k_B \sum_e \frac{1}{\Omega} \ln\left(\frac{1}{\Omega}\right) = k_B \ln \Omega$$

------ $\forall$ egyensúlyi rendszert klasszikusan

Harmonikus oszcillátor: $\varepsilon_k = \hbar\omega \cdot \left(k + \frac{1}{2}\right)$

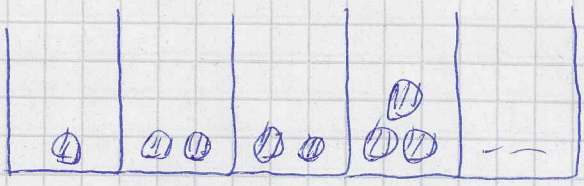
$$E = \sum_k \left(k + \frac{1}{2}\right) \hbar\omega \cdot n_k = \hbar\omega \sum_k k \cdot n_k + E_0$$

$$N = \sum_k n_k \qquad \varepsilon = \frac{E - E_0}{\hbar\omega}$$

$\Downarrow$

gerjesztési kvantumok száma

Hányféleképpen oszthatsz szét ε gerjesztési kvantumot N részecske közt?



1 2 — — — N



1 2 3 4

$\varepsilon + N - 1$ golyó + fal

$\varepsilon + N - 1$ üres helyből ki kell választani a falak helyét:

$$\Omega = \binom{\varepsilon + N - 1}{N - 1} = \frac{(\varepsilon + N - 1)!}{(N-1)!\,\varepsilon!}$$

$$S = k_B \ln \Omega = k_B \left\{ (\varepsilon + N - 1) \ln (\varepsilon + N - 1) - \varepsilon \ln \varepsilon - (N-1) \ln (N-1) \right\}$$

$$\frac{\partial S}{\partial E} = \frac{\partial S}{\partial \varepsilon} \cdot \frac{\partial \varepsilon}{\partial E} = \frac{k_B}{\hbar\omega} \ln \left(\frac{\varepsilon + N - 1}{\varepsilon} \right) = \frac{1}{T}$$

$$\Rightarrow \quad \mathcal{E} = \frac{N-1}{e^{\beta\hbar\omega}-1} \approx \frac{N}{e^{\beta\hbar\omega}-1}$$

$$E = E_0 + \frac{N\hbar\omega}{e^{\beta\hbar\omega}-1}$$

kl. lineáris: $e^{\beta\hbar\omega} - 1 \approx \beta\hbar\omega$

$$E = \cancel{E_0} + N k_B T$$

$N \to 3N$ térbeli oszcillátorok

$$E = 3N k_B T$$

kl. lineáris: $(\mathcal{E} \to \infty)$

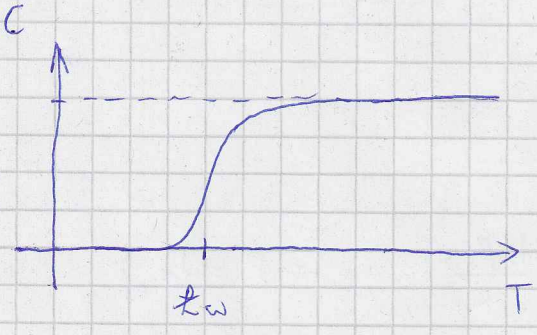
$$S = 3N k_B \ln \mathcal{E} + 3N k_B (1 - \ln 3N) + \dots$$

klasszikusan levezethető $S_{kl} = 3N k_B \ln\left(\frac{E}{\hbar\omega}\right) + S_0$

$\Rightarrow$ a klasszikus statisztikus fizikán a $\hbar$-val jelölt állandót a Planck-állandónak kell választani

$$\frac{\partial E}{\partial T} = N\hbar\omega \cdot \frac{e^{\frac{\hbar\omega}{k_B T}}}{\left(e^{\frac{\hbar\omega}{k_B T}} - 1\right)^2} \cdot \frac{\hbar\omega}{k_B} \cdot \frac{1}{T^2} = C$$

$$C = N k_B \left(\frac{\hbar\omega}{k_B T}\right)^2 \cdot \frac{e^{\frac{\hbar\omega}{k_B T}}}{\left(e^{\frac{\hbar\omega}{k_B T}} - 1\right)^2} \longrightarrow \begin{cases} N k_B & , \text{ha } T \to \infty \\ N k_B \left(\frac{\hbar\omega}{k_B T}\right)^2 e^{-\frac{\hbar\omega}{k_B T}} & T \to 0 \end{cases}$$



2 állapotú rendszer

↳ volt ber. statfizen

negy: populációinverzió

gerjesztett nívón több atom

további gerjesztésnél S csökken ⇒ T negatív

Kanonikus sokaság: adott $\langle \mathcal{H} \rangle$

$$S = -k_B \sum_e \uparrow_e \ln \uparrow_e = \max$$

$$\sum_e \uparrow_e = 1$$

$$\langle \mathcal{H} \rangle = \sum_e \uparrow_e \langle \Psi_e | \mathcal{H} | \Psi_e \rangle = \sum_e \uparrow_e E_e = \text{adott}$$

$$\uparrow_e = \frac{1}{Z} e^{-\beta E_e} \qquad \mathcal{R}(E_e) \text{ degeneráció foka}$$

$$Z = \sum_{\ell} e^{-\beta E_\ell} = \sum_{E} \Omega(E)\, e^{-\beta E}$$

$$\beta = \frac{1}{k_B T} \quad , \quad F = -k_B T \ln Z$$

Oszillátor rendszer

$$E_\ell = \sum_{k=1}^{N} n_k \hbar\omega + \frac{N\hbar\omega}{2} \qquad \ell = \{n_k\}$$

$$Z = \sum_{\ell} e^{-\beta E_\ell} = \sum_{\{n_k\}} e^{-\beta \sum_k n_k \hbar\omega - \beta \frac{N\hbar\omega}{2}} =$$

$$= e^{-\beta \frac{N\hbar\omega}{2}} \cdot \sum_{\{n_k\}} \prod_{k=1}^{N} e^{-\beta \hbar\omega \cdot n_k} =$$

$$= e^{-\beta \frac{N\hbar\omega}{2}} \cdot \prod_{k=1}^{N} \left(\sum_{n_k} e^{-\beta \hbar\omega \cdot n_k} \right)$$

$$Z = e^{-\beta \frac{N\hbar\omega}{2}} \cdot \zeta^N \qquad \zeta = \sum_{n=0}^{\infty} e^{-\beta \hbar\omega \cdot n} = \frac{1}{1 - e^{-\beta\hbar\omega}}$$

$$F = -k_B T \ln Z = \frac{N\hbar\omega}{2} - k_B T N \cdot \ln \zeta =$$

$$= \frac{N\hbar\omega}{2} + k_B T N \ln\left(1 - e^{-\beta\hbar\omega}\right)$$

$$\langle \mathcal{H} \rangle = \frac{\partial \ln Z}{\partial(-\beta)} = \frac{N\hbar\omega}{2} + \frac{N e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}} \hbar\omega =$$

$$= \frac{N\hbar\omega}{2} + \frac{N\hbar\omega}{e^{\beta\hbar\omega} - 1}$$

Általánosítás: különböző frekvenciájú oszcillátorok

$$E = \sum_{k=1}^{N} n_k \hbar\omega + E_0$$

$$F = F_0 + k_B T \sum_{k=1}^{N} \ln\left(1 - e^{-\beta\hbar\omega_k}\right)$$

Kvantumstatisztikus sokaság

$n_{\ell,N}$ ⟶ részecskeszám

energiaszintek indexe

$$\langle A \rangle = \sum_{N,\ell} n_{\ell,N} \langle \psi_\ell^{(N)} | A | \psi_\ell^{(N)} \rangle$$

$$S = -k_B \sum_{N,\ell} n_{\ell,N} \ln n_{\ell,N} = \max$$

$$\sum_{N,\ell} n_{\ell,N} = 1$$

$$\sum_{N,\ell} n_{\ell,N} \langle \psi_\ell^{(N)} | \mathcal{H} | \psi_\ell^{(N)} \rangle = \sum_{N,\ell} n_{\ell,N} E_\ell^{(N)} = \langle \mathcal{H} \rangle = \text{adott}$$

$$\sum_{N,\ell} N \cdot \uparrow_{\ell,N} = \langle N \rangle = \text{adott}$$

$$\uparrow_{\ell,N} = \frac{1}{Q} e^{-\beta\left(E_\ell^{(N)} - \mu N\right)}, \quad Q = \sum_{N,\ell} e^{-\beta\left(E_\ell^{(N)} - \mu N\right)}$$

$$-k_B T \ln Q = \Phi = -\uparrow V$$

Fermi és Bose gáz:

nincs kölcsönhatás, az energia egyrészecske-energiák összege

$\ell = \{n_r\}$

$$E_\ell^{(N)} = \sum_r n_r \cdot \varepsilon_r \qquad E_\ell^{(N)} \; N \text{ függése} \qquad \sum_r n_r = N$$

$$Q = \sum_{N,\ell} e^{-\beta\left(E_\ell^{(N)} - \mu N\right)} = \sum_{N,\ell} e^{-\beta \sum_r (\varepsilon_r - \mu) n_r}$$

$$Q = \sum_{\{n_r\}} e^{-\beta \sum_r n_r(\varepsilon_r - \mu)} = \sum_{\{n_r\}} \prod_r e^{-\beta n_r (\varepsilon_r - \mu)} =$$

$$= \prod_r \sum_{n_r} e^{-\beta(\varepsilon_r - \mu) n_r}$$

Fermi-Dirac: $n_r = 0, 1$

Bose-Einstein: $n_r = 0, 1, 2, 3, \ldots$

F.D. $\longrightarrow$ $\prod_r \left(1 + e^{-\beta(\varepsilon_r - \mu)}\right)$

B.E. $\longrightarrow$ $\prod_r \left(1 - e^{-\beta(\varepsilon_r - \mu)}\right)^{-1}$

$$\frac{\partial \ln Q}{\partial(-\beta\varepsilon_r)} = \langle n_r \rangle = \frac{\partial}{\partial(\beta\varepsilon_r)} (\pm 1) \sum_r \ln\left(1 \pm e^{-\beta(\varepsilon_r - \mu)}\right) =$$

$$= \frac{e^{-\beta(\varepsilon_r - \mu)}}{1 \pm e^{-\beta(\varepsilon_r - \mu)}} = \frac{1}{e^{\beta(\varepsilon_r - \mu)} \pm 1}$$

$$\langle N \rangle = \sum_r \langle n_r \rangle = \sum_r \frac{1}{e^{\beta(\varepsilon_r - \mu)} \pm 1}$$

$$\langle \mathcal{H} \rangle = \sum_r \varepsilon_r \cdot \langle n_r \rangle = \sum_r \frac{\varepsilon_r}{e^{\beta(\varepsilon_r - \mu)} \pm 1}$$

ha az r nívó degenerációja $g(\varepsilon_r)$

$$\langle \mathcal{H} \rangle = \sum_\varepsilon g(\varepsilon)\, n(\varepsilon) = \sum_\varepsilon \frac{g(\varepsilon)\,\varepsilon}{e^{\beta(\varepsilon - \mu)} \pm 1}$$

$$\sum_r \ldots = (2s+1) \sum_{r_1, r_2, r_3} \ldots$$

spin

(ha nincs mágneses tér, akkor az energiaszintek nem függnek tőle, ezért leválasztható)

$$\langle N \rangle = (2s+1) \sum_{r_1 r_2 r_3} \frac{1}{\exp(\ldots) \pm 1} = (2s+1) \sum_{r_1 r_2 r_3} \frac{1}{\exp(\ldots) \pm 1} \Delta_{r_1} \Delta_{r_2} \Delta_{r_3}$$

1 1 1

$$r_i \frac{\lambda_i}{2} = L \qquad \uparrow_i = \frac{2}{\lambda_i} = r_i \frac{R}{2L} \qquad \Delta\uparrow_i = \Delta r_i \cdot \frac{R}{2L}$$

$$\varepsilon_{\uparrow}(r_1, r_2, r_3) = \frac{R^2}{4L^2 \cdot 2m} \left(r_1^2 + r_2^2 + r_3^2\right)$$

részek L élhosszúságú dobozban

$$\langle N \rangle = (2s+1) \cdot \left(\frac{2L}{R}\right)^3 \frac{1}{8} \sum_{\uparrow_1 \uparrow_2 \uparrow_3} \langle n_{\uparrow} \rangle \Delta\uparrow_1 \Delta\uparrow_2 \Delta\uparrow_3 =$$

