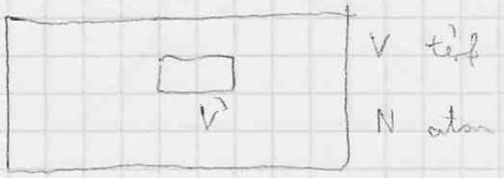
## Sűrűségingadozás

www.complex.elte.hu/~szovri/
/bevstat.ptf




$V'$ térfogatban hány atom? várhatóan $\frac{N}{V}\cdot V'$

$p(n)$ valószínűség: $n$ db atom $V'$-ben

1 atom $\frac{V'}{V}$ valószínűséggel van $V'$-ben

atomok egymástól függetlenek

$$p(n) = \binom{N}{n}\cdot\left(\frac{V'}{V}\right)^{n}\left(1-\frac{V'}{V}\right)^{N-n}$$ binomiális eloszlás

$$\bar{n} = \sum_{n=0}^{N} p(n)\cdot n \qquad \overline{n^2} = \sum_{n=0}^{\infty} p(n)\cdot n^2$$

$$\overline{\Delta n^2} = \overline{n^2} - \bar{n}^2$$

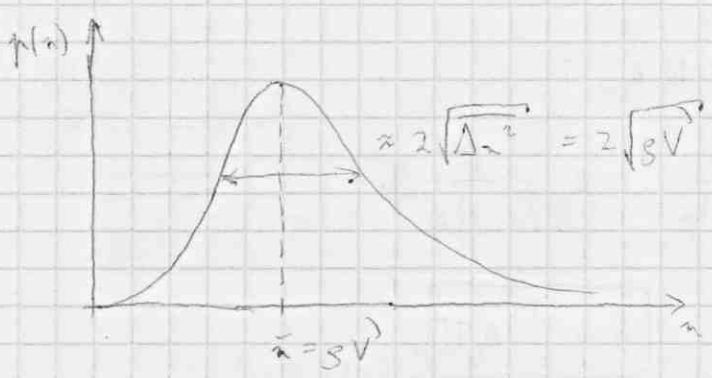
Generátor-függvény: $$G(z) = \sum_{n=0}^{N} p(n)\, e^{nz} = \sum_{\ell=0}^{\infty}\frac{1}{\ell!}\underbrace{\left(\sum_{n=0} p(n)\, n^{\ell}\right)}\, z^{\ell}$$

$$\left.\frac{d^{\ell}G(z)}{dz^{\ell}}\right|_{z=0} = \sum_{n=0}^{N} p(n)\cdot n^{\ell} = \overline{n^{\ell}}$$

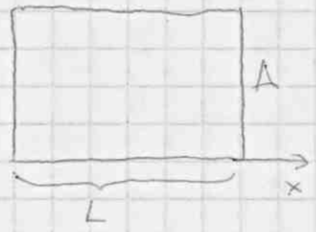
$\overline{n^{\ell}}$ momentum

$$G(z) = \sum_{n=0}^{N}\binom{N}{n}\left(\frac{V'}{V}\right)^{n}\left(1-\frac{V'}{V}\right)^{N-n} e^{nz} = \left[\frac{V'}{V}e^{z} + \left(1-\frac{V'}{V}\right)\right]^{N}$$

$$\bar{n} = \left.\frac{dG}{dz}\right|_{z=0} = N\left[\ \dots\ \right]^{N-1}\cdot\left.\frac{V'}{V}e^{z}\right|_{z=0} = \frac{N}{V}\cdot V'$$




<u>állapotegyenlet:</u> $p$ nyomás




átadott impulzus: $2|p_x|$

2 ütközés közötti idő: $\frac{2L}{\frac{|p_x|}{m}} = \frac{2mL}{|p_x|}$

$\Delta t$ idő alatt átadott impulzus: $2|p_x| \frac{\Delta t}{\frac{2mL}{|p_x|}} = \frac{p_x^2}{mL} \Delta t$

x normálisú lapra ható erő:

$$F_x = pA = \sum_{\alpha=1}^{N} \frac{p_{x\alpha}^2}{mL}$$

nyomás: $p = \frac{1}{V} \sum_{\alpha=1}^{N} \frac{p_{x\alpha}^2}{m} = \frac{N}{V} \frac{\overline{p_x^2}}{m}$ $\qquad \overline{p_x^2} = \frac{1}{N} \sum_{\alpha=1}^{N} p_{x\alpha}^2$

nincs kitüntetett irány: $\overline{p_x^2} = \overline{p_y^2} = \overline{p_z^2}$

(x, y, z ekvivalensek)

$$\overline{p_x^2} = \frac{1}{3} \overline{\left(p_x^2 + p_y^2 + p_z^2\right)} = \frac{\overline{p^2}}{3} = \frac{2m}{3} \overline{\varepsilon}$$

$$\boxed{p = \frac{N}{V} \cdot \frac{2}{3} \overline{\varepsilon}}$$

termodinamika: $pV = nRT = N k_B T$

$$n = \frac{N}{N_A} \qquad k_B = \frac{R}{N_A}.$$

$$pV = N \cdot \frac{2}{3} \bar{\varepsilon} = N k_B T \implies \boxed{\bar{\varepsilon} = \frac{3}{2} k_B T}$$

hőmérséklet kinetikus értelmezése

átlagos távolság: $\left(\frac{V}{N}\right)^{\frac{1}{3}} \gg r_0$ hatótávolság

$\implies$ nincs kölcsönhatás a részecskék között

Viriáltétel

$$\dot{p}_\alpha = F_\alpha \qquad \alpha = 1, \ldots, N$$

$$\frac{d}{dt}\left(\sum_{\alpha=1}^{N} p_\alpha r_\alpha\right) = \sum_\alpha \left(\dot{p}_\alpha r_\alpha + p_\alpha \dot{r}_\alpha\right) =$$

$$= \sum_\alpha F_\alpha r_\alpha + \sum_\alpha \frac{p_\alpha^2}{m} = \sum_\alpha F_\alpha r_\alpha + 2 \sum_\alpha \varepsilon_\alpha$$

időbeli átlag: $$\bar{A} = \lim_{T \to \infty} \frac{1}{T} \int_{t-\frac{T}{2}}^{t+\frac{T}{2}} A(t') \, dt'$$

$$\overline{\frac{dA}{dt}} = \lim_{T \to \infty} \frac{1}{T} \int_{t-\frac{T}{2}}^{t+\frac{T}{2}} \frac{dA(t')}{dt'} \, dt' = \lim_{T \to \infty} \frac{1}{T}\left[A\left(t+\frac{T}{2}\right) - A\left(t-\frac{T}{2}\right)\right] = 0$$

, ha A korlátos

$$\implies 0 = \overline{\frac{d}{dt}\left(\sum_\alpha p_\alpha r_\alpha\right)} = \underbrace{\overline{\sum_\alpha F_\alpha r_\alpha}}_{\text{viriál}} + 2 \overline{\sum_\alpha \varepsilon_\alpha}$$

ideális gázban:

$$\overline{\sum_\alpha \underline{F}_\alpha \underline{r}_\alpha} = - \int_S p (\underline{n}\, \underline{r})\, df = - p \int \underbrace{\operatorname{div} \underline{r}}_{3}\, dV = -3pV$$

$$-3pV + 2 \underbrace{\sum_\alpha \varepsilon_\alpha}_{N \cdot \overline{\varepsilon}} = 0$$

$$\Rightarrow \boxed{p = \frac{N}{V} \cdot \frac{2}{3}\, \overline{\varepsilon}}$$

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$$-2 \sum_\alpha \varepsilon_\alpha = \overline{\sum_\alpha \underline{F}_\alpha \underline{r}_\alpha} \rightarrow \text{felület: } -3pV$$

$$\downarrow$$

kölcsönhatás: $\underline{F}_\alpha = \sum_{\alpha'} F_{\alpha\alpha'} (\underline{r}_{\alpha'} - \underline{r}_\alpha)$ $\qquad \underline{F}_{\alpha\alpha'} = -\underline{F}_{\alpha'\alpha}$

$$\sum_\alpha \sum_{\substack{\alpha' \\ (\alpha' \neq \alpha)}} \underline{F}_{\alpha\alpha'} \underline{r}_\alpha = \frac{1}{2} \sum_\alpha \sum_{\substack{\alpha' \\ (\alpha' \neq \alpha)}} \underbrace{\underline{F}_{\alpha'\alpha}}_{= -\underline{F}_{\alpha\alpha'}} \underline{r}_{\alpha'} + \frac{1}{2} \sum_\alpha \sum_{\substack{\alpha' \\ (\alpha' \neq \alpha)}} \underline{F}_{\alpha\alpha'} \underline{r}_\alpha =$$

$$= \frac{1}{2} \sum_\alpha \sum_{\substack{\alpha' \\ \alpha' \neq \alpha}} \underline{F}_{\alpha\alpha'} (\underline{r}_\alpha - \underline{r}_{\alpha'})$$

erő $\sim \frac{1}{r^{7}}$ $\qquad$ összeg $\sim \frac{1}{r^6}$ $\qquad$ gáz ritka $\Rightarrow$ elhanyagolható

# Sebességeloszlás


$$d^3v = dv_x\, dv_y\, dv_z$$

$$P(\underline{v}, d^3v) = f(\underline{v})\, d^3v = f(v_x, v_y, v_z)\, dv_x\, dv_y\, dv_z$$

1) $f(\underline{v})$ csak $|\underline{v}|$-től függ

2) $v_x, v_y, v_z$ változók függetlenek: $f(v_x, v_y, v_z) = g(v_x)\, g(v_y)\, g(v_z)$

1) $\Rightarrow$ $\nabla f \parallel \underline{v}$

$$\frac{1}{v_x}\frac{\partial f}{\partial v_x} = \frac{1}{v_y}\frac{\partial f}{\partial v_y} = \frac{1}{v_z}\frac{\partial f}{\partial v_z} \qquad /:f$$

$$\frac{1}{v_x}\frac{g'(v_x)}{g(v_x)} = \frac{1}{v_y}\frac{g'(v_y)}{g(v_y)} = \frac{1}{v_z}\frac{g'(v_z)}{g(v_z)} = -2\alpha^2$$

$$\frac{g'(v_x)}{g(v_x)} = -2\alpha^2 v_x \qquad \int dv_x$$

$$\ln g(v_x) = -\alpha^2 v_x^2 + \ln C \qquad g(v_x) = C e^{-\alpha^2 v_x^2}$$

normálás: $$\int_{-\infty}^{+\infty} g(v_x)\, dv_x = C \int_{-\infty}^{+\infty} e^{-\alpha^2 v_x^2}\, dv_x = C\sqrt{\frac{\pi}{\alpha^2}} = 1 \Rightarrow C = \sqrt{\frac{\alpha^2}{\pi}}$$

$$\uparrow$$

$$\int_{-\infty}^{+\infty} e^{-a y^2}\, dy = \sqrt{\frac{\pi}{a}}$$

$$g(v_x) = \sqrt{\frac{\alpha^2}{\pi}}\, e^{-\alpha^2 v_x^2}$$

$$f(v_x, v_y, v_z) = \left(\frac{\alpha^2}{\pi}\right)^{\frac{3}{2}} e^{-\alpha^2\left(v_x^2 + v_y^2 + v_z^2\right)}$$

$$\overline{n^2} = \frac{d^2 G}{dz^2}\Big|_{z=0} = \left( N(N-1)\left[\ \ldots\ \right]^{N-2} \left(\frac{V'}{V} e^{z}\right)^2 + N \left[\ \ldots\ \right]^{N-1} \cdot \frac{V'}{V} e^{z} \right)\Big|_{z=0} =$$

$$= N(N-1)\left(\frac{V'}{V}\right)^2 + N \cdot \frac{V'}{V}$$

$$\overline{\Delta n^2} = \overline{n^2} - \bar{n}^2 = N\frac{V'}{V} - N\left(\frac{V'}{V}\right)^2 = N\frac{V'}{V}\left(1 - \frac{V'}{V}\right)$$

termodinamikai határeset (makroszkopikus rendszer)

$$N \to \infty \qquad \frac{N}{V} = \text{állandó}$$

$$\bar{n} = \frac{N}{V}\cdot V' \qquad \overline{\Delta n^2} = N \cdot \frac{V'}{V}$$

$$\frac{\overline{\Delta n^2}}{\bar{n}^2} = \frac{\frac{N}{V}V'}{\left(\frac{N}{V}V'\right)^2} = \frac{1}{\bar{n}}.$$

eloszlás fv.: $\quad p(n) = \binom{N}{n}\left(\frac{V'}{V}\right)^n \left(1 - \frac{V'}{V}\right)^{N-n} =$

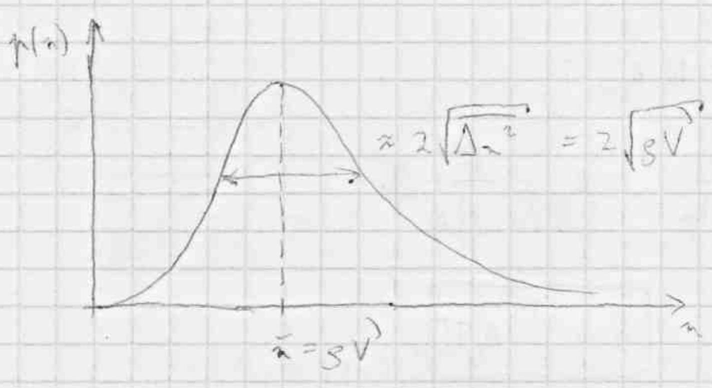
$$= \frac{N(N-1)(N-2)\cdot\ldots\cdot(N-n+1)}{n!}\cdot\frac{1}{N^n}\left(\frac{N}{V}V'\right)^n \underbrace{\left(1 - \frac{1}{N}\frac{N}{V}V'\right)^N}_{\downarrow} \underbrace{\left(1 - \frac{V'}{V}\right)^{-n}}_{\downarrow\ 1}$$

$$p(n) = \frac{1}{n!}\underbrace{\frac{N(N-1)(N-2)\cdot\ldots\cdot(N-n+1)}{N^n}}_{\downarrow\ 1}\left(\frac{N}{V}V'\right)^n e^{-\frac{N}{V}V'}$$

$$\lim_{N\to\infty}\left(1 + \frac{x}{N}\right)^N = e^x$$

$$p(n) = \frac{1}{n!}\left(\frac{N}{V}V'\right)^n e^{-\frac{N}{V}V'} = \frac{1}{n!}(\varrho V')^n e^{-\varrho V'}$$

$$\varrho = \frac{N}{V}$$

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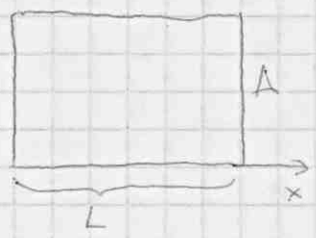


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kölcsönhatás: $\underline{F}_\alpha = \sum_{\alpha'} F_{\alpha\alpha'}(\underline{r}_\alpha - \underline{r}_{\alpha'})$ $\qquad \underline{F}_{\alpha\alpha'} = -\underline{F}_{\alpha'\alpha}$

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$$\uparrow$$

$$\int_{-\infty}^{+\infty} e^{-ay^2}\, dy = \sqrt{\frac{\pi}{a}}$$

$$g(v_x) = \sqrt{\frac{\alpha^2}{\pi}}\, e^{-\alpha^2 v_x^2}$$

$$f(v_x, v_y, v_z) = \left(\frac{\alpha^2}{\pi}\right)^{\frac{3}{2}} e^{-\alpha^2 (v_x^2 + v_y^2 + v_z^2)}$$

Bernoulli formula: $p = \frac{N}{V} \cdot \frac{2}{3} \bar{\varepsilon} = \frac{N}{V} \frac{m}{3} \overline{v^2} = \frac{N}{V} \underbrace{m \overline{v_x^2}}$

állapotegyenlet $\longrightarrow k_B T$

$$\overline{v_x^2} = \frac{k_B T}{m}$$

$$\overline{v_x^2} = \int_{-\infty}^{+\infty} g(v_x)\, v_x^2 \, dv_x = \sqrt{\frac{\alpha^2}{\pi}} \int_{-\infty}^{+\infty} v_x^2 e^{-\alpha^2 v_x^2} \, dv_x =$$

$$= \sqrt{\frac{\alpha^2}{\pi}} \cdot \frac{\sqrt{\pi}}{2\alpha^3} = \frac{1}{2\alpha^2} = \frac{k_B T}{m}$$

$$\int_{-\infty}^{+\infty} y^2 e^{-\alpha^2 y^2} = \frac{\sqrt{\pi}}{2\alpha^3}$$

$$\alpha^2 = \frac{m}{2 k_B T}$$

$$\boxed{\begin{aligned} g(v_x) &= \sqrt{\frac{m}{2\pi k_B T}}\, e^{-\frac{m v_x^2}{2 k_B T}} \\ f(v) &= \left(\frac{m}{2\pi k_B T}\right)^{\frac{3}{2}} e^{-\frac{m v^2}{2 k_B T}} \end{aligned}}$$

Maxwell-féle sebességeloszlás

$$\overline{v_x^2} = \frac{k_B T}{m} \qquad \overline{v^2} = \overline{v_x^2} + \overline{v_y^2} + \overline{v_z^2} = \frac{3 k_B T}{m}$$

$H_2$: $\sqrt{\overline{v^2}} = 1886 \frac{m}{s}$ $\qquad$ $O_2$: $\sqrt{\overline{v^2}} = 453 \frac{m}{s}$