$r_1, r_2, r_3 \geq 0$ miatt csak egy térnyolcadra

vagy az eredeti $\sum$

Ezt kiterjesztjük a teljes térre $\Rightarrow \frac{1}{8}$-os kompenzáló faktor

$$= (2s+1) \cdot \frac{V}{R^3} \int \langle n_{\uparrow} \rangle \, d^3\uparrow =$$

$$= (2s+1) \frac{V}{R^3} \int d^3\uparrow \, \frac{1}{e^{\beta(\varepsilon_{\uparrow} - \mu)} \pm 1} \qquad \varepsilon_{\uparrow} = \frac{\uparrow^2}{2m}$$

Vizsgáljuk az klasszikus képletekkel való korrespondenciát

$s = 0$ $\qquad d^3\uparrow \to 4\pi \uparrow^2 d\uparrow$

$$\frac{\langle N \rangle}{V} = \frac{4\pi}{R^3} \int_0^{\infty} d\uparrow \cdot \uparrow^2 \, \frac{1}{e^{\beta\left(\frac{\uparrow^2}{2m} - \mu\right)} \pm 1} =$$

$$= \frac{4\pi}{h^3}\left(2 m k_B T\right)^{\frac{3}{2}} \cdot \int_0^\infty dx \; \frac{x^2}{e^{x^2 - \frac{\mu}{k_B T}} \pm 1}$$

$$\frac{\vec{p}^2}{2 m k_B T} \Rightarrow x^2 \qquad \frac{\vec{p}^2}{2m} \sim \frac{1}{2} k_B T$$

$$\tilde{p} \sim \sqrt{m k_B T} \qquad \frac{\langle N \rangle}{V} \sim \frac{1}{r_0^3}$$

$$\Rightarrow \frac{h^3}{\tilde{p}^3 \cdot r_0^3} = \int_0^\infty dx \cdot \frac{x^2}{e^{x^2 - \frac{\mu}{k_B T}} \pm 1} = f\left(-\frac{\mu}{k_B T}\right)$$

$\Downarrow$

mint cöökler

Klassikus liter feltétele:

$$\Delta_p \ll \tilde{p}, \quad \Delta_r \ll r_0, \quad \Delta_p \cdot \Delta_r \sim h$$

$$\Rightarrow h \ll \tilde{p} \cdot r_0$$

$$f\left(-\frac{\mu}{k_B T}\right) \ll 1 \Rightarrow -\frac{\mu}{k_B T} \gg 1$$

$$\Rightarrow \int_0^\infty dx \cdot \frac{x^2}{e^{x^2 - \frac{\mu}{k_B T}} \pm 1} \approx \int_0^\infty dx \cdot x^2 \cdot e^{-x^2 + \frac{\mu}{k_B T}}$$

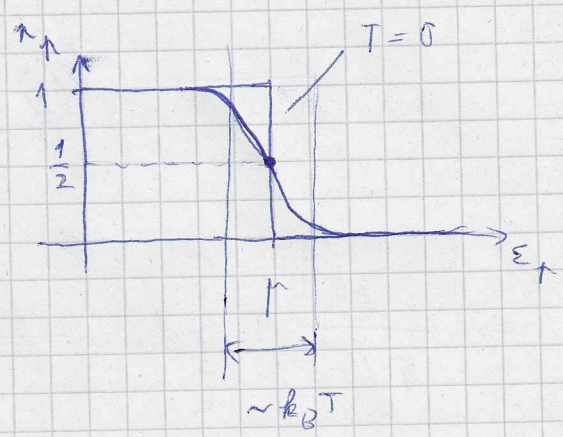
Mikor: $\lambda_T = \frac{h}{\tilde{p}} \ll r_0$

Még írjuk fel: $\frac{1}{2}\frac{\hbar^2}{m r_0^2} \ll \frac{1}{2} k_B T$

↑ lokalizációból eredő kinetikai energia

Fermi - eloszlás

$$n_r = \frac{1}{e^{\beta(\varepsilon_r - \mu)} + 1}$$



$T = 0 \Rightarrow \mu = \varepsilon_F$ Fermi - energia

$$\langle \mathcal{H} \rangle = (2s+1)\frac{V}{\hbar^3} 4\pi \int_0^\infty dp \cdot p^2 \cdot \frac{p^2}{2m} \cdot \frac{1}{e^{\frac{p^2}{2m k_B T} - \frac{\mu}{k_B T}} \pm 1} =$$

$$x = \frac{p}{\sqrt{2m k_B T}}$$

$$= (2s+1)\frac{4\pi V}{\hbar^3} k_B T (2m k_B T)^{\frac{3}{2}} \cdot \int_0^\infty dx \cdot \frac{x^4}{e^{x^2 - \frac{\mu}{k_B T}} \pm 1}$$

$$\langle N \rangle = (2s+1)\frac{4\pi V}{\hbar^3} \cdot (2m k_B T)^{\frac{3}{2}} \cdot \int_0^\infty dx \cdot \frac{x^2}{e^{x^2 - \frac{\mu}{k_B T}} \pm 1}$$

$$\frac{\langle \mathcal{H} \rangle}{\langle N \rangle} = k_B T \cdot f_\pm\left(-\frac{\mu}{k_B T}\right)$$

$$\mathcal{H}: \quad -\frac{\mu}{k_B T} \to \infty \qquad f_\pm \to \frac{3}{2}$$

ekvipartíció - tétel

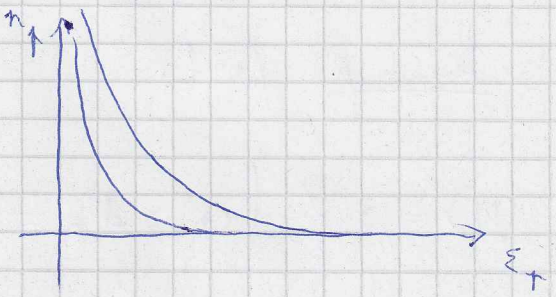
klassz. határesetben nincs degeneráció

csak a Fermi-energia közeli, betölthető részecskékre

jut $k_B T$ energia

Bose-Einstein

$$n_{\uparrow} = \frac{1}{e^{\beta(\varepsilon_{\uparrow} - \mu)} - 1}$$



$$\ln Q = \pm \sum_r \ln\left(1 \pm e^{-\beta(\varepsilon_r - \mu)}\right) =$$

$$= \pm (2s+1) \frac{4\pi V}{h^3} \int_0^{\infty} dp \cdot p^2 \ln\left(1 \pm e^{-\beta\left(\frac{p^2}{2m} - \mu\right)}\right)$$

$$= \frac{2}{3} \beta \cdot \langle \mathcal{H} \rangle$$

$$\uparrow$$

$$\uparrow V = -\Phi = k_B T \cdot \ln Q = \frac{2}{3} \langle \mathcal{H} \rangle$$

$$\uparrow V = \frac{2}{3} \langle \mathcal{H} \rangle = \frac{2}{3} k_B T \langle N \rangle f_{\pm}\left(-\frac{\mu}{k_B T}\right)$$

$$f_{\pm}\left(-\frac{\mu}{k_B T}\right) = \frac{\int_0^{\infty} dx \cdot \frac{x^{\frac{1}{2}}}{e^{x^2 - \frac{\mu}{k_B T}} \pm 1}}{\int_0^{\infty} dx \cdot \frac{x^2}{e^{x^2 - \frac{\mu}{k_B T}} \pm 1}}$$

Állapotegyenlet alacsony hőmérsékleten

$$pV = NkT\left(1 \pm \frac{\pi^{\frac{3}{2}}}{2(2s+1)} \frac{N\lambda^3}{V(n k_B T)^{\frac{3}{2}}}\right)$$

Fermionok $\left(s=\frac{1}{2}\right)$

$$\langle N\rangle = 2\cdot\frac{V}{h^3}\int \langle n_p\rangle d^3p = 2\cdot\frac{4\pi V}{h^3}\int_0^\infty dp\cdot p^2\langle n_p\rangle =$$

$$p = \sqrt{2m\varepsilon}$$

$$= 2\cdot\frac{4\pi V}{h^3}(2m)^{\frac{3}{2}}\cdot\frac{1}{2}\int_0^\infty d\varepsilon \frac{\varepsilon^{\frac{1}{2}}}{e^{\frac{\varepsilon-\mu}{k_B T}}+1}$$

$$\langle E\rangle = 2\cdot\frac{4\pi V}{h^3}(2m)^{\frac{3}{2}}\cdot\frac{1}{2}\int_0^\infty d\varepsilon \frac{\varepsilon^{\frac{3}{2}}}{e^{\frac{\varepsilon-\mu}{k_B T}}+1}$$

$T=0$

$$\langle N\rangle = \frac{4\pi V}{h^3}(2m)^{\frac{3}{2}}\int_0^\mu \varepsilon^{\frac{1}{2}} d\varepsilon = \frac{4\pi V}{h^3}(2m)^{\frac{3}{2}}\frac{\mu^{\frac{3}{2}}}{\frac{3}{2}}$$

$$\mu = \left(\frac{3}{8\pi}\right)^{\frac{2}{3}}\cdot h^2\cdot\left(\frac{N}{V}\right)^{\frac{2}{3}}\cdot\frac{1}{2m} = \varepsilon_F = \frac{p_F^2}{2m}$$

$$p_F = \left(\frac{3}{8\pi}\right)^{\frac{1}{3}}\cdot h\cdot\left(\frac{N}{V}\right)^{\frac{1}{3}} = \left(\frac{9}{32\pi^2}\right)^{\frac{1}{3}}\cdot\frac{h}{r_0}$$

$$r_0 = \left(\frac{3}{4\pi}\cdot\frac{V}{N}\right)^{\frac{1}{3}}$$

$$\langle \mathcal{H} \rangle = \frac{4\pi V}{h^3} \cdot (2m)^{\frac{3}{2}} \cdot \int_0^{\mu} \varepsilon^{\frac{3}{2}} d\varepsilon = \frac{4\pi V}{h^3} (2m)^{\frac{3}{2}} \cdot \frac{\mu^{\frac{3}{2}}}{\frac{3}{2}} \cdot \frac{3}{2} \cdot \frac{\mu}{\frac{5}{2}} =$$

$$= \frac{3}{5} \mu N \qquad \langle N \rangle \to N$$

$$\frac{\langle \mathcal{H} \rangle}{\langle N \rangle} = \frac{3}{5} \varepsilon_F = \frac{3}{5} \mu = \bar{\varepsilon}$$

$$\uparrow V = \frac{2}{3} \langle \mathcal{H} \rangle \Rightarrow \uparrow = \frac{2}{5} \frac{N}{V} \mu \neq 0$$

$$\uparrow_F \sim \hbar \cdot \rho^{\frac{1}{3}} \qquad \rho = \frac{N}{V}$$

$$\Downarrow$$

$$N \propto \frac{V \cdot \uparrow_F^3}{h^3} \qquad \varepsilon_F \sim \frac{\hbar^2}{2m} \rho^{\frac{2}{3}}$$

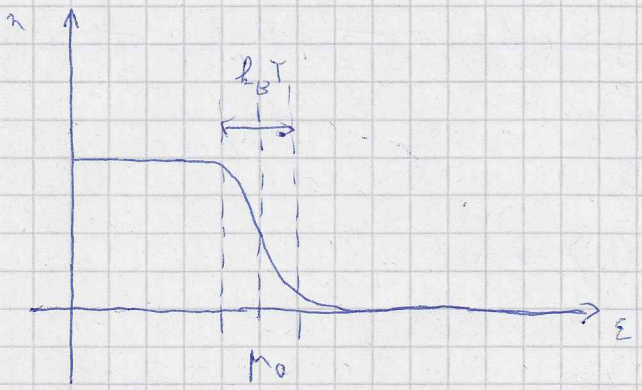
$$E \sim N \varepsilon_F \sim N \cdot \frac{\hbar^2}{2m} \rho^{\frac{2}{3}} = \frac{\hbar^2}{2m} N^{\frac{5}{3}} \cdot V^{-\frac{2}{3}}$$

$$\uparrow V = \frac{2}{3} E \Rightarrow \uparrow \sim \frac{\hbar^2}{2m} \rho^{\frac{5}{3}}$$

T bassa : $k_B T_F \equiv \mu_0 = \varepsilon_F \qquad T \ll T_F$

$$r_0 \sim 10^{-10} \text{ m} \qquad \uparrow_F \approx \frac{\hbar}{r_0} \sim 10^{-24} \sim \frac{h\rho}{3}$$

$$\mu = \frac{\uparrow_F^2}{2m} \sim 10^{-18} \text{ J} \qquad T_F = \frac{\mu}{k_B} \sim 10^5 \text{ K}$$