<u>sebesség nagyság szerinti eloszlás:</u>

$$P(v, dv) = F(v)\, dv = f(v) \cdot 4\pi v^2 \, dv$$

$$\boxed{F(v) = \left(\frac{m}{2\pi k_B T}\right)^{\frac{3}{2}} \cdot 4\pi v^2 e^{-\frac{m v^2}{2 k_B T}}}$$

legvalószínűbb sebesség: $v^2 e^{-\frac{mv^2}{2k_BT}} = \max$

$$\cancel{2}v \cdot \cancel{e^{-\frac{mv^2}{2k_BT}}} + v^2 \cancel{e^{-\frac{mv^2}{2k_BT}}} \cdot \left(-\frac{m}{2k_BT}\right) \cdot \cancel{2}v = 0$$

$$v^2 = \frac{2k_BT}{m} \Rightarrow \boxed{v^* = \sqrt{\frac{2k_BT}{m}}}$$

$$\bar{v} = \int_0^\infty F(v)\, v\, dv = \left(\frac{m}{2\pi k_BT}\right)^{\frac{3}{2}} \cdot 4\pi \int_0^\infty v^3 e^{-\frac{mv^2}{2k_BT}}\, dv$$

$$\int_0^\infty y^n \cdot e^{-ay^2}\, dy = \frac{\Gamma\left(\frac{n+1}{2}\right)}{2a^{\frac{n+1}{2}}} \qquad \Gamma(n+1) = n!$$

$$\int_0^\infty y^3 \cdot e^{-ay^2}\, dy = \frac{\Gamma(2)}{2a^2} = \frac{1}{2a^2}$$

$$\bar{v} = \left(\frac{m}{2\pi k_BT}\right)^{\frac{3}{2}} \cdot 4\pi \cdot \frac{1}{2\left(\frac{m}{2k_BT}\right)^2} = \sqrt{\frac{k_BT}{m}} \cdot \frac{1}{\sqrt{\pi}}\; 8 \cdot \frac{1}{2} \cdot \frac{1}{\sqrt{2}} = \sqrt{\frac{8}{\pi} \cdot \frac{k_BT}{m}}$$

$$\boxed{\bar{v} = \sqrt{\frac{8}{\pi} \cdot \frac{k_BT}{m}}}$$


$$h\nu_0 = E_\gamma - E_0$$

Doppler-effektus: $\nu = \nu_0\left(1 + \frac{v_x}{c}\right) \qquad v_x = \frac{c}{\nu_0}(\nu - \nu_0)$

$$I(\nu)\, d\nu = g(v_x)\, dv_x = g\left(\frac{c}{\nu_0}(\nu - \nu_0)\right) \frac{c}{\nu_0}\, d\nu$$

$$I(\nu) = \left(\frac{m}{2\pi k_B T}\right)^{\frac{1}{2}} \cdot \frac{c}{\nu_0} \, e^{-\frac{m}{2 k_B T} \frac{c^2}{\nu_0^2}(\nu-\nu_0)^2}$$

<u>harmonikus oszcillátor</u>

$$H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 \cdot x^2 \qquad E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

térbeli: $$H = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + \frac{1}{2} m\omega^2 \left(x^2 + y^2 + z^2\right)$$

$$E(n_x, n_y, n_z) = \hbar\omega\left(n_x + n_y + n_z + \frac{3}{2}\right)$$

$$E_0 = \frac{3}{2}\hbar\omega \qquad g_0 = 1$$

g: multiplicitás

$$E_1 = \frac{5}{2}\hbar\omega \qquad g_1 = 3$$

$$E_2 = \frac{7}{2}\hbar\omega \qquad g_3 = 6$$

$$\vdots \qquad \qquad \vdots$$

<u>N db 2 állapotú, független atom</u>

$$\underline{\quad N_+ \quad} \; +\varepsilon$$

$$\overline{\quad N_- \quad} \; -\varepsilon$$

$N_+, N_-$ : betöltési szám

$$N = N_+ + N_- \qquad E = \underbrace{(N_+ - N_-)}_{M} \varepsilon$$

$$N_+ = \frac{N+M}{2} \qquad N_- = \frac{N-M}{2} \qquad E = M\varepsilon$$

<u>multiplicitás:</u> $$g(N, N_+) = \binom{N}{N_+} = \frac{N!}{N_+! \cdot N_-!}$$

$$\sum_{N_+=0}^{N} \binom{N}{N_+} = \sum_{N_+=0}^{N} \binom{N}{N_+} \cdot 1^{N_+} \cdot 1^{N_-} = (1+1)^N = 2^N$$

termodinamikai határeset: $N \to \infty$ $\quad \frac{E}{N} = \underbrace{\frac{M}{N}}_{\text{áll}} \varepsilon =$ állandó

Stirling-formula: $n! = \left(\frac{n}{e}\right)^n \cdot \sqrt{2\pi n} \left(1 + O\left(\frac{1}{n}\right)\right)$

$$\ln(n!) = n \ln n - n + \frac{1}{2} \ln(2\pi n) + \ldots = n \ln n - n + O(\ln n)$$

$$\ln g(N, N_+) = \ln N! - \ln N_+! - \ln N_-! =$$

$$= \underbrace{N \ln N}_{N_+ \ln N + N_- \ln N} - \cancel{N} - N_+ \ln N_+ + \cancel{N_+} - N_- \ln N_- + \cancel{N_-} + O(\ln N)$$

$$\ln g(N, N_+) = -N_+ \ln \frac{N_+}{N} - N_- \ln \frac{N_-}{N} + O(\ln N)$$

$$\ln g(N, N_+) = N \underbrace{\left[ -\frac{N_+}{N} \ln \frac{N_+}{N} - \frac{N_-}{N} \ln \frac{N_-}{N} \right]}_{N \to \infty \text{-nél állandó}} + O(\ln N)$$

$$\frac{N_+}{N} = \frac{1 + \frac{M}{N}}{2} \qquad \frac{N_-}{N} = \frac{1 - \frac{M}{N}}{2}$$

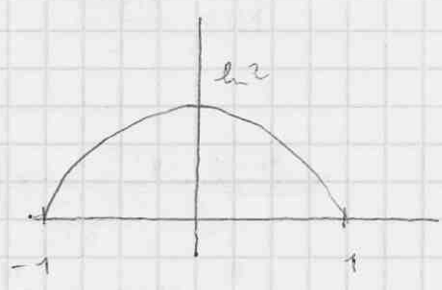
$$\ln g(N, N_+) = N \left[ -\frac{1 + \frac{M}{N}}{2} \ln \frac{1 + \frac{M}{N}}{2} - \frac{1 - \frac{M}{N}}{2} \ln \frac{1 - \frac{M}{N}}{2} \right] + O(\ln N)$$

$$\ln g(N, N_+) \approx N \cdot \phi\left(\frac{M}{N}\right) \qquad \phi(x) = -\frac{1+x}{2} \ln \frac{1+x}{2} - \frac{1-x}{2} \ln \frac{1-x}{2}$$

extenzív mennyiség

$$\phi(0) = -\frac{1}{2} \ln\left(\frac{1}{2}\right) - \frac{1}{2} \ln\left(\frac{1}{2}\right) = \ln 2$$

$$\phi(+1) = 0 \qquad \phi(-1) = 0$$

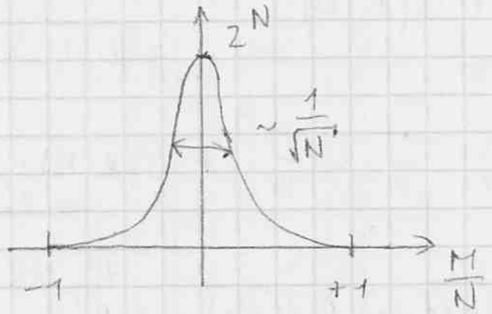


$$\phi'(x) = -\frac{1}{2}\ln\frac{1+x}{2} + \frac{1}{2}\ln\frac{1-x}{2} - \cancel{\frac{1+x}{2}}\cdot\cancel{\frac{2}{1+x}}\cdot\frac{1}{2} + \cancel{\frac{1-x}{2}}\cdot\cancel{\frac{2}{1-x}}\cdot\frac{1}{2}$$

$$\phi''(x) = -\frac{1}{2}\cdot\frac{2}{1+x}\cdot\frac{1}{2} - \frac{1}{2}\,\frac{2}{1-x}\cdot\frac{1}{2} = -\frac{1}{2}\cdot\frac{1}{1+x} - \frac{1}{2}\cdot\frac{1}{1-x}$$

$$\phi'(0) = 0 \qquad \phi''(0) = -1 \qquad \phi(x) \approx \ln 2 - \frac{1}{2}x^2 + \ldots \qquad |x| \ll 1$$

$$g(N, N_+) \approx e^{N\phi\left(\frac{M}{N}\right)} \approx e^{N\ln 2 - \frac{N}{2}\cdot\left(\frac{M}{N}\right)^2} = 2^N \cdot e^{-\frac{1}{2}\frac{M^2}{N}}$$