$T \ll T_F$ feltételt kapjuk ezért részecskék száma

$$N' \sim \frac{4\pi V}{h^3} (2m)^{\frac{3}{2}} \cdot \varepsilon_F^{\frac{1}{2}} \cdot kT \sim$$

$T = 0 - n$

$$N = \frac{4\pi V}{h^3} (2m)^{\frac{3}{2}} \int_0^{\mu} \varepsilon^{\frac{1}{2}} d\varepsilon$$

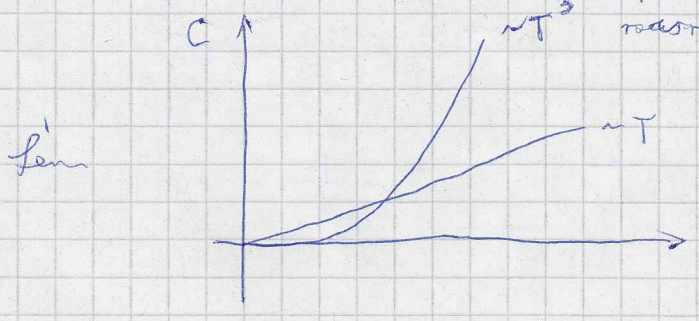
kiintegrálva

$$\sim \underbrace{\frac{4\pi V}{h^3} (2m)^{\frac{3}{2}} \cdot \frac{\varepsilon_F^{\frac{3}{2}}}{\frac{3}{2}}}_{N} \cdot \frac{kT}{\varepsilon_F} \sim N \cdot \frac{k_B T}{\varepsilon_F} = N \cdot \frac{T}{T_F} \ll N$$

Ezek az N' részecskék kielégítik a Boltzmann-statisztikát

$$E \approx E_0 + \text{const} \cdot N' \cdot k_B T = E_0 + \text{const} \cdot N \cdot \frac{(kT)^2}{\varepsilon_F}$$

$$\frac{\partial E}{\partial T} = C = \text{const} \cdot \frac{N k_B^2 T}{k_B T_F} = \text{const} \cdot N k_B \cdot \frac{T}{T_F}$$



Susceptibilität des Gases der Leitungselektronen

$k_B T \ll \varepsilon_F$ $\quad$ $\mu_B H \ll k_B T$ $\quad$ $\mu_B = \frac{e\hbar}{2mc}$

$$M = -\left(\frac{\partial \Phi}{\partial H}\right)_{T,V,\mu} \qquad \varepsilon = \frac{\hbar^2}{2m} \pm \mu_B H$$

$\varepsilon - \mu$

$$\mu \to \mu \mp \mu_B H$$

$$\Phi = \frac{1}{2}\Phi_0(\mu + \mu_B H) + \frac{1}{2}\Phi_0(\mu - \mu_B H)$$

$$\Phi = \Phi_0 + \frac{1}{2}\mu_B^2 H^2 \cdot \frac{\partial^2 \Phi_0}{\partial \mu^2}$$

$$M = -H\mu_B^2 \cdot \frac{\partial^2 \Phi_0}{\partial \mu^2} \qquad \frac{\partial \Phi_0}{\partial \mu} = -N$$

$$\chi = \frac{\mu_B^2}{V}\left(\frac{\partial N}{\partial \mu}\right)_{T,V}$$

$T = 0$: $\quad N = V \cdot \frac{(2m\mu)^{\frac{3}{2}}}{3\pi^2\hbar^3} \Rightarrow \chi = \frac{\mu_B^2 \cdot F^m}{\pi^2 \hbar^3}$



Bose-gáz

pl.: szuperfolyékony hélium
alkálifoldfémek gőzei

$T = 0$ $\quad \langle n_0 \rangle = \langle N \rangle$

$\langle n_r \rangle = 0 \qquad r \neq 0$

$\varepsilon_0 - \mu \geq 0$

$$n_0 = \frac{1}{e^{\beta(\varepsilon_0 - \mu)} - 1}$$

$$e^{\frac{\varepsilon_0 - \mu}{kT}} = 1 + \frac{1}{n_0} \qquad \frac{\varepsilon_0 - \mu}{kT} = \ln\left(1 + \frac{1}{n_0}\right) \to \ln\left(1 + \frac{1}{N}\right)$$

$$\varepsilon_0 - \mu = \frac{kT}{N} + kT \cdot O\left(\frac{1}{N^2}\right)$$

$$n_1 = \frac{1}{e^{\left(\varepsilon_0 + \frac{\hbar^2}{mL^2} - \mu\right)/kT} - 1}$$

, ha $\varepsilon_0 = \mu$ $\qquad n_1 \sim \frac{mL^2 kT}{\hbar^2} \ll N$

$$N = \frac{2\pi V (2m)^{3/2}}{h^3} \int_0^\infty d\varepsilon \cdot \frac{\varepsilon^{\frac{1}{2}}}{e^{\frac{\varepsilon - \mu}{k_B T}} - 1} =$$

$$= \frac{2\pi V (2m k_B T)^{3/2}}{h^3} \underbrace{\int_0^\infty \frac{x^{1/2}\, dx}{e^{x + \frac{|\mu|}{k_B T}} - 1}}_{F\left(\frac{|\mu|}{k_B T}\right)}$$

$$F(0) = \int_0^\infty dx \cdot \frac{x^{\frac{1}{2}}}{e^x - 1} = \int_0^\infty dx\, x^{\frac{1}{2}} \cdot \frac{e^{-x}}{1 - e^{-x}} = \int_0^\infty dx \cdot x^{\frac{1}{2}} \cdot e^{-x} \cdot \sum_{n=0}^\infty e^{-nx}$$

$$= \sum_{n=0}^\infty \int_0^\infty dx\, x^{\frac{1}{2}} \cdot e^{-(n+1)x} =$$

$$= \underbrace{\sum_{n=0}^\infty \frac{1}{(n+1)^{\frac{3}{2}}}}_{\downarrow} \underbrace{\int_0^\infty dy \cdot y^{\frac{1}{2}} \cdot e^{-y}}_{\to \Gamma\left(\frac{3}{2}\right) = \frac{\sqrt{\pi}}{2}} = A \text{ véges érték}$$

$\downarrow$

$\zeta\left(\frac{3}{2}\right)$

$T \to 0$, $|\mu| \to 0$ integrál véges

, de előtte $T^{\frac{3}{2}} \to 0$

$\Rightarrow$ A képlet nem tudja reprodukálni N-t.

Miből jön a probléma? Legalsó nívó betöltöttsége makroszkopikus

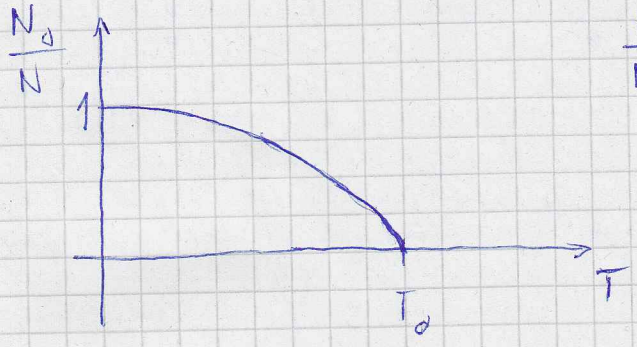
$$N = \frac{2\pi V (2m)^{\frac{3}{2}} (kT_c)^{\frac{3}{2}}}{h^3} A \longrightarrow \text{a } T_c \text{ kritikus Bose-sűrűségben}$$

$$\| \qquad \|$$

$$N = N_0 + \frac{2\pi A (2m kT)^{\frac{3}{2}} \cdot V}{h^3} \quad , \text{ ha } T < T_c$$

N fix $\Rightarrow$ két képlet ugyanaz kell adjon

$$N_0 = \frac{2\pi V (2m)^{\frac{3}{2}} \cdot A}{h^3} k_B^{\frac{3}{2}} \left(T_c^{\frac{3}{2}} - T^{\frac{3}{2}} \right)$$



$$\frac{N}{N_0} = 1 - \left(\frac{T}{T_c} \right)^{\frac{3}{2}}$$

Na^{23}, $T_c = 2\,\mu K$, 10^6 atom - 10^8 atom, $\rho \sim 10^{14}/cm^3$

Rb^{87}, $T_c = 170\,nK$, 10^5 - 10^6 atom, $\rho \sim 10^{12}/cm^3$

$T \approx 0$

$E \sim V T^{\frac{5}{4}} \sim p V \sim \Phi$

$S = -\frac{\partial \Phi}{\partial T} \sim T^{\frac{3}{2}} \to 0, \quad T \to 0$

Üreges üst rugósság tér

$$\omega = c k = \frac{2\pi c}{\lambda} \qquad n \frac{\lambda_n}{2} = L = \frac{L}{\pi} k_n$$

$$\omega_{n_1 n_2 n_3} = \frac{\pi c}{L} \sqrt{n_1^2 + n_2^2 + n_3^2}$$

$$F = F_0 + k_B T \sum_k \ln\left(1 - e^{-\beta \hbar \omega_k}\right)$$

$$\sum_k \ldots = 2 \sum_{n_1 n_2 n_3 > 0} \ldots \Delta n_1 \Delta n_2 \Delta n_3 =$$

↑ polarizációs irányok

$$= 2 \sum_{k_i > 0} \ldots \left(\frac{L}{\pi}\right)^3 \Delta k_1 \Delta k_2 \Delta k_3 \to 2 \left(\frac{L}{\pi}\right)^3 \int_{k_i > 0} d^3k \ldots =$$

$$= 2 \left(\frac{L}{\pi}\right)^3 \frac{1}{8} \int_{k_i > 0} d^3k \ldots =$$

$$= 2 \cdot \frac{V}{8\pi^3} \int d^3k \ldots = \frac{2V}{8\pi^3} \cdot 4\pi \int_0^\infty dk \cdot k^2 \ldots =$$

$$= \frac{2V}{2\pi^2 c^3} \int_0^\infty d\omega \cdot \omega^2 \cdot \ldots = \int_0^\infty d\omega \, g(\omega) \ldots$$

$$g(\omega)\, d\omega = \frac{V}{\pi^2 c^3} \omega^2 d\omega$$

$$F = F_0 + k_B T \int_0^\infty d\omega\, g(\omega) \ln\left(1 - e^{-\beta\hbar\omega}\right)$$

$$\frac{\partial F}{\partial T} = -S = k_B \int_0^\infty d\omega\, g(\omega) \ln\left(1 - e^{-\beta\hbar\omega}\right) +$$

$$+ k_B T \int_0^\infty d\omega\, g(\omega) \frac{-e^{-\beta\hbar\omega} \cdot \hbar\omega}{1 - e^{-\beta\hbar\omega}} \cdot \frac{1}{k_B T^2}$$

$$= k_B \int_0^\infty d\omega\, g(\omega) \ln\left(1 - e^{-\beta\hbar\omega}\right) + \frac{1}{T} \int_0^\infty d\omega\, g(\omega) \cdot \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1}$$

$$F = E - T \cdot S$$

$$E = E_0 + \int_0^\infty d\omega\, g(\omega) \cdot \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1}$$

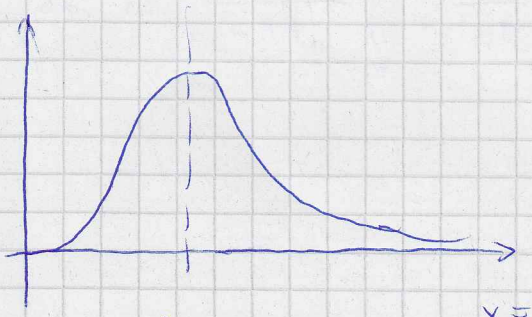
$$\frac{E}{V} = \frac{E_0}{V} + \int_0^\infty d\omega\, f(\omega) \qquad f(\omega) = \frac{\omega^2}{\pi^2 c^3} \cdot \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1}$$