N db. lineáris oszcillátor azonos frekvenciával

$$E = \hbar\omega\cdot\sum_{i=1}^{N}\left(n_i + \frac{1}{2}\right) = M\cdot\hbar\omega + N\cdot\frac{1}{2}\hbar\omega$$

$$M = \sum_{i=1}^{N} n_i \qquad n_i = 0, 1, 2, \ldots$$

multiplicitás: M golyó elhelyezése N dobozba

$\downarrow$ $\hbar\omega$ gerjesztési kvantum

$\downarrow$ oszcillátorok

$\circ\circ\circ \mid \circ\circ \mid \circ\circ\circ\circ \mid \circ\circ \mid \circ$ M golyó, N-1 fal

$$g(N, M) = \frac{(M+N-1)!}{M!\cdot(N-1)!}$$

termodinamikai határeset: $N \to \infty$ $\quad \dfrac{E}{N} \simeq \dfrac{1}{2}\hbar\omega + \underbrace{\dfrac{M}{N}}_{\text{áll}}\hbar\omega = \text{áll}$

$$\ln g(N,M) = \ln (M+N-\cancel{1})! - \ln M! - \ln (N-\cancel{1})! =$$

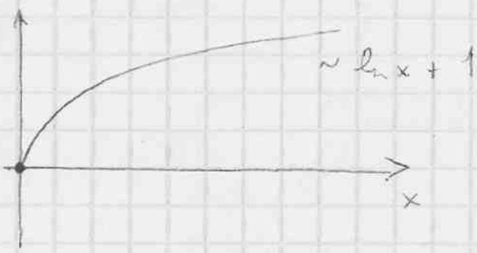
$$= (M+N)\ln(M+N) - \cancel{(M+N)} - M\ln M + \cancel{M} - \underbrace{N\ln N}_{(N+M)\ln N - M\ln N} + \cancel{N} + O(\ln N) =$$

$$= (N+M)\ln\left(\frac{N+M}{N}\right) - M\ln\frac{M}{N} + O(\ln N)$$

$$\ln g(N,M) \simeq N\left[\left(1+\frac{M}{N}\right)\ln\left(1+\frac{M}{N}\right) - \frac{M}{N}\ln\frac{M}{N}\right] + O(\ln N)$$

$$\ln g(N,M) \approx N\cdot\phi\left(\frac{M}{N}\right) \qquad \phi(x) = (1+x)\ln(1+x) - x\ln x$$

$$\phi'(x) = \ln(1+x) + x\underbrace{\ln\left(\frac{1+x}{x}\right)}_{\ln\left(1+\frac{1}{x}\right) \approx \frac{1}{x}\ ,\ \text{ha } x\to\infty} \approx \ln x + 1 \quad ,\ \text{ha } x \to \infty$$




$\phi(0) = 0$

$$\ln g(N,M) = N\cdot\phi\left(\frac{M}{N}\right) \qquad \text{extenzív mennyiség}$$

$$\ln g(\lambda N,\lambda M) = \lambda N\cdot\phi\left(\frac{M}{N}\right) = \lambda\cdot\ln g(N,M)$$

↘ homogén elsőfokú függvény

entrópia: $S = k_B \ln g$

$$\ln g(N,M) = N\,\Phi\left(\frac{M}{N}\right) + O(\ln N)$$

$\uparrow$

termodinamikai határeset: $N \to \infty \quad \frac{M}{N} = \text{áll}$

Boltzmann: $S(E,N) = k_B \ln g(N,E)$ statisztikus entrópia

$$\frac{1}{T} = \frac{\partial S(E,N)}{\partial E}$$ statisztikus hőmérséklet

$$S = k_B N\,\Phi\left(\frac{E}{N}\right) \Rightarrow \frac{1}{T} = k_B\,\Phi'\left(\frac{E}{N}\right)$$

zárt rendszer egyensúlyi állapota

makroállapot: makroszkópikus adatok rögzítése

mikroállapot: teljes részletességgel meghatározott állapot

pl.: bináris atomok

- makroállapot: $N, E$ (vagy $N, N_+$)
- mikroállapot: tudom, melyik $N_+$ atom van gerjesztve

Az $(N,E)$ makroállapotot $g(N,E)$ mikroállapot valósítja meg

posztulátum: Egyensúlyi állapotban minden, az adott makroállapotot megvalósító mikroállapot egyenlő valószínűségű.

$\uparrow$

alapozás: - információelmélet

- ergodikus tételek

| | |
|---|---|
| $N_1$, $E_1$ | $N_2$, $E_2$ |

$$N_1 + N_2 = N \qquad E_1 + E_2 = E$$

gyenge kölcsönhatás

$$P(E_1) = \frac{g_1(E_1, N_1)\, g_2(E_2, N_2)}{g(E,N)} = \max$$

$$\ln P(E_1) = \underbrace{\ln g_1(E_1, N_1) + \ln g_2(E_2, N_2)}_{=\max} - \ln g(E,N)$$

$$N \to \infty \qquad \frac{N_1}{N}, \frac{E}{N} = \text{állandó}$$

$$S_1(E_1, N_1) + S_2(E_2, N_2) = \max$$

$$E_2 = E - E_1 \qquad \frac{\partial E_2}{\partial E_1} = -1$$

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

$$\frac{1}{T_1(E_1, N_1)} = \frac{1}{T_2(E_2, N_2)}$$

$$\frac{\partial^2 S_1}{\partial E_1^2} - \frac{\partial^2 S_2}{\partial E_2^2} \cdot \underbrace{\left(\frac{\partial E_2}{\partial E_1}\right)^2}_{-1} = \frac{\partial^2 S_1}{\partial E_1^2} + \frac{\partial^2 S_2}{\partial E_2^2} < 0$$

tetszőleges 2 rendszerre

megkövetelve: tagonként $< 0$

egyensúly (max. valósz. létezése) feltétele:

$$\frac{\partial^2 S}{\partial E^2} < 0 \qquad \frac{\partial \left(\frac{1}{T}\right)}{\partial E} = -\frac{1}{T^2}\frac{\partial T}{\partial E} < 0 \implies \boxed{\frac{\partial T}{\partial E} > 0}$$

$$\ln P(E_1) = \ln g_1(E_1,N_1) + \ln g_2(E_2,N_2) + \text{const.} =$$

$$= \frac{1}{k_B}\left[S_1(E_1,N_1) + S_2(E_2,N_2)\right] + \text{const.} =$$

sorfejtés a legvalószínűbb érték körül: $E_1^*$, $E_2^* = E - E_1^*$

$$= \frac{1}{k_B}\left[S_1(E_1^*) + \left.\frac{\partial S_1}{\partial E_1}\right|_*(E_1-E_1^*) + \frac{1}{2}\left.\frac{\partial^2 S_1}{\partial E_1^2}\right|_*(E_1-E_1^*)^2 + \right.$$

$$\left. S_2(E_2^*) + \left.\frac{\partial S_2}{\partial E_2}\right|_*(E_2-E_2^*) + \frac{1}{2}\left.\frac{\partial^2 S_2}{\partial E_2^2}\right|_*(E_2-E_2^*)^2\right] + \text{const} =$$

$$E_2 - E_2^* = -(E_1 - E_1^*)$$

$$= \frac{1}{k_B}\left[S_1(E_1^*) + S_2(E_2^*) + \underbrace{\left(\left.\frac{\partial S_1}{\partial E_1}\right|_* - \left.\frac{\partial S_2}{\partial E_2}\right|_*\right)}_{0}(E_1-E_1^*) + \right.$$

$$\left. + \frac{1}{2}\left[\frac{\partial^2 S_1}{\partial E_1^2} + \frac{\partial^2 S_2}{\partial E_2^2}\right]_* (E_1-E_1^*)^2 + \ldots\right] + \text{const}$$

$$\ln P(E_1) = \frac{1}{2k_B}\underbrace{\left[\frac{\partial^2 S_1}{\partial E_1^2} + \frac{\partial^2 S_2}{\partial E_2^2}\right]_*}_{-\frac{k_B}{\Delta^2} < 0} (E_1-E_1^*)^2 + \underbrace{\text{const}}_{\ln C}$$

$$P(E_1) = C\, e^{-\frac{(E_1-E_1^*)^2}{2\Delta^2}}$$ Gauss-eloszlás

$$\bar{E}_1 = E_1^* \qquad \overline{\Delta E_1^2} = \Delta^2$$

$$S = k_B N \phi\left(\frac{E}{N}\right) \qquad \frac{\partial S}{\partial E} = k_B \phi'\left(\frac{E}{N}\right) \qquad \frac{\partial^2 S}{\partial E^2} = \frac{k_B}{N}\phi''\left(\frac{E}{N}\right)$$

$$\frac{\partial^2 S_1}{\partial E_1^2} + \frac{\partial^2 S_2}{\partial E_2^2} = -\frac{a^2}{N_1} - \frac{b^2}{N_2} = -\frac{k_B}{\Delta^2} \qquad \Delta^2 \sim N$$

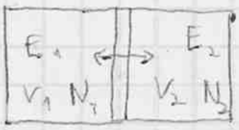
$E_1^* \sim N \qquad \Delta^2 \sim N$

$$\frac{\overline{\Delta E_1^2}}{\overline{E}_1^2} \sim \frac{N}{N^2} = \frac{1}{N} \to 0 \quad \Rightarrow \text{termodinamikai határesetben}$$

eltűnnek a fluktuációk

sorfejtés következő tagja:

$$\underbrace{\frac{1}{3!}\left(\frac{\partial^3 S_1}{\partial E_1^3} - \frac{\partial^3 S_2}{\partial E_2^3}\right)_*}_{\sim \frac{1}{N^2}} \cdot \underbrace{\left(E_1 - E_1^*\right)^3}_{\sim (\Delta^2)^{\frac{3}{2}} \sim N^{\frac{3}{2}}} \sim \frac{1}{\sqrt{N}} \to 0 \Rightarrow \text{Gauss-eloszlás jó közelítés}$$




termikus és mechanikai kölcsönhatás:

$$S_1(E_1, V_1, N_1) + S_2(E_2, V_2, N_2) = \max$$

$$\frac{\partial S_1}{\partial E_1} = \frac{\partial S_2}{\partial E_2} \to \frac{1}{T_1} = \frac{1}{T_2} \qquad \text{def.: } \frac{1}{T} = \frac{\partial S}{\partial E}$$

$$\frac{\partial S_1}{\partial V_1} = \frac{\partial S_2}{\partial V_2} \to \frac{p_1}{T_1} = \frac{p_2}{T_2} \qquad \text{def.: } \frac{p}{T} = \frac{\partial S}{\partial V}$$