Planck

$$\frac{E}{V} = \frac{E_0}{V} + \int_0^\infty d\nu\, \tilde{f}(\nu) \qquad \tilde{f}(\nu) = \frac{8\pi h \nu^3}{c^3} \cdot \frac{1}{e^{\frac{h\nu}{k_B T}} - 1}$$

$$\tilde{f}(\nu) = \frac{8\pi}{c^3 h^2 (k_B T)^3} \cdot \frac{\left(\frac{h\nu}{k_B T}\right)^3}{e^{\frac{h\nu}{k_B T}} - 1}$$

$$\frac{c^3 h^2 (k_B T)^3}{8\pi} \cdot \tilde{f}$$



$$\frac{h\nu_{max}}{k_B T} = 2{,}82$$

↖ Wien

$$\nu_{max} = 2{,}82 \cdot \frac{k_B T}{h} = 5{,}3 \cdot 10^{10} \cdot \frac{T}{1.\,Kel}$$

$$E = E_0 + V \cdot \frac{8\pi}{c^3 \cdot h^3} (k_B T)^4 \cdot \underbrace{\int_0^\infty \frac{x^3\,dx}{e^x - 1}}_{\frac{\pi^4}{15}}$$

$$\frac{E}{V} = \frac{\cancel{E_0}}{\cancel{V}} + \frac{8\pi^5 k_B^4}{15 h^3 c^3} T^4 \qquad \text{Stefan-Boltzmann}$$

$$\frac{E}{V} = 7{,}56 \cdot 10^{-16} \frac{J}{K^4 m^3} \cdot T^4$$

$$C = \frac{\partial E}{\partial T} \sim T^3$$

$$p = -\left(\frac{\partial F}{\partial V}\right)_T = -\frac{k_B T}{\pi^2 c^3} \int_0^\infty d\omega \cdot \omega^2 \cdot \ln\left(1 - e^{-\beta \hbar \omega}\right)$$

$$= \frac{1}{3\pi^2 c^3} \int_0^\infty \frac{\hbar \omega}{e^{\beta \hbar \omega} - 1} \omega^2 \, d\omega = \frac{1}{3} \cdot \frac{E}{V}$$

$$\frac{E}{V} = \frac{E_0}{V} + \int_0^\infty d\omega \, f(\omega) \quad \Rightarrow [f] = \frac{J}{m^3} = \frac{kg}{m \cdot s} = kg^{+1} \, m^{-1} \cdot s^{-1}$$

$\hbar$ bevezetése nélkül:

3 db lineáris független vektorunk van $\Rightarrow$ bázis

f egyértelműen előállítható ebből

	kg	m	s
f	1	-1	-1
ω	0	0	-1
c	0	1	-1
$k_B T$	1	2	-2

$$\begin{pmatrix} 1 \\ -1 \\ -1 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ -2 \end{pmatrix} - 3 \cdot \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix} + 2 \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix} \quad \Rightarrow \frac{\omega^2}{c^3} k_B T \sim f$$

$$f = \frac{\omega^2}{c^3} k_B T \cdot g(__)$$

nem lehet konstans: $\int_0^\infty d\omega \cdot \omega^2 = +\infty$

↯

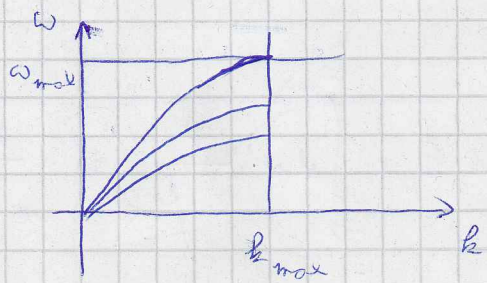
$$g = g\left(\frac{\omega}{k_B T}, k\right)$$

$$\left[\frac{\omega}{k_B T}\right] = \frac{J}{kg \cdot m^2} \qquad [k] \stackrel{!}{=} \frac{kg \cdot m^2}{J}$$

g lesz az integrált

$$\omega_m \sim T$$

Részletesen



$\omega = c \cdot k$, ha $k \to 0$

$$k_{max} \sim \frac{2\pi}{\lambda_{min}} \sim \frac{2\pi}{a} \sim 10^{-10}\ m$$

$$\omega_{max} \sim c \cdot k_{max} \sim \frac{c}{a} \sim 10^3 \frac{m}{s} / 10^{-10}\ m$$

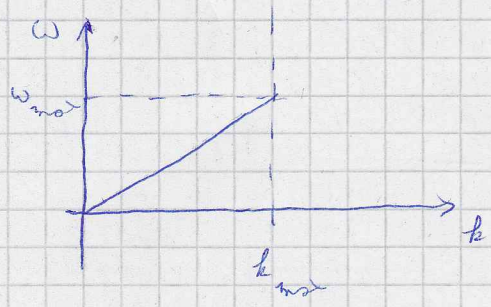
$$\sim 10^{13}\ s^{-1}$$

$$\hbar \omega_{max} \sim 10^{-34} \cdot 10^{13} \sim k_B T_0 \sim 10^{-24} T_0 \Rightarrow T_0 \sim 100\ K$$

alacsony hőmérsékleten csak a fonon hullámhossz

fonok gerjesztődnek

Debye



te oszillátorok száma:

$$G = \int_0^{\omega_{max}} d\omega\, g(\omega) = \int_0^{\omega_{max}} d\omega\, \frac{V}{\pi^2 \cdot c_{ate}^3}\, \omega^2 = \frac{V}{\pi^2 \cdot c_{ate}^3} \cdot \frac{\omega_{max}^3}{3} = 3 \cdot N_A$$

$$\frac{1}{c_{ate}^3} = \frac{1}{c_l^3} + \frac{2}{c_t^2} \qquad \Rightarrow \; k_B T_D = \hbar \omega_{max}$$

$$E = E_0 + \int_0^{\omega_{max}} d\omega\, g(\omega) \cdot \frac{\hbar\omega}{e^{\frac{\hbar\omega}{k_B T}} - 1} = E_0 + \int_0^{\omega_{max}} d\omega \cdot \frac{V}{\pi^2 \cdot c_{ate}^3} \cdot \omega^2 \cdot \frac{\hbar\omega}{e^{\frac{\hbar\omega}{k_B T}} - 1}$$

$$= E_0 + \frac{V \cdot \hbar^{-3}}{\pi^2 \cdot c_{ate}^3} (k_B T)^4 \int_0^{\frac{\hbar\omega_{max}}{k_B T}} dx \cdot \frac{x^3}{e^x - 1}$$

$$E = E_0 + \frac{V \cdot \hbar^{-3}}{\pi^2 \cdot c_{ate}^3} \cdot (k_B T)^4 \underbrace{\int_0^{\frac{\hbar\omega_{max}}{k_B T}} dx \cdot \frac{x^3}{e^x - 1}}$$

$$\rightarrow \int_0^{\infty} dx \cdot \frac{x^3}{e^x - 1} = \frac{\pi^4}{15}, \quad \text{ha } \hbar\omega_{max} \gg k_B T$$

$$\Rightarrow C \sim T^3$$

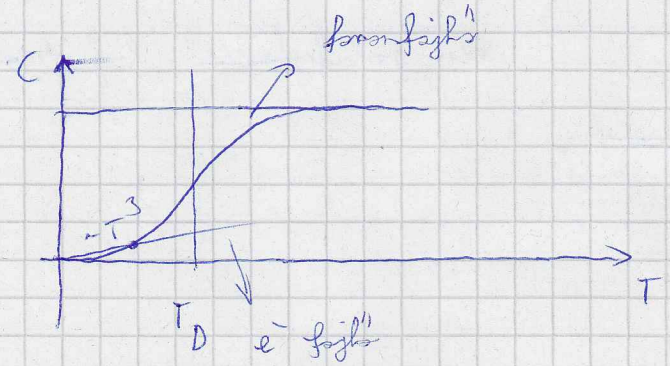
$\hbar\omega_{max} \ll k_B T$ magas hőmérséklet

$$\frac{x^3}{e^x - 1} \approx \frac{x^3}{x} = x^2$$

$$E = E_0 + \underbrace{\frac{V \cdot \hbar^{-3}}{\pi^2 \cdot c_{ate}^3} (k_B T)^4 \cdot \frac{1}{3} \left(\frac{\hbar\omega_{max}}{k_B T}\right)^3}_{3 N_A k_B T}$$

$$\Downarrow$$

$$C = 3 N_A k_B$$



Ritka klasszikus gáz → korrekciók az állapotegyenletben

$$-\beta F = \ln Z$$

$$Z = \frac{1}{N! \hbar^{3N}} \int d^{(3N)} p \, d^{(3N)} q \; e^{-\beta \mathcal{H}(p,q)}$$

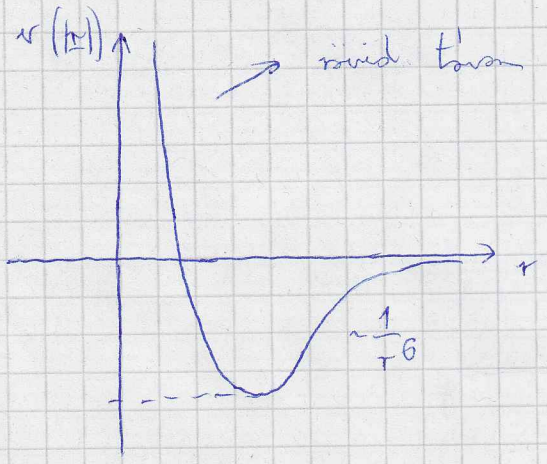
klasszikus

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 \quad , \quad \mathcal{H}_0 = \sum_i \frac{p_i^2}{2m} \qquad \mathcal{H}_1 = \frac{1}{2} \sum_{i \neq j} v_{ij}$$

$$Z_0 = \frac{V^N}{N! \lambda^{3N}}$$, ahol λ a termikus de-Broglie hullámhossz

$$\lambda = \frac{h}{\sqrt{2\pi k_B T}}$$

$$\frac{Z}{Z_0} = \frac{1}{V^N} \int d^3 r_1 \cdots d^3 r_N \cdot e^{-\frac{1}{2}\beta \sum_{i \neq j} v(\underline{r}_i - \underline{r}_j)}$$



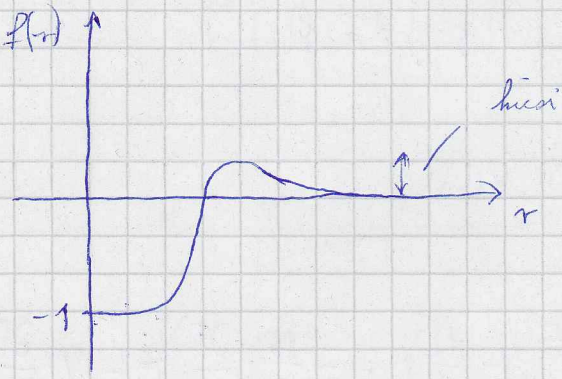
rövid távon divergencia

exp sorbafejtésével baj van

$$\frac{Z}{Z_0} = \frac{1}{V^N} \int d^3 r_1 \cdots d^3 r_N \cdot \prod_{i \neq j} e^{-\frac{\beta}{2} v_{ij}} =$$

$$= \frac{1}{V^N} \int d^3 r_1 \cdots d^3 r_N \cdot \prod_{i<j} e^{-\beta \cdot v_{ij}}$$

$$\to \frac{1}{V^N} \int d^3 r_1 \cdots d^3 r_N \cdot \prod_{i<j} \left(\underbrace{e^{-\beta v_{ij}} - 1}_{f_{ij}} + 1 \right)$$



$$= 1 + \frac{1}{V^N} \int d^3r_1 \cdots d^3r_N \cdot \left(\underbrace{\sum_{i<j} f_{ij}}_{\text{(összegzés)}} + \sum_{i \neq j} \sum_{l \neq e} f_{ij} f_{le} + \cdots \right)$$

a sor a sűrűség hatványai szerint rendeződik

$$= 1 + \frac{1}{V^2} \int d^3r_i \, d^3r_j \, f_{ij} \cdot \frac{N(N-1)}{2} + \cdots =$$

$$\underline{r}_i, \underline{r}_j \rightarrow \underline{r}_i - \underline{r}_j, \ \frac{\underline{r}_i + \underline{r}_j}{2} \qquad \underline{r} = \underline{r}_i - \underline{r}_j$$

$$= 1 + \frac{N(N-1)}{2} \frac{1}{V} \int d^3r \, f(\underline{r}) =$$

$$= 1 + \frac{1}{2} N g \cdot \int d^3r \, f(\underline{r}) \qquad g = \frac{N}{V}$$

$$\ln\left(\frac{Z}{Z_0}\right) = \ln\left(1 + \frac{1}{2} N g \int f(\underline{r}) \, d^3r + \cdots\right) = \frac{1}{2} N g \int d^3r \, f(\underline{r})$$

↑ kicsi

$$\ln Z - \ln Z_0 = -\beta F + \beta F_0 = \frac{1}{2} N \rho \cdot \int d^3 r \, f(r)$$

$$F = F_0 - \frac{1}{2} k_B T \cdot N \cdot \rho \cdot \int d^3 r \, f(r)$$

$$\rho \frac{\partial F}{\partial \rho} = \rho \cdot \frac{\partial F}{\partial V} \cdot \frac{\partial V}{\partial \rho} = \rho \cdot \frac{\partial F}{\partial \rho} \cdot \left(-\frac{N}{\rho^2} \right) = -\frac{N}{\rho} \cdot \frac{\partial F}{\partial V} = -V \cdot \frac{\partial F}{\partial V} =$$

$$= \uparrow \cdot V$$

$$\rho \frac{\partial F}{\partial \rho} = \rho \cdot \frac{\partial F_0}{\partial \rho} - \frac{1}{2} k_B T \, N \cdot \rho \int d^3 r \, f(r)$$

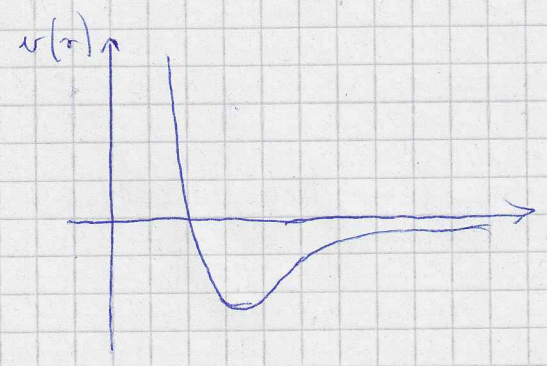
$$\uparrow V = N k_B T - \frac{1}{2} k_B T \, N \cdot \rho \int d^3 r \, f(r)$$

$$\frac{\uparrow V}{N k_B T} = 1 - \frac{1}{2} \int d^3 r \, f(r) \cdot \rho \equiv 1 + B_2(T) \rho + \dots$$

$\uparrow$

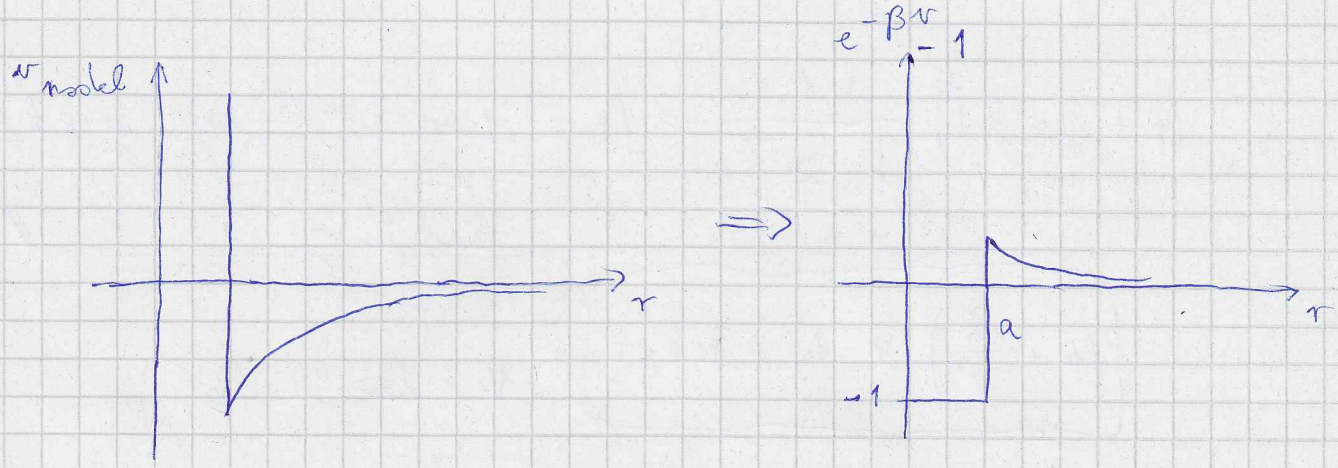
2. virial-koefficiens

$$B_2(T) = -\frac{1}{2} \int d^3 r \left(e^{-\beta v(r)} - 1 \right)$$



modellberink

egyszerűbbel



$$\int d^3r \left(e^{-\beta v} - 1\right) = -\frac{4\pi}{3} a^3 + 4\pi \int_a^\infty dr \cdot r^2 \left(e^{-\beta v(r)} - 1\right)$$

a sugara gömbön belül

$\hat{=} -\beta v(r)$

itt már v gyenge $\Rightarrow$ $\Rightarrow$ sorbafejthetünk

$$= -\frac{4\pi}{3} a^3 + \underbrace{4\pi \int_a^\infty dr \cdot r^2 \cdot \left(-\beta v(r)\right)}_{-\frac{\bar{v}}{k_B T}}$$

$$\bar{v} = \int_a^\infty dr \cdot 4\pi r^2 \cdot v(r)$$

$$\frac{pV}{N k_B T} = 1 + \frac{1}{2} \rho \frac{4\pi}{3} a^3 + \frac{1}{2} \rho \cdot \frac{\bar{v}}{k_B T}$$

$$p = \rho k_B T + \frac{1}{2} \cdot \frac{4\pi}{3} \cdot a^3 \cdot k_B T \cdot \rho^2 + \frac{1}{2} \rho^2 \cdot \bar{v}$$

$$p - \underbrace{\frac{1}{2} \rho^2 \cdot \bar{v}}_{>0} = \rho k_B T \left(1 + \frac{2\pi}{3} a^3 \rho\right)$$

$$\left(1 + \frac{1}{2}\rho^2|\bar{v}|\right)\frac{1}{1+\frac{2\pi}{3}a^3\rho} \approx \left(1+\frac{1}{2}\rho^2|\bar{v}|\right)\left(1-\frac{2\pi}{3}a^3\rho\right) = \rho k_B T \quad / \cdot V$$

rendezés

$$\boxed{\left(1+\frac{\tilde{a}}{V^2}\right)(V-b) = N k_B T}$$

Van der Waals

$$\frac{\tilde{a}}{V^2} = \frac{1}{2}\rho^2|\bar{v}| = \frac{N^2|\bar{v}|}{2V^2} \qquad b = \frac{2\pi}{3}a^3 N$$

kis sűrűség: $\frac{2\pi}{3}a^3\rho = \frac{2\pi}{3}a^3\cdot\frac{N}{V} \ll 1$

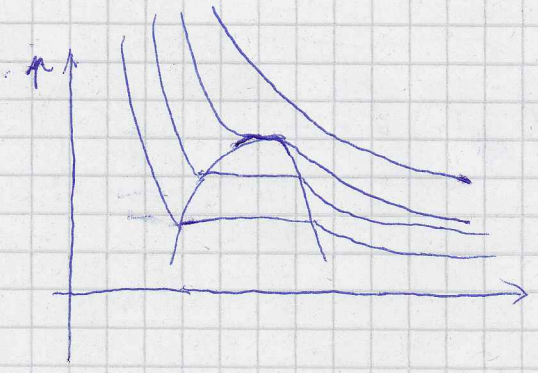
$$\bar{v} = \int_a^\infty dr \cdot 4\pi r^2 \cdot v(r)$$

$$v(r) \sim r^{-\alpha}$$

szingulás részecskék: $\alpha = 6 \rightarrow \nexists\, \bar{v}$

tiltott — " — : $\alpha = 1 \rightarrow$ divergens

nem jó!

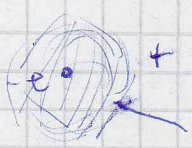


Van der Waals egyenlet

Töltés leárnyékolása

$-e$ töltés az origóban

$$\phi(r) = \frac{e^2}{r}$$



pozitív töltésű felhő

$$\phi_{eff}(r) = \phi(r) + \int v(\underline{r} - \underline{r}') \left(\rho(\underline{r}') - \rho_0\right) d^3r'$$

$\frac{e^2}{|\underline{r} - \underline{r}'|}$ ↑ elektronok sűrűsége ↑ ion sűrűsége

$$\rho(r) = \rho_0 \cdot e^{-\frac{\phi(r)}{k_B T}}$$

volna kölcsönhatás nélkül. (klasszikus)

$$\Rightarrow \rho(r) = \rho_0 \, e^{-\frac{\phi_{eff}(r)}{k_B T}}, \quad \phi_{eff} \text{ gerjeszt}$$

$$\rho(r) = \rho_0 - \rho_0 \frac{\phi_{eff}(r)}{k_B T}$$

$$\Phi_{eff}(\underline{r}) = \Phi(\underline{r}) - \frac{\rho_0}{k_B T} \int v(\underline{r}-\underline{r}') \, \Phi_{eff}(\underline{r}') \, d^3 r'$$

Fourier-trafó:

$$\Phi(\underline{k}) = \int \Phi(\underline{r}) \, e^{-i \underline{k} \underline{r}} \, d^3 r$$

$$\Phi_{eff}(\underline{k}) = \int \Phi_{eff}(r) \, e^{-i \underline{k} \underline{r}} \, d^3 r$$

$$\Phi_{eff}(\underline{k}) = \Phi(\underline{k}) - \frac{\rho_0}{k_B T} v(\underline{k}) \, \Phi_{eff}(\underline{k})$$

↑

konvolúció-tétel: konvolúció Fourier-transzformáltja szorzat

⇓

$$\Phi_{eff}(\underline{k}) = \frac{\Phi(\underline{k})}{1 + \frac{\rho_0}{k_B T} v(\underline{k})}$$

$\Phi(\underline{k}) = v(\underline{k})$ → külső forrásra ér egyrészről vett válasz arány

$$\boxed{\Phi_{eff}(\underline{k}) = \frac{v(\underline{k})}{1 + \frac{\rho_0}{k_B T} v(\underline{k})}}$$

$$\phi_{eff}(r) = \frac{e^2}{r} \cdot e^{-\kappa r}$$ ekr. Debaya

$$\phi_{eff}(\underline{k}) = \int \phi_{eff}(\underline{r}) \cdot e^{-i\underline{k}\underline{r}} \, d^3r =$$

$$= \int_0^\infty dr \cdot r^2 \cdot \frac{e^2}{r} \int_0^\pi d\vartheta \sin\vartheta \, e^{-ikr\cos\vartheta} \cdot 2\pi$$

(##)

$$-\int_{kr}^{-kr} dx \cdot e^{-ix} = \int_{-kr}^{+kr} dx \cdot e^{-ix} =$$

$x = kr\cos\vartheta$

$$= \frac{e^{-ix}}{-i}\Big|_{-kr}^{+kr} = 2\sin(kr)$$

$$\phi_{eff}(k) = \frac{4\pi e^2}{k} \int_0^\infty dr \, e^{-\kappa r} \sin(kr) =$$

$t = kr$

$$= \frac{4\pi e^2}{k^2} \int_0^\infty dt \, e^{-\frac{\kappa}{k}t} \sin t$$

$$I_\alpha = \int_0^\infty dt \, e^{-\alpha t} \cdot \sin t$$

$$I_\alpha = -e^{-\alpha t}\cos t\Big|_0^\infty + \int_0^\infty dt\,(-\alpha)\, e^{-\alpha t}\cos t =$$

$$= 1 - \alpha \int_0^\infty dt \, e^{-\alpha t}\cos t$$

mamrecht:

$$I_\alpha = \frac{e^{-\alpha t}}{-\alpha} \sin t \Big|_0^\infty - \int_0^\infty dt \, \frac{e^{-\alpha t}}{-\alpha} \cos t =$$

$$= \frac{1}{\alpha} \int_0^\infty dt \, e^{-\alpha t} \cos t$$

$$\bar{I}_\alpha = 1 - \alpha \int_0^\infty dt \, e^{-\alpha t} \cos t = \frac{1}{\alpha} \int_0^\infty dt \, e^{-\alpha t} \cos t$$

$$\int_0^\infty dt \, e^{-\alpha t} \cos t = \frac{\alpha}{1+\alpha^2}$$

$$I_\alpha = \frac{1}{1+\alpha^2}$$

$$\boxed{\phi_{eff}(k) = \frac{4\pi e^2}{k^2} \frac{1}{1+\frac{\varkappa^2}{k^2}} = \frac{4\pi e^2}{k^2+\varkappa^2}}$$

$\varkappa \to 0$

$$\phi(k) = \frac{4\pi e^2}{k^2} = v(k)$$

$$\phi_{eff}(k) = \frac{v(k)}{1 + \frac{\rho_0}{k_B T} v(k)} = \frac{4\pi e^2}{k^2 + \frac{\rho_0}{k_B T}(4\pi e^2)} \Rightarrow \varkappa = \frac{4\pi e^2 \rho_0}{k_B T}$$

$$r_D = \sqrt{\frac{k_B T}{4\pi e^2 \rho_0}}$$

$$\boxed{\phi_{eff}(r) = \frac{4\pi e^2}{r} e^{-\frac{r}{r_D}}}$$

Debye – Hückel amplitudos

Spin $S_i = \pm 1$ Ising-spin

zárt részecskéket tartunk: $\mathcal{H} = -H \sum_i S_i$

$$Z = \sum_{\{S_i\}} e^{\beta H \sum_i S_i} = \prod_i \sum_{S_i = \pm 1} e^{\beta H S_i} = \left(2 \operatorname{ch}(\beta H)\right)^N$$

$$F = -k_B T \ln Z = -\frac{N}{\beta} \ln\left(2 \operatorname{ch}(\beta H)\right)$$

$$E = -\frac{\partial}{\partial \beta}(\ln Z) = -NH \cdot \operatorname{th}\left(\frac{H}{k_B T}\right)$$