+ anyagi kölcsönhatás: $\frac{\partial S_1}{\partial N_1} = \frac{\partial S_2}{\partial N_2} \to \frac{\mu_1}{T_1} = \frac{\mu_2}{T_2} \qquad \text{def.: } \frac{\mu}{T} = -\frac{\partial S}{\partial N}$

$$S(E, V, N) \qquad dS = \frac{1}{T} dE + \frac{p}{T} dV - \frac{\mu}{T} dN$$

$$dE = T\,dS - p\,dV + \mu\,dN$$

bináris atomok rendszere: $S = k_B \ln g(N,E) = k_B N \phi\left(\frac{M}{N}\right) \overset{E = M\varepsilon}{=} k_B N \phi\left(\frac{E}{N\varepsilon}\right)$

$$\phi(x) = -\frac{1+x}{2} \ln \frac{1+x}{2} - \frac{1-x}{2} \ln \frac{1-x}{2}$$

$$S = N k_B \left( - \frac{1+\frac{E}{N\varepsilon}}{2} \ln \frac{1+\frac{E}{N\varepsilon}}{2} - \frac{1-\frac{E}{N\varepsilon}}{2} \ln \frac{1-\frac{E}{N\varepsilon}}{2} \right)$$

$$\frac{1}{T} = \frac{\partial S}{\partial E} = N k_B \cdot \frac{1}{N\varepsilon} \left( -\frac{1}{2} \ln \frac{1+\frac{E}{N\varepsilon}}{2} + \frac{1}{2} \ln \frac{1-\frac{E}{N\varepsilon}}{2} \right) = \frac{k_B}{2\varepsilon} \ln \left( \frac{1-\frac{E}{N\varepsilon}}{1+\frac{E}{N\varepsilon}} \right)$$

$$E = - N\varepsilon \frac{e^{\frac{2\varepsilon}{kT}} - 1}{e^{\frac{2\varepsilon}{kT}} + 1} = - N\varepsilon \frac{e^{\frac{\varepsilon}{kT}} - e^{-\frac{\varepsilon}{kT}}}{e^{\frac{\varepsilon}{kT}} + e^{-\frac{\varepsilon}{kT}}}$$

$$\boxed{E = - N\varepsilon \, \mathrm{th}\left(\frac{\varepsilon}{k_B T}\right)}$$

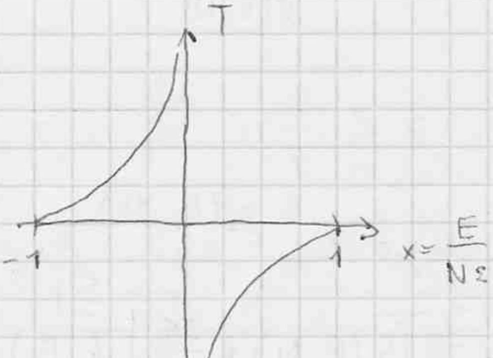
$$N_+ + N_- = N \qquad N_+ - N_- = M \qquad N_+ = \frac{N+M}{2} \qquad M = \frac{E}{\varepsilon}$$

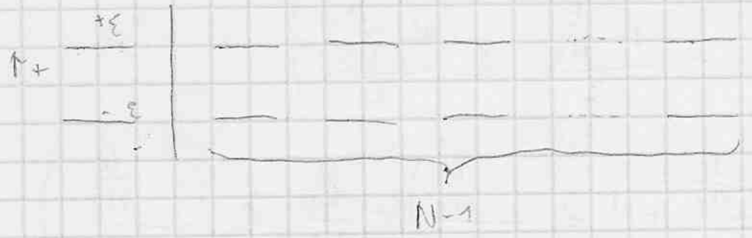
$$\frac{N_+}{N} = \frac{1+\frac{M}{N}}{2} = \frac{1+\frac{E}{N\varepsilon}}{2} = \frac{1}{2}\left(1 - \frac{e^{\frac{\varepsilon}{kT}} - e^{-\frac{\varepsilon}{kT}}}{e^{\frac{\varepsilon}{kT}} + e^{-\frac{\varepsilon}{kT}}}\right)$$

$$\frac{N_+}{N} = \frac{e^{-\frac{\varepsilon}{kT}}}{e^{\frac{\varepsilon}{kT}} + e^{-\frac{\varepsilon}{kT}}} \qquad \frac{N_-}{N} = 1 - \frac{N_+}{N} = \frac{e^{\frac{\varepsilon}{kT}}}{e^{\frac{\varepsilon}{kT}} + e^{-\frac{\varepsilon}{kT}}}$$

$$\boxed{\frac{N_+}{N_-} = e^{-\frac{2\varepsilon}{kT}}}$$

$$\frac{1}{T} = \frac{1}{\varepsilon} k_B \cdot \phi\left(\frac{E}{N\varepsilon}\right)$$






$N, E$

$$p_+ = \frac{\binom{N-1}{N_+-1}}{\binom{N}{N_+}} = \frac{\dfrac{(N-1)!}{(N_+-1)!\,N_-!}}{\dfrac{N!}{N_+!\cdot N_-!}}$$

$$p_+ = \frac{N_+}{N} = \frac{e^{-\frac{\varepsilon}{kT}}}{e^{\frac{\varepsilon}{kT}} + e^{-\frac{\varepsilon}{kT}}} \qquad p_- = 1 - p_+ = \frac{e^{\frac{\varepsilon}{kT}}}{e^{\frac{\varepsilon}{kT}} + e^{-\frac{\varepsilon}{kT}}}$$

| | |
|---|---|
| $N_1$ | $N_2$ |
| $E_1$ | $E_2$ |

zárt rendszer

termodin. határesetben:

$N_2 \to \infty \qquad \frac{E_2}{N_2} =$ áll

$$P(E_1) = \frac{g_1(E_1, N_1)\, g_2(E_2, N_2)}{g(E, N)} \qquad E_1 + E_2 = E \qquad N_1 + N_2 = N$$

$$E_2 \gg E_1$$

$$E_2 = E - E_1$$

$$g_2(E_2, N_2) = e^{\ln g_2(E_2, N_2)} = e^{\frac{1}{k_B} S_2(E_2, N_2)} =$$

$$= e^{\frac{1}{k_B}\left[S_2(E, N_2) + \underbrace{\left.\frac{\partial S}{\partial E_2}\right|_E}_{\frac{1}{T_2(E)}}(-E_1) + \dots\right]} = e^{\frac{1}{k_B} S_2(E, N_2)} \cdot e^{-\frac{E_1}{k_B T_2}}$$

$$P(E_1) = g_1(E_1, N_1)\, e^{-\frac{E_1}{k_B T_2}} \cdot C$$

$\uparrow$ $E_1$-től független

egyetlen $E_1$ energiájú állapot valószínűsége: $C\, e^{-\frac{E_1}{k_B T_2}}$

<u>kanonikus eloszlás</u>: fiz. rendszer $T$ hőmérsékletű környezetben

$n$-ik energiaállapot: $E_n$

$\downarrow$

valószínűsége: $\boxed{p(E_n) = \frac{1}{Z}\, e^{-\frac{E_n}{k_B T}}}$

$\Downarrow$ normálási tényező

$$\boxed{Z = \sum_n e^{-\frac{E_n}{k_B T}}}$$ <u>állapot összeg</u>

annak valószínűsége, hogy $E$ energiája legyen:

$$P(E) = \frac{1}{Z}\, e^{-\frac{E}{k_B T}} \cdot g(E, N)$$

energia várható értéke:

$$\bar{E} = \sum_n p(E_n) E_n = \frac{1}{Z} \sum_n E_n e^{-\frac{E_n}{k_B T}} = \frac{1}{Z} \sum_n E_n e^{-\beta E_n} =$$

$$= \frac{\sum_n E_n e^{-\beta E_n}}{\sum_n e^{-\beta E_n}} = \frac{-\frac{\partial}{\partial \beta}\left(\sum_n e^{-\beta E_n}\right)}{\sum_n e^{-\beta E_n}} = \frac{-\frac{\partial Z}{\partial \beta}}{Z} =$$

$$\boxed{\bar{E} = -\frac{\partial}{\partial \beta}\left(\ln Z\right)}$$

Bináris atom $T$ hőm. környezetben

——— $+\varepsilon$

——— $-\varepsilon$

$$Z = e^{-\frac{\varepsilon}{kT}} + e^{+\frac{\varepsilon}{kT}} = e^{\beta\varepsilon} + e^{-\beta\varepsilon} = 2\,\mathrm{ch}(\beta\varepsilon)$$

$$\bar{E} = -\frac{\partial}{\partial\beta} \ln(2\,\mathrm{ch}\,\beta\varepsilon) = -\frac{2\,\mathrm{sh}(\beta\varepsilon)}{2\,\mathrm{ch}(\beta\varepsilon)}\,\varepsilon$$

$$\bar{E} = -\varepsilon\,\mathrm{th}(\beta\varepsilon)$$

definícióból: $$E = \varepsilon\,\frac{e^{-\beta\varepsilon}}{Z} + (-\varepsilon)\,\frac{e^{\beta\varepsilon}}{Z} = -\varepsilon\,\frac{e^{\beta\varepsilon} - e^{-\beta\varepsilon}}{e^{\beta\varepsilon} + e^{-\beta\varepsilon}}$$

<u>Hőkapacitás</u>:

$$C = \frac{\partial\bar{E}}{\partial T} = \frac{\partial\bar{E}}{\partial\beta}\cdot\frac{\partial\beta}{\partial T} = -\varepsilon\,\frac{\varepsilon}{\mathrm{ch}^2(\beta\varepsilon)}\cdot\left(-\frac{1}{k_B T^2}\right) = k_B\cdot\frac{(\beta\varepsilon)^2}{\mathrm{ch}^2(\beta\varepsilon)}$$

$$C = k_B\left(\frac{\varepsilon}{k_B T}\right)^2 \frac{1}{\mathrm{ch}^2\left(\frac{\varepsilon}{k_B T}\right)}$$

$\dfrac{x^2}{\mathrm{ch}^2 x}$ $\quad x \ll 1 \quad \mathrm{ch}\,x \approx 1$

$x \gg 1 \quad \mathrm{ch}\,x \approx \frac{1}{2}e^x \qquad \dfrac{x^2}{\mathrm{ch}^2 x} \approx (2x)^2 e^{-2x}$

$\dfrac{\varepsilon}{k_B T} \ll 1 \qquad C \approx k_B\left(\dfrac{\varepsilon}{k_B T}\right)^2$

$\dfrac{\varepsilon}{k_B T} \gg 1 \qquad C \approx k_B\left(\dfrac{2\varepsilon}{k_B T}\right)^2 e^{-\frac{2\varepsilon}{k_B T}}$


$\dfrac{\varepsilon}{k_B T} \sim O(1)$

$E_n$

$E_0$

T hőm. környezetben: $P(E_n) = \frac{1}{Z} e^{-\beta E_n}$

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

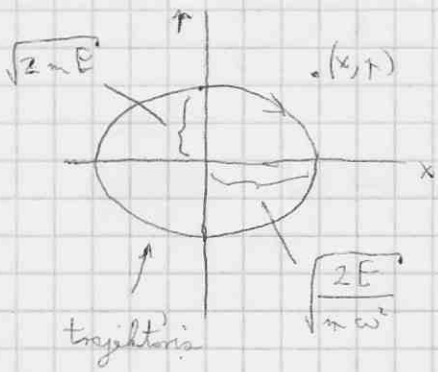
$$\bar{E} = -\frac{\partial}{\partial \beta} \ln Z$$

$$\frac{P(E_n)}{P(E_0)} = e^{-\beta(E_n - E_0)}$$

$$T \to 0 \qquad \beta = \frac{1}{kT} \to \infty \qquad \frac{P(E_n)}{P(E_0)} \to 0$$

<u>Klasszikus mech. rendszer</u>

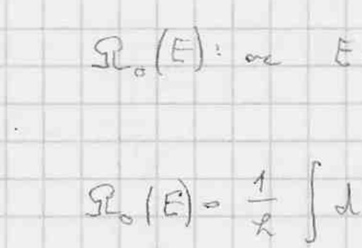
lin. oszcillátor: $H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2$




fázistér

$H = E$ felület $\quad \frac{p^2}{2mE} + \frac{m\omega^2 x^2}{2E} = 1$

$$\Delta x \cdot \Delta p \gtrsim h$$

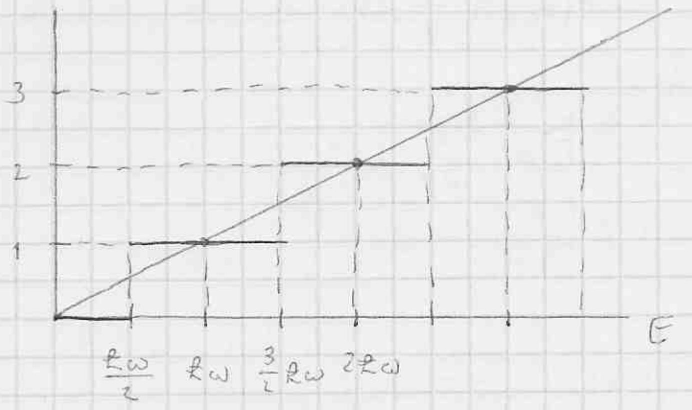



$\longrightarrow$ fáziscella = 1 állapot

$$\Delta x \cdot \Delta p = h$$

$\Omega_0(E)$: az $E$-nél kisebb energiájú áll. száma

$$\Omega_0(E) = \frac{1}{h} \int_{H(x,p)<E} dx\, dp = \frac{1}{h} \sqrt{2mE} \sqrt{\frac{2E}{m\omega^2}} = \frac{2\pi}{h} \cdot \frac{E}{\omega} = \frac{E}{\hbar \omega}$$




f szabadsági fokú klasszikus mech. rendszer:

$$q=(q_1,\dots,q_f) \qquad p=(p_1,\dots,p_f)$$ fázistér: 2f dimenziós

$$H(p,q) \qquad \dot q = \frac{\partial H}{\partial p} \qquad \dot p = -\frac{\partial H}{\partial q}$$

$$\Omega_0(E) = \frac{1}{h^f}\int_{H<E} dq_1 \dots dq_f \, dp_1 \dots dp_f$$

$$Z = \frac{1}{h^f}\int dq\, dp\; e^{-\beta H(p,q)}$$

$$\overline{A(p,q)} = \frac{\int dq\, dp\; A(p,q)\, e^{-\beta H(p,q)}}{\int dq\, dp\; e^{-\beta H(p,q)}}$$

<u>lineáris oszcillátor T hőmérséklete:</u>

<u>klasszikus:</u> $H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2$

$$Z = \frac{1}{h}\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dp \; e^{-\frac{\beta p^2}{2m}} \cdot e^{-\frac{\beta m \omega^2 x^2}{2}} =$$

$$= \frac{1}{h}\int_{-\infty}^{+\infty} dx \; e^{-\frac{\beta m \omega^2 x^2}{2}} \int_{-\infty}^{+\infty} dp \; e^{-\frac{\beta p^2}{2m}}$$

$$\int_{-\infty}^{+\infty} e^{-ay^2} dy = \sqrt{\frac{\pi}{a}}$$

$$= \frac{1}{h}\sqrt{\frac{2\pi}{\beta m \omega^2}}\sqrt{\frac{2m\pi}{\beta}} = \frac{2\pi}{h}\cdot\frac{1}{\beta\omega}$$

$$Z = \frac{1}{\beta \hbar \omega} \qquad \boxed{\overline{E} = -\frac{\partial}{\partial\beta}\ln Z = \frac{\partial}{\partial\beta}\ln(\beta\hbar\omega) = \frac{1}{\beta} = k_B T}$$

$$C = \frac{\partial \overline{E}}{\partial T} = k_B$$

$N_A$ db atom $\rightarrow$ $3N_A$ oszcillátor $\rightarrow$ $C = 3N_A k_B = 3R$

<u>Dulong - Petit - szabály</u>

$\overline{x^2} = ?$

valószínűség: $\sim e^{-\frac{\beta p^2}{2m}} \cdot e^{-\frac{\beta m \omega^2 x^2}{2}}$