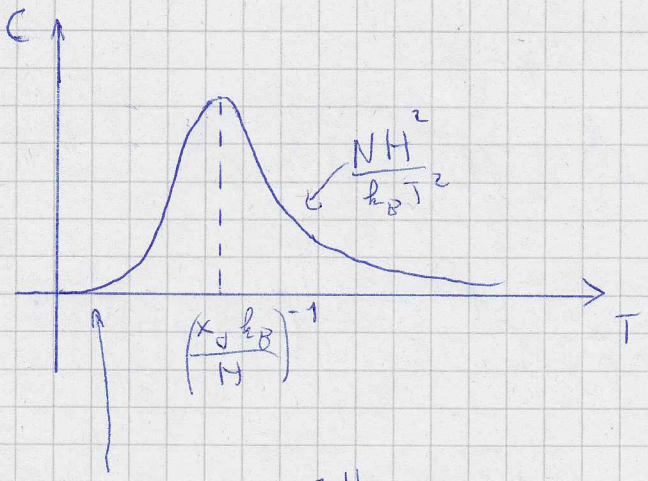
$$M = \frac{\partial}{\partial H}(\ln Z) = N \cdot \operatorname{th}\left(\frac{H}{kT}\right)$$

$$C(T) = \frac{\partial E}{\partial T} = k_B T \cdot \frac{(H/kT)^2}{\operatorname{ch}^2\left(\frac{H}{k_B T}\right)}$$

$$\chi = \frac{\partial M}{\partial H} = \frac{N}{k_B T} \cdot \frac{1}{\operatorname{ch}^2\left(\frac{H}{k_B T}\right)}$$

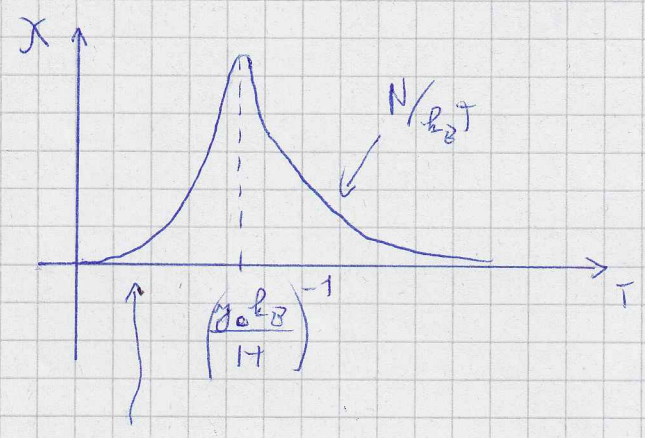
$$(\Delta \mathcal{H})^2 = \langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2 = \frac{\partial^2}{\partial \beta^2}(\ln Z) = -\frac{\partial E}{\partial \beta} = kT^2 \cdot \frac{\partial E}{\partial T} = kT^2 \cdot C(T)$$

$$(\Delta M)^2 = \langle M^2 \rangle - \langle M \rangle^2 = \frac{\partial^2}{\partial (\beta H)^2} \ln Z = k_B T \cdot \frac{\partial \langle M \rangle}{\partial H} = kT \cdot \chi$$



$\frac{4NH^2}{k_B T^2} e^{-\frac{2H}{k_B T}}$

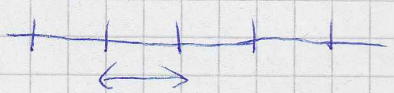
$\frac{H}{k_B T} = x_0 \qquad x_0 = \text{cth}\, x_0$



$\frac{N}{k_B T} e^{-\frac{2H}{k_B T}}$

$y_0 = \frac{1}{2}\,\text{cth}\, y_0$

1d Ising modello:



$\mathcal{H} = -J \sum_i S_i S_{i+1}$ $\quad J>0$ ferro $\quad J<0$ antiferro

$$Z_N = \sum_{\{S_i\}} e^{K \sum_{i=1}^{N-1} S_i S_{i+1}}$$

$K = \beta J$

$$Z_{N+1} = \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \cdots \sum_{\sigma_N=\pm 1} e^{K \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1}} \underbrace{\sum_{\sigma_{N+1}=\pm 1} e^{K \sigma_N \sigma_{N+1}}}_{2 \operatorname{ch} K}$$

független S_N-től

$$= 2 \cdot \operatorname{ch} K \cdot Z_N$$

$$Z_1 = \sum_{\sigma_1=\pm 1} e^0 = 2$$

$$\boxed{Z_N = 2^N \cdot (\operatorname{ch} K)^{N-1}}$$

$$E = -\frac{\partial}{\partial \beta} (\ln Z) = -J \cdot \frac{\partial}{\partial K} \ln Z$$

$$\ln Z = N \ln 2 + (N-1) \ln \operatorname{ch} K$$

$$E(T) = -(N-1) J \operatorname{th} K \approx -N J \operatorname{th} K$$

$T \to 0 : \quad E \to -(N-1) J$

$T \to \infty : \quad E \to -0$

fajhő

$$C = \frac{\partial E}{\partial T} = (N-1) k_B \frac{K^2}{\operatorname{ch}^2 K}$$

entrópia

$$S = k_B \ln Z + \frac{1}{T} E = N k_B \ln 2 + (N-1) k_B \ln \operatorname{ch} K$$

$$-(N-1) k_B \cdot K \cdot \operatorname{th} K$$

$K \to 0 \quad (J \to 0 \text{ vagy } T \to \infty)$:

$$S \to N k_B \ln 2 = k_B \ln\left(2^N\right)$$ ← független spinek 2^N állapot összes valószínűséggel

$K \to \infty \quad (T \to 0)$:

$$\ln(\operatorname{ch} K) = \ln\left(\frac{1}{2} e^K \left(1 + e^{-2K}\right)\right)$$

$$= K - \ln 2 + \dots$$

$$K \operatorname{th} K \to K \quad \Rightarrow \quad S = k_B \ln 2$$

↑ minden ismert spinek $\Rightarrow$ 2 állapot (mind ↑, mind ↓)

Korrelációs függvény:

$$C_k(r) = \langle S_k S_{r+k} \rangle = \frac{1}{Z_N} \sum_{\{S_i\}} S_k S_{r+k} \, e^{+K \sum_{i=1}^{N-1} S_i S_{i+1}}$$

Trükk: $\mathcal{H} = -\sum_{i=1}^{N-1} J_i \cdot S_i \cdot S_{i+1}$

↑ pontról pontra változó csatolási állandó

$$Z_{N+1} = 2 \operatorname{ch} K_N \cdot Z_N \quad , \quad Z_1 = 2$$

$$Z_N = 2^N \prod_{i=1}^{N-1} \operatorname{ch} K_i$$

$$C_k(r) = \langle S_k S_{k+r} \rangle = \frac{1}{Z_N} \left(\sum_{\{S_i\}} \right) \frac{\partial}{\partial K_k} \frac{\partial}{\partial K_{k+1}} \cdots \frac{\partial}{\partial K_{k+r-1}} Z_N \Big|_{K_i = K}$$

Mert: $\frac{\partial}{\partial K_i} Z_N = \sum_{\{S_k\}} S_i S_{i+1} \, e^{\sum_{\ell=1}^{N-1} K_\ell S_\ell S_{\ell+1}}$

$$\frac{\partial}{\partial K_k} \cdot \frac{\partial}{\partial K_{k+1}} \cdots \frac{\partial}{\partial K_{k+r-1}} Z_N =$$

$$= \sum_{\{S\}} (S_k S_{k+1})(S_{k+1} S_{k+2}) \cdots (S_{k+r-1} S_{k+r}) \cdot e^{\sum_{\ell=1}^{N-1} K_\ell S_\ell S_{\ell+1}}$$

$(S_{k+1} S_{k+2}) = 1$, $(S_{k+r-1} S_{k+r}) = 1$

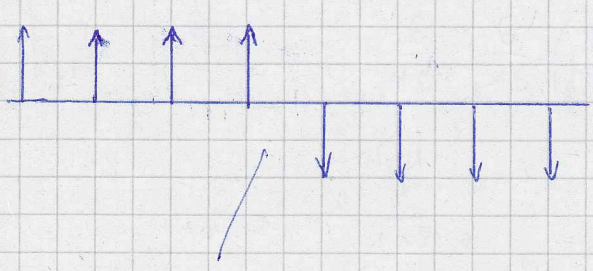
$S_i^2 = 1 \quad \forall i$

$$= \sum_{\{S\}} S_k S_{k+r} \, e^{\sum_{\ell=1}^{N-1} K_\ell S_\ell S_{\ell+1}}$$

$C_k(r) = \text{th}^r K$ független k-tól

$C(r) = e^{r \ln \text{th} K} \equiv e^{-\frac{r}{\xi}}$

$\xi = \frac{1}{|\ln \text{th} K|} \longrightarrow \begin{cases} 0 & , K \to 0 \\ \infty & , K \to \infty \end{cases}$



$\Delta E = 2J$

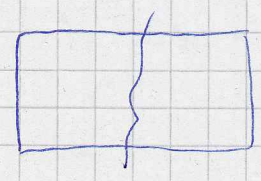
$\Delta S \sim \ln N$

$\Delta F = \Delta E - T \Delta S$

a törésponttól csökkentik a rendezettségi

$\Rightarrow$ rendeződés $\emptyset$

2d:



$\Delta E \sim \sqrt{N}$

a fenti érv nem működik

2d-ben tud rendeződni a rendszer

1D Ising-modell, $H \neq 0$, periodikus kötésfeltételek

$$S_{N+1} \equiv S_1$$

$$Z_N = \sum_{\{s_i\}} e^{\sum_i K s_i s_{i+1} + \frac{h}{2} \sum_i (s_i + s_{i+1})}$$

$\Downarrow$ szimmetrikusan szerepelnek

$$h = \frac{H}{k_B T} \qquad K = \frac{J}{k_B T}$$

Def.: transzfer mátrix

$$T_{ss'} = e^{K s s' + \frac{h}{2}(s + s')}$$

$$\begin{pmatrix} T_{++} & T_{+-} \\ T_{-+} & T_{--} \end{pmatrix} = \begin{pmatrix} e^{K+h} & e^{-K} \\ e^{-K} & e^{K-h} \end{pmatrix}$$

$$Z = \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \cdots \sum_{s_N=\pm 1} T_{s_1 s_2} T_{s_2 s_3} \cdots T_{s_N s_1} =$$

$$= \sum_{s_1=\pm 1} \left(T^N\right)_{s_1 s_1} = \mathrm{Sp}\left(T^N\right)$$

T sajátértékei: λ_1, λ_2

$$\mathrm{Sp}\, T = \lambda_1 + \lambda_2$$

$$\mathrm{Sp}\, T^N = \lambda_1^N + \lambda_2^N$$

$$0 = \begin{vmatrix} e^{K+h} - \lambda & e^{-K} \\ e^{-K} & e^{K-h} - \lambda \end{vmatrix} = \lambda^2 - 2\lambda e^K \mathrm{ch}(h) + \underbrace{e^{2K} - e^{-2K}}_{2\,\mathrm{sh}(2K)}$$

$$\lambda_{1,2} = e^K \mathrm{ch}(h) \pm \sqrt{e^{2K}\,\mathrm{sh}^2(h) + e^{-2K}} \qquad \lambda_1 > \lambda_2$$

Specializáció: $h = 0$ $\quad \lambda_{1,2} = e^K \pm e^{-K} = \begin{cases} 2\,\mathrm{ch}\,K \\ 2\,\mathrm{sh}\,K \end{cases}$

$$Z_N = 2^N \left(\mathrm{ch}^N K + \mathrm{sh}^N K\right) = 2^N \mathrm{ch}^N K \left(1 + \mathrm{th}^N K\right)$$

$\mathrm{th}\, K < 1$ $\qquad \downarrow N \to \infty$ $\qquad 0$

Z_N a két esetben:

- zárt végek esetén: $Z^N ch^{N-1} K \to 2^N \cdot ch^N K$
- periodikus határfeltétel esetén:

$$2^N ch^N K (1 + th^N K) \to 2^N ch^N K$$

általában: elhanyagolható a határfeltételek, ha a lánc elég hosszú

$$Z_N = \lambda_1^N \left(1 + \left(\frac{\lambda_2}{\lambda_1}\right)^N\right) \approx \lambda_1^N$$