$p, x$ független valószínűségi változók

Gauss-eloszlás

$$\overline{x} = \frac{\int_{-\infty}^{+\infty} dx \cdot x \cdot e^{-\frac{\beta m \omega^2 x^2}{2}}}{\int_{-\infty}^{+\infty} dx \cdot e^{-\frac{\beta m \omega^2 x^2}{2}}} = 0$$

$$Z = \frac{1}{h} \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dp \; e^{-\frac{\beta p^2}{2m}} \cdot e^{-\frac{\beta m \omega^2 x^2}{2}} =$$

$$= \frac{1}{h} \int_{-\infty}^{+\infty} dx \; e^{-\frac{\beta m \omega^2 x^2}{2}} \int_{-\infty}^{+\infty} dp \; e^{-\frac{\beta p^2}{2m}}$$

$$\int_{-\infty}^{+\infty} e^{-a y^2} dy = \sqrt{\frac{\pi}{a}}$$

$$= \frac{1}{h} \sqrt{\frac{2\pi}{\beta m \omega^2}} \sqrt{\frac{2m\pi}{\beta}} = \frac{2\pi}{h} \cdot \frac{1}{\beta \omega}$$

$$Z = \frac{1}{\beta \hbar \omega} \qquad \boxed{\bar{E} = -\frac{\partial}{\partial \beta} \ln Z = \frac{\partial}{\partial \beta} \ln(\beta \hbar \omega) = \frac{1}{\beta} = k_B T}$$

$$\overline{x^2} = \frac{\int\limits_{-\infty}^{+\infty} dx \cdot x^2 \cdot e^{-\frac{\beta m \omega^2 x^2}{2}}}{\int\limits_{-\infty}^{+\infty} dx \cdot e^{-\frac{\beta m \omega^2 x^2}{2}}} = \frac{\frac{1}{2}\sqrt{\pi}\left(\frac{2}{m\omega^2\beta}\right)^{\frac{3}{2}}}{\sqrt{\frac{2\pi}{\beta m \omega^2}}} = \frac{1}{m\omega^2\beta} = \frac{k_B T}{m\omega^2}$$

$$\int\limits_{-\infty}^{+\infty} dy \cdot y^2 \cdot e^{-ay^2} = -\frac{\partial}{\partial a}\int\limits_{-\infty}^{+\infty} dy \cdot e^{-ay^2} = -\frac{\partial}{\partial a}\sqrt{\frac{\pi}{a}} = \frac{\sqrt{\pi}}{2\, a^{\frac{3}{2}}}$$

$$\boxed{\frac{1}{2} m\omega^2 \cdot \overline{x^2} = \frac{1}{2} k_B T} \qquad \boxed{\frac{1}{2}\frac{\overline{p^2}}{m} = \frac{1}{2} k_B T}$$

ekvipartíció tétele

$$\overline{p^2} = \frac{\int\limits_{-\infty}^{+\infty} dp \cdot p^2 \cdot e^{-\frac{\beta p^2}{2m}}}{\int\limits_{-\infty}^{+\infty} dp \cdot e^{-\frac{\beta p^2}{2m}}} = m k_B T$$

<u>kvantum:</u> $\quad E_n = \hbar\omega\left(n + \frac{1}{2}\right) \qquad n = 0, 1, 2, \ldots$

$$Z = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(n+\frac{1}{2}\right)} = e^{-\frac{\beta\hbar\omega}{2}} \sum_{n=0}^{\infty} e^{-\beta\hbar\omega \cdot n} =$$

$$= \frac{e^{-\frac{\beta\hbar\omega}{2}}}{1 - e^{-\beta\hbar\omega}} = \frac{1}{e^{\frac{\beta\hbar\omega}{2}} - e^{-\frac{\beta\hbar\omega}{2}}} = \frac{1}{2\,\mathrm{sh}\left(\frac{\beta\hbar\omega}{2}\right)}$$

$$\overline{E} = -\frac{\partial}{\partial\beta}\left(\ln Z\right) = -\frac{\partial}{\partial\beta}\left(-\frac{\beta\hbar\omega}{2} - \ln\left(1 - e^{-\beta\hbar\omega}\right)\right)$$

$$\boxed{\bar{E} = \frac{\hbar\omega}{2} + \frac{-e^{-\beta\hbar\omega}(-\hbar\omega)}{1-e^{-\beta\hbar\omega}} = \frac{\hbar\omega}{2} + \frac{\hbar\omega}{e^{\beta\hbar\omega}-1}}$$

$$\boxed{\bar{n} = \frac{1}{e^{\beta\hbar\omega}-1}}$$

$$C = \frac{\partial\bar{E}}{\partial T} = \hbar\omega\,\frac{-1}{(e^{\beta\hbar\omega}-1)^2}\,e^{\beta\hbar\omega}\cdot\hbar\omega\cdot\underbrace{\frac{\partial\beta}{\partial T}}_{-\frac{1}{k_B T^2}} =$$

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

$k_B T \ll \hbar\omega \qquad \beta\hbar\omega \gg 1$

$$\bar{E} = \frac{\hbar\omega}{2} + \hbar\omega\, e^{-\beta\hbar\omega} + \ldots$$

$$C = k_B\left(\frac{\hbar\omega}{k_B T}\right)^2\cdot e^{-\frac{\hbar\omega}{k_B T}} + \ldots$$

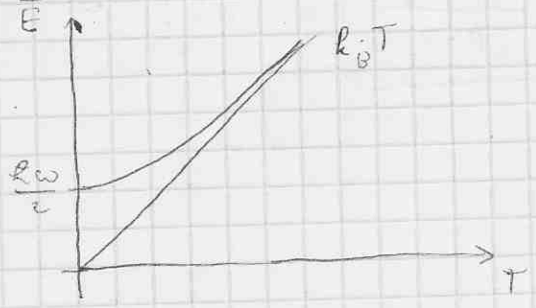
$k_B T \gg \hbar\omega \qquad \beta\hbar\omega \ll 1$

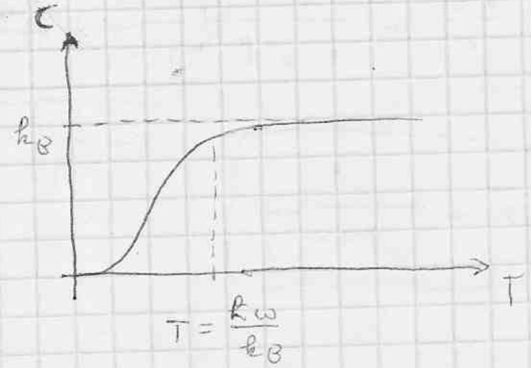
$$e^{\beta\hbar\omega} - 1 = \beta\hbar\omega + \frac{1}{2}(\beta\hbar\omega)^2 + \ldots$$

$$\bar{E} = \frac{\hbar\omega}{2} + \frac{\cancel{\hbar\omega}}{\beta\cancel{\hbar\omega}} + \ldots = k_B T + \ldots$$

$$\bar{E} = k_B T\left(1 + \left(\frac{\hbar\omega}{k_B T}\right)^2\cdot\frac{1}{12} + \ldots\right)$$

$$C = k_B\left(\frac{\hbar\omega}{k_B T}\right)^2\cdot\frac{1}{(\beta\hbar\omega)^2} = k_B + \ldots$$




<u>Ekvipartíció tétele</u>

f szabadsági fokú klasszikus rendszer

x: egy koordináta vagy impulzus

$$H = \alpha x^2 + H' \text{ (többi impulzus és koordináta)}$$

$$e^{-\beta H} = e^{-\beta\alpha x^2} \cdot e^{-\beta H'}$$

$$\overline{\alpha x^2} = \frac{\int_{-\infty}^{+\infty} dx \cdot \alpha x^2 \cdot e^{-\beta\alpha x^2}}{\int_{-\infty}^{+\infty} dx \, e^{-\beta\alpha x^2}} = \frac{-\frac{\partial}{\partial\beta}\int_{-\infty}^{+\infty} e^{-\beta\alpha x^2}\,dx}{\int_{-\infty}^{+\infty} e^{-\beta\alpha x^2}\,dx} =$$

$$= -\frac{\partial}{\partial\beta} \ln \int_{-\infty}^{+\infty} e^{-\beta\alpha x^2}\,dx = -\frac{\partial}{\partial\beta} \ln\sqrt{\frac{\pi}{\beta\alpha}} = \frac{\partial}{\partial\beta}\frac{1}{2}\ln\frac{\beta\alpha}{\pi} =$$

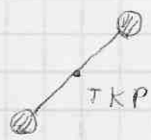
$$= \frac{1}{2\beta} = \frac{1}{2} k_B T \qquad \boxed{\overline{\alpha x^2} = \frac{1}{2} k_B T}$$

$$\overline{\frac{p^2}{2m}} + \overline{\frac{1}{2} m\omega^2 x^2} = \frac{k_B T}{2} + \frac{k_B T}{2}$$

$$\frac{\overline{p^2}}{2m} = \frac{\overline{p_x^2}}{2m} + \frac{\overline{p_y^2}}{2m} + \frac{\overline{p_z^2}}{2m} = \frac{3}{2} k_B T$$

kétatomos molekula

(merev súlyzó modell)




$$\overline{E} = \frac{\overline{p^2}}{2m} + \overline{\frac{1}{2}\Theta\left(\omega_1^2 + \omega_2^2\right)} = \frac{3}{2} k_B T + 2 \cdot \frac{k_B T}{2} = \frac{5}{2} k_B T$$