$\lambda_1 > \lambda_2$ $\Rightarrow$ 0

legnagyobb sajátérték N hatványa adja az állapotösszeget (általában)

$$\ln Z_N = N \ln \lambda_1 = N \ln\left(e^K ch k + \sqrt{e^{2K} sh^2(k) + e^{-2K}}\right)$$

$$M = \underbrace{\frac{\partial}{\partial(\beta H)}}_{\ell} \ln Z \approx N \frac{e^K sh(k) + \frac{e^{2K} sh(k) ch(k)}{\sqrt{e^{2K} sh^2(k) + e^{-2K}}}}{e^K ch(k) + \sqrt{e^{2K} sh^2(k) + e^{-2K}}}$$

$$= N \cdot \underbrace{\frac{e^K sh(k)}{\sqrt{e^{2K} sh^2(k) + e^{-2K}}}} \cdot \frac{e^K ch(k) + \sqrt{\cdots}}{e^K ch(k) + \sqrt{\cdots}}$$

$\to 1$

$K \to 0$ $(T \to \infty$ v. $J \to 0)$ esetén

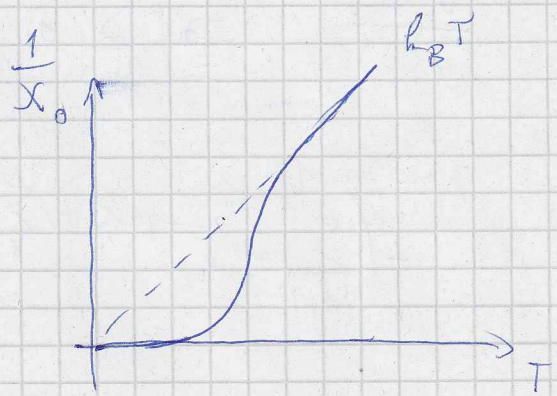
$$\ln Z = N \ln(2\cosh(h))$$

$$M = N \cdot \tanh(h)$$ ezt már tudtuk

$$M(T, H=0) = 0$$

$$M(T=0) = N \cdot \operatorname{sgn}(H)$$

$$\chi_0 = \left.\frac{\partial M}{\partial H}\right|_{H=0} = \frac{N}{k_B T} e^{\frac{2J}{k_B T}}$$



$H = 0$, $T = 0$ lényegi szingularitás

$$\chi(T, H) = \frac{1}{k_B T} \frac{e^{-K}\cosh(h)}{\left(e^{2K}\sinh^2(h) + e^{-2K}\right)^{3/2}}$$

Most lapunk, ha más sorrendben tartunk a 0-hoz

Korreláció - válasz tétel

$\mathcal{H}$ többlépés, $h_i = \frac{H_i}{k_B T}$ dimenziótlan

$$Z = \sum_{\{s_j\}} e^{-\beta H + \sum_j h_j s_j}$$

$$\frac{\partial \ln Z}{\partial h_i} = \frac{1}{Z} \sum_{\{s_j\}} s_i \cdot e^{-\beta \mathcal{H} + \sum_j h_j s_j} = \langle s_i \rangle$$

$$\frac{\partial^2 \ln Z}{\partial h_i \partial h_k} = \frac{1}{Z^2} \left[\sum_{\{s_j\}} s_i s_k e^{-\beta \mathcal{H} + \sum_j h_j s_j} \cdot Z - \right.$$

$$\left. - \left(\sum_{\{s_j\}} s_i e^{-\beta \mathcal{H} + \sum_j h_j s_j} \right) \left(\sum_{\{s_j\}} s_k e^{-\beta \mathcal{H} + \sum_j h_j s_j} \right) \right] =$$

$$= \boxed{\langle s_i s_k \rangle - \langle s_i \rangle \langle s_k \rangle = \frac{\partial \langle s_i \rangle}{\partial h_k}}$$ korrelációs fv

nemzine tűnik el i várható értéke, ha j-be megjósoljuk a rendszert → nézi a korrelációt

$$\sum_{i,j} \left(\langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle \right) = \left\langle \sum_i s_i \sum_j s_j \right\rangle - \left\langle \sum_i s_i \right\rangle \left\langle \sum_j s_j \right\rangle$$

$$= \langle M^2 \rangle - \langle M \rangle^2 \quad , \text{ hol } M = \sum_i s_i$$

$$\frac{\partial \ln Z}{\partial (\beta H)} = \langle M \rangle = \left\langle \sum_i s_i \right\rangle$$

$$\frac{\partial^2 \ln Z}{\partial(\beta H)^2} = k_B T \cdot \frac{\partial \langle M \rangle}{\partial H} = k_B T \chi$$

$$\frac{\partial \langle M \rangle}{\partial(\beta H)} = \frac{\partial}{\partial(\beta H)} \left(\frac{1}{Z} \sum_{\{s\}} \left(\sum_i s_i \right) e^{-\beta \mathcal{H} + \beta H \sum_j s_j} \right) =$$

$$= \left\langle \sum_i s_i \sum_k s_k \right\rangle - \left\langle \sum_i s_i \right\rangle \left\langle \sum_j s_j \right\rangle = \langle M^2 \rangle - \langle M \rangle^2$$

$$\sum_{i,j} \left(\langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle \right) = k_B T \chi$$

korrelációs fv. kiösszegzve = $k_B T \cdot$ szuszceptibilitás

$\Rightarrow$ kitérjedt korrelációk nagy érzékenységet és nagy fluktuációkat okoznak

(fázisátalakulásban: korreláció $\to \infty$
$\Rightarrow$ érzékenység $\to \infty$ a kritikus pontban)

1D antiferromágnes

$$\mathcal{H} = |J| \sum s_i s_{i+1} - H \sum s_i$$

$\uparrow\downarrow\uparrow\downarrow \ldots$ szerkezet beállni alapállapotban ($H = 0$)

$$\ln Z = N \ln(2 \operatorname{ch} K) \quad K < 0$$

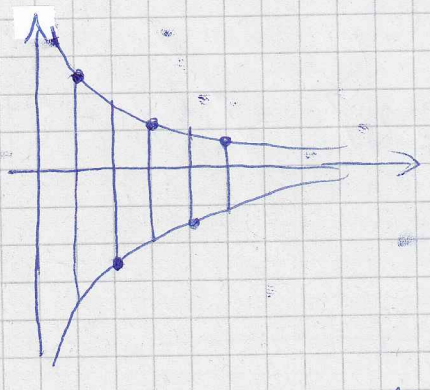
korrelációs fv.: $C_z(r) = \text{th}^r(K)$

$$|C_z(r)| = \text{th}^r|K| = e^{-r|\ln \text{th}|K||} = e^{-\frac{r}{\xi}}$$

$$\ln|\text{th}|K|| < 0$$

$$\xi = \frac{1}{|\ln \text{th}|K||}$$

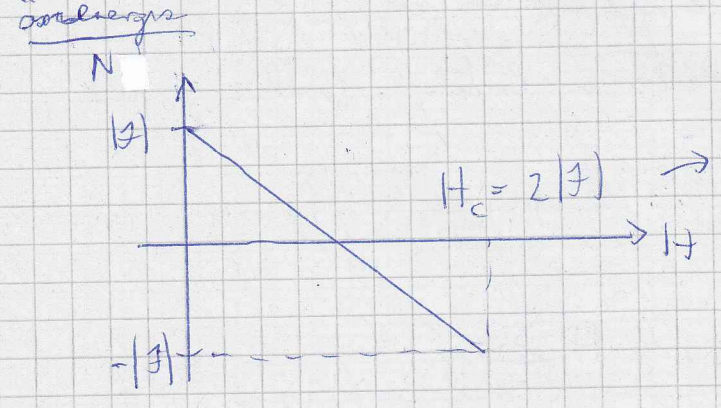
korrelációs hossz



ha bekapcsolok a külső teret, az be akarja állítani a spineket

$H \neq 0$

		energiája
alapállapot	$\uparrow\downarrow\uparrow\downarrow\uparrow\cdots$	$-|J|N$
	$\uparrow\uparrow\uparrow\uparrow\uparrow\cdots$	$(|J| - H)N$

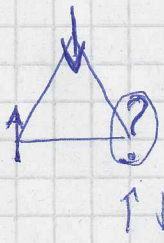


attól az értéktől kezdve átáll

ha pont $H = H_c$-nél vagyunk, akkor mindegy, hogy állnak a spinek → exponenciálisan sok alapállapot

van rácsból is előfordul

Δ - rács



→ frusztráció: nincs kielégítve a csatolás

↑↓

rácsrendszerhez entrópia szorul a rendszerbe

az antiferromágneses spektrum a fejét tetejére állította

ferromágneses spektrum → az alapállapot a legnagyobb multiplicitású és a legnagyobb energiaszint 2-szeresen degenerált

átlagtér-elmélet

Hamiltonfüggvény: Hartree

$$\mathcal{H} = -\frac{1}{2} J \sum_{(i,j)} s_i s_j - H \sum_i s_i \qquad \text{(több dim)}$$

↑ első szomszédokra

átlag fluktuációs (kicsi)

$$s_i s_j = \left(\langle s_i \rangle + (s_i - \langle s_i \rangle)\right)\left(\langle s_j \rangle + (s_j - \langle s_j \rangle)\right) =$$

$$= \langle s_i \rangle \langle s_j \rangle + \langle s_i \rangle (s_j - \langle s_j \rangle) + \langle s_j \rangle (s_i - \langle s_i \rangle) +$$

$$+ (s_i - \langle s_i \rangle)(s_j - \langle s_j \rangle) = \langle s_i \rangle s_j + \langle s_j \rangle s_i - \langle s_i \rangle \langle s_j \rangle$$

másodrendben kicsi

tmit elhanyagoltunk: $(s_i - \langle s_i \rangle)(s_j - \langle s_j \rangle)$ → fluktuációk szorzata

Ez akkor tehető meg, ha 1 spin sokat változik. (Nagy. Számolásnál - tétel működik)

Legyen $\langle s_i \rangle = m$

$$\mathcal{H} = -\frac{1}{2} J \sum_{(i,j)} \left(s_i \langle s_j \rangle + s_j \langle s_i \rangle - \langle s_i \rangle \langle s_j \rangle \right) - H \sum_i s_i =$$

$$= \frac{1}{2} J N q m^2 - (H + J q m) \sum_i s_i$$

q: legközelebbi szomszédok száma

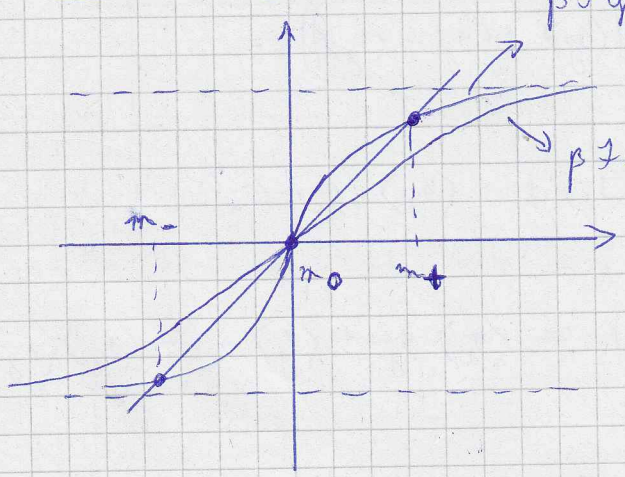
$$Z = e^{-\frac{1}{2} \beta J N q m^2} \cdot 2^N \operatorname{ch}^N \left(\beta (H + J q m) \right)$$

$$\langle s_i \rangle = m = \operatorname{th} \left(\beta (H + J q m) \right)$$

belső tér

$F = -k_B T \ln Z$ $\quad \frac{\partial F}{\partial m} = 0$ stacionárius állapot

$H = 0$ grafikus



1. $\beta \mathcal{J}_q < 1$, $k_B T > \mathcal{J}_q \longrightarrow m_0 = 0$

2. $\beta \mathcal{J}_q > 1$, $k_B T < \mathcal{J}_q \longrightarrow m_0 = 0$, $m_\pm \neq 0$

$m_- = -m_+$

spontán szimmetriasértés: két nem szimmetrikus megoldás jelenik meg, amelyek egymás tükörképei

$$m = \langle s_i \rangle = \frac{1}{Z} \sum_{\{s\}} s_i \cdot e^{-\beta \mathcal{H}(s)} \equiv 0$$

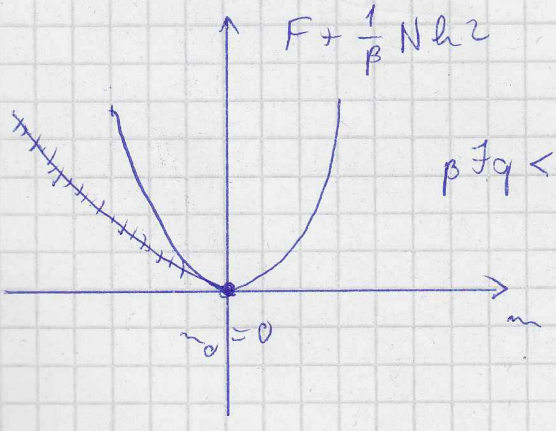
s_i: tükrözésnél előjelet vált

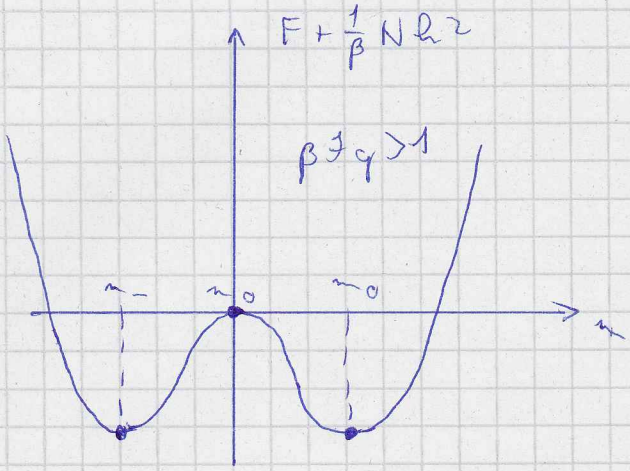
$\mathcal{H}(s)$: tükrözésnél nyereséget

Paradoxon: m-et a $\langle \rangle$ formulájával számolva csak az $m_0 = 0$ -t kapjuk meg.

$$-F = \frac{1}{2} q N m^2 + k_B N T \ln 2 + N k_B T \ln \operatorname{ch}\left(\frac{H + \mathcal{J}_q m}{k_B T}\right)$$

↑ szabadenergia





m_0 - ben F-nek maximuma van → lesznek visszafelé görbébe

hol ben az ergodicitással: a pálya nem járja be az

egész fázisteret

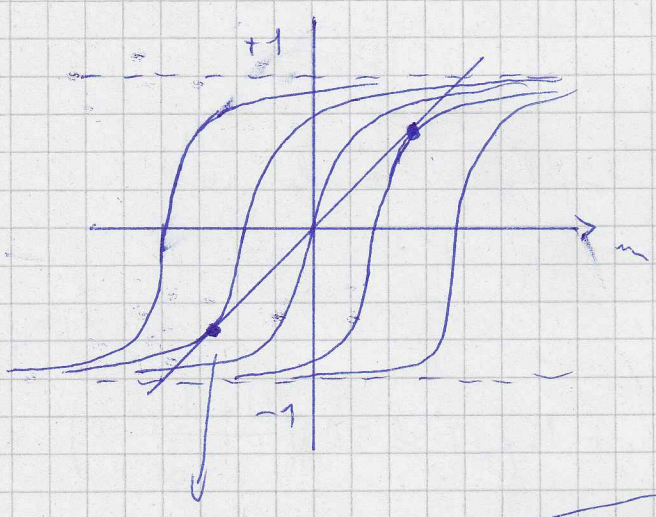
( ) fennállhat csak a fázistér egy részére belül

összegezni → hiján $m_\pm$

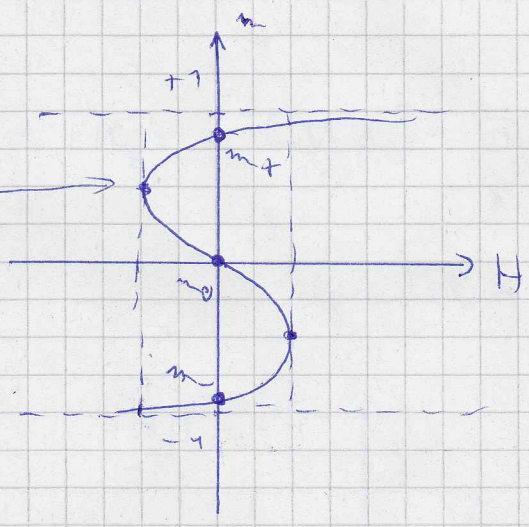
gyakorlati megoldás: harcsánduk egy kis "külső"

perturbáló teret, amivel $\to 0$

$H \neq 0$ $\quad m = \text{th}\left(\beta(H + J q m)\right)$



érintési pont



Susceptibilitás

$$\chi = \frac{\partial m}{\partial H} = m' = \frac{\beta + \beta J q m'}{\cosh^2(\beta(H + J q m))} = (\beta + \beta J q m')(1 - \underbrace{\tanh^2 \ldots}_{m})$$

$$= (\beta + \beta J q m')(1 - m^2) \rightarrow m' \text{ kifejezhető}$$

$$m' = \frac{\beta(1-m^2)}{1 - \beta J q (1-m^2)} = \frac{\chi_0}{1 - J q \chi_0} = \chi$$

, ahol $\chi_0 = \beta(1-m^2)$

$m_0 = 0$, $\beta J q \to 1-$ $\Rightarrow \chi \to \infty$

A fázisátalakulás kritikus pontján a rendszer hiperérzékennyé válik

T_c felett az állapotegyenlet $\beta_c = \frac{1}{J q}$

$$\left(\frac{\beta}{\beta_c} - 1\right) m + \beta H - \frac{1}{3}\left(\frac{\beta}{\beta_c} m + \beta H\right)^3 = 0$$

$$\frac{\beta}{\beta_c} - 1 \equiv \tau \;,\; |\tau| \ll 1 \;,\; |H| \ll m \ll 1$$

$$\tau \cdot m + H \beta_c = \frac{1}{3} m^3 \qquad / \cdot \tau^{-3/2}$$

$$\frac{m}{\tau^{1/2}} + \frac{H \beta_c}{\tau^{3/2}} = \frac{1}{3} \cdot \left(\frac{m}{\tau^{1/2}}\right)^3$$

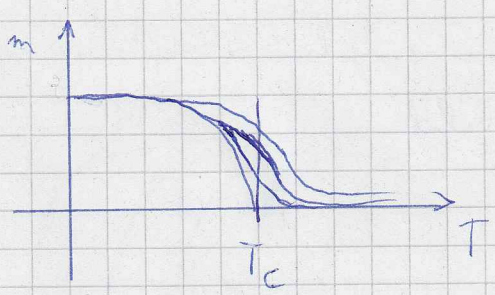
$$\Rightarrow \frac{m}{\tau^{1/2}} = f\left(\frac{H}{\tau^{3/2}}\right)$$

$$m\,\tau^{1/2} = f\left(\frac{H}{\tau^{3/2}}\right)$$

általában: $m = \tau^{\beta} \cdot f\left(\frac{H}{\tau^{\beta\delta}}\right)$ $\rightarrow$ $\beta = 1/2$, $\delta = 3$

Ezek a számok nem egészek, mert a kicsiket túl egyszerűen vettük

$H = 0$: $\tau m = \frac{1}{3} m^3$ $\quad m \sim \tau^{1/2}$



$T < T_c$ $\quad m \neq 0$

$\tau = 0$: $H\beta_c = \frac{1}{3} m^3$, $m \sim H^{1/3}$, $\delta = 3$

~~(Gauss)~~ Szuszceptibilitás:

$$\chi = \frac{\beta}{1 - \beta J q} = \frac{\beta}{1 - \frac{\beta}{\beta_c}} = \frac{1}{k_B T_c} \cdot \frac{1}{\frac{T}{T_c} - 1} = -\frac{1}{k_B T_c} \cdot \frac{1}{\tau}$$

$\Downarrow$ $\gamma = 1$

$\beta = \frac{1}{k_B T}$

$\chi \sim \tau^{-\gamma}$

$T \lesssim T_c$, $H = 0$

$$\frac{F}{N} = -\frac{1}{\beta} \ln z - \frac{1}{\beta}\left[\frac{1}{2}(\beta J q m)^2 - \frac{1}{2}\beta J q m^2\right] =$$

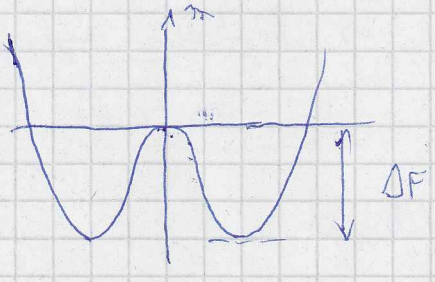
$$= -\frac{1}{\beta} \ln z - \frac{Jq}{2} m^2 (\beta J q - 1)$$

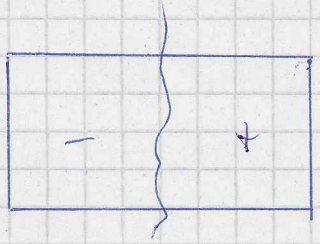
$$= \left(\frac{F}{N}\right)_{m=0} - \frac{Jq}{2} m^2 \frac{\beta - \beta_c}{\beta_c} + \dots$$

$\uparrow O(m^4)$

$$\Delta\left(\frac{F}{N}\right) = \left(\frac{F}{N}\right)_{m=0} - \left(\frac{F}{N}\right)_{m} =$$

$$= \frac{Jq}{4} \cdot m^2 \cdot \tau \qquad \Delta F = \frac{3}{4} N J q \cdot \tau^2$$





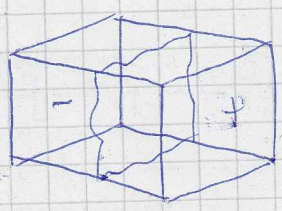
2 dim

$\sqrt{N}$ - részecske ill a változótérszám

$$\Delta F \sim k_B T_c N^{1/2}$$

általában $\Delta F \sim N^{d}$

3 dim



$\sim N^{2/3}$

$$t_{erg} \sim e^{\frac{\Delta F}{k_B T}} = e^{(\sim) \frac{N^{\alpha}}{k_B T}}$$

$$t_{erg} \sim 10^{-12} \cdot e^{(\ )N^{\alpha}}$$

$N \sim 10^{24}$

→ kb. elveszíti ergodicitását

Univerzum 10^{17} s élettartam

a rendszer nem hagyja el a potenciálgödröt ⇒

⇒ ergodicitás sérül

kísérletben rendszert vizsgálunk ⇒ átfordulás megfigyelhető

átlagtér-elmélet nyújt kitűnőket ad

$C \sim |\tau|^{-\alpha}$ | $m \sim |\tau|^{+\beta}$ ↑ $H \to 0$ | $\chi \sim |\tau|^{-\gamma}$

$m \sim |H|^{1/\delta} \quad \leftarrow \tau = 0$

$\xi \sim |\tau|^{-\nu}$ $\qquad C(r) \sim \frac{1}{r^{d-2+\eta}} f\left(\frac{r}{\xi}\right)$

↓

korrelációhossz

$F = \tau^{2-\alpha}\, \tilde{F}\left(\frac{h}{\tau^{\beta\delta}}\right)$ általában homogén függvénye a változóinak

$h = 0 \quad F \sim \tau^{2-\alpha} \Rightarrow C \sim \tau^{-\alpha}$

$\frac{\partial F}{\partial h} = m = \tau^{2-\alpha-\beta\delta}\, \tilde{F}'\left(\frac{h}{\tau^{\beta\delta}}\right)$

$m \sim \tau^{2-\alpha-\beta\delta} = \tau^{\beta}$, ha $h = 0$

$$\boxed{2-\alpha-\beta\delta = \beta}$$

$\frac{\partial^2 F}{\partial h^2} = \frac{\partial m}{\partial h} = \chi = \tau^{\beta-\beta\delta}\, \tilde{F}''\left(\frac{h}{\tau^{\beta\delta}}\right)$

$h = 0 \quad \chi \sim \tau^{\beta-\beta\delta} = \tau^{-\gamma}$

$$\boxed{\gamma = \beta(\delta-1)}$$

mean-field elmélet $\alpha = 0$, $\beta = \frac{1}{2}$, $\delta = 3$

$\Rightarrow$ teljesíti a fenti skálatörvényeket

Lyon-skálatörvények

$d\nu = 2-\alpha$ $\qquad d\frac{\delta-1}{\delta+1} = 2-\eta$

főiskolai universitási osztályokba soroltak

Kitűnő kitűnő egy osztályon belül marad

oklevelező osztályokon átvehetik

versenyzési csoport → nagyon fontos!