$p$: TKP impulzusa

$M$: teljes tömeg

<u>ekvipart. alkalmazása</u>

1) oszcillátor $\overline{E} = k_B T$ $\quad C = k_B$

2) N db oszcillátor $\overline{E} = N k_B T$ $\quad C = N k_B$

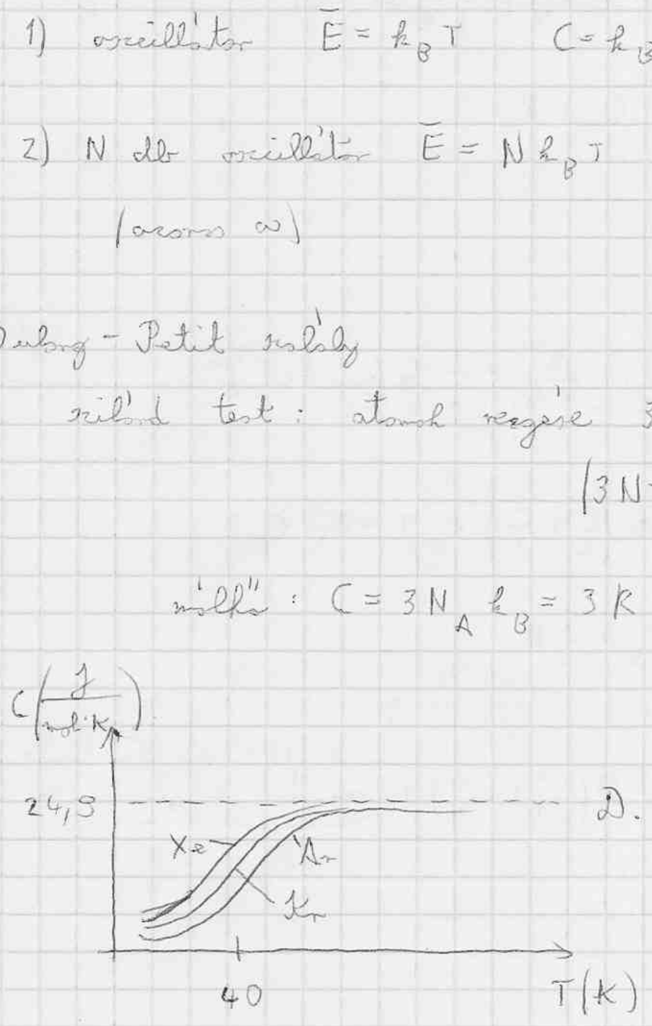
(azonos $\omega$)

Dulong – Petit szabály

szilárd test: atomok rezgése 3N db oszcillátor

(3N − 6)

mólhő: $C = 3 N_A k_B = 3R$



alacsony hőmérsékleten kvantumszámítások !

$$\bar{E} = \sum_{l=1}^{3N-6} \left( \frac{1}{2}\hbar\omega_l + \frac{\hbar\omega_l}{e^{\beta\hbar\omega_l}-1} \right)$$

3) egyatomos gáz $\quad \varepsilon \approx \frac{p^2}{2m} \quad \bar{\varepsilon} = \frac{3}{2} k_B T$

gáz: $\bar{E} = N \cdot \frac{3}{2} k_B T$

mólhő: $C_V = \frac{3}{2} N_A k_B = \frac{3}{2} R$ (állandó térf.)

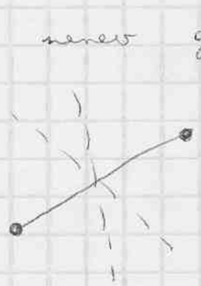
állandó nyomáson: $C_p = \left(\frac{\partial H}{\partial T}\right)_p = \left(\frac{\partial (E + pV)}{\partial T}\right)_p$

$$H = \frac{3}{2} N k_B T + N k_B T = \frac{5}{2} N k_B T$$

$$C_p = \frac{5}{2} R = C_V + R$$

4) kétatomos gáz

merev golyó modell: $\frac{p^2}{2m} + \frac{1}{2}\Theta(\omega_1^2 + \omega_2^2)$



$$\bar{\varepsilon} = \left(\frac{3}{2} + \frac{2}{2}\right) k_B T = \frac{5}{2} k_B T$$

$$C_V = \frac{5}{2} R$$

rezgő súlyzó $\quad \frac{p^2}{2m} + \frac{1}{2}\Theta(\omega_1^2 + \omega_2^2) + \underbrace{\text{rezgési energia}}_{k_B T}$

$$\underline{L} = \underline{\underline{\Theta}}\,\underline{\omega} = \begin{pmatrix} \Theta & & \\ & \Theta & \\ & & 0 \end{pmatrix} \begin{pmatrix} \omega_1 \\ \omega_2 \\ 0 \end{pmatrix} = \begin{pmatrix} \Theta\omega_1 \\ \Theta\omega_2 \\ 0 \end{pmatrix}$$

$$\frac{1}{2}\Theta\left(\omega_1^2 + \omega_2^2\right) = \frac{1}{2}\frac{L^2}{\Theta}$$

$$\underline{L}^2 = \hbar^2\, l(l+1) \qquad l = 0, 1, 2, \ldots$$

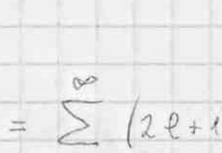
$$L_z = \hbar \cdot m \qquad m = -l, \ldots, l$$

első gerjesztett állapot: $\sim \dfrac{\hbar^2}{\Theta}$

$k_B T \gg \dfrac{\hbar^2}{\Theta}$ klasszikus viselkedés

$k_B T \lesssim \dfrac{\hbar^2}{\Theta}$ kvantumos viselkedés

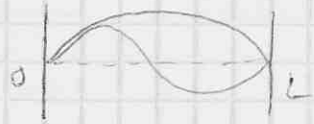
$H_2$:




$$\Theta = 2m\left(\frac{d}{2}\right)^2 = \frac{1}{2} m d^2$$

$$T = \frac{\hbar^2}{k_B \cdot \Theta} = 87\ \mathrm{K}$$

$$Z = \sum_{l=0}^{\infty} (2l+1) \cdot e^{-\beta \frac{\hbar^2 l(l+1)}{2\Theta}}$$



$\lambda = \frac{h}{p}$ de Broglie - hullámhossz

$p = \frac{h}{\lambda} \qquad \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2}$

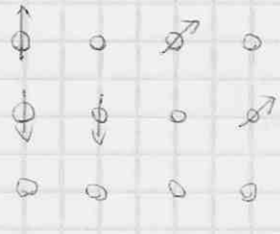
energiaszintek távolsága: $\frac{h^2}{mL^2}$

$T \to 0$ degenerált kvantumgázok

kvantumstatisztika

(megkülönböztethetetlen részecskék)

<u>bináris atomok alkalmazása</u>



atomok mágneses momentummal

$\underline{B}$ mágneses térben

$E = -\underline{m}\,\underline{B}$

$\underline{m} = \mu\,\underline{S}$

$\frac{1}{2}$ spin: $S_z = \pm \frac{\hbar}{2}$

$\underline{B} \parallel z \qquad \bar{E} = -\mu S_z B = \begin{cases} -m_0 B & m \uparrow\uparrow B \\ +m_0 B & m \downarrow\uparrow B \end{cases}$

$m_0 = \mu \cdot \frac{\hbar}{2}$

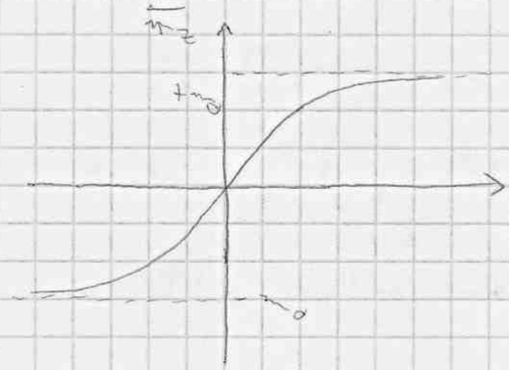
$+\varepsilon$

$-\varepsilon$

$\bar{E} = -\varepsilon \, \mathrm{th}\left(\frac{\varepsilon}{k_B T}\right)$

$\bar{E} = N\left(-m_0 B \, \mathrm{th}\left(\frac{m_0 B}{k_B T}\right)\right)$

$\bar{E} = -N \cdot \bar{m}_z \cdot B \qquad \bar{m}_z = m_0 \, \mathrm{th}\left(\frac{m_0 B}{k_B T}\right)$




$\frac{m_0 B}{k_B T} \gg 1$

$\bar{m}_z \approx m_0$ (telítés)

$\frac{m_0 B}{k_B T} \ll 1 \qquad \mathrm{th}\, x \approx x$

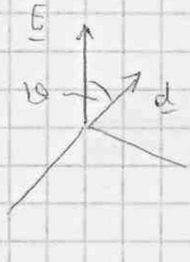
$\bar{m}_z = \frac{m_0^2 B}{k_B T}$

$\chi = \frac{m_0^2}{k_B T}$ szuszceptibilitás (mágneses)

(Curie - tv.)

egész anyag szuszceptibilitása: $N \cdot \frac{m_0^2}{k_B T}$

elektromos dipólus elektromos térben




$\underline{d} \qquad U = -\underline{d}\,\underline{E} = -d E \cos\vartheta = -d_z E$

$e^{-\beta U} = e^{\beta d \cos\vartheta \cdot E}$

térszög: $d\Omega = d\vartheta \cdot \sin\vartheta \, d\varphi$

$$Z = \int d\Omega \, e^{-\beta U} = \int_0^{\pi} d\vartheta \int_0^{2\pi} d\varphi \, \sin\vartheta \cdot e^{\beta \cdot d \cdot \cos\vartheta \cdot E}$$

$s = \cos\vartheta \qquad ds = -\sin\vartheta \cdot d\vartheta$

$\vartheta = 0 \qquad s = 1$

$\vartheta = \pi \qquad s = -1$

$$Z = 2\pi \int_{-1}^{1} ds \; e^{\beta d E s} = 2\pi \left[ \frac{e^{\beta d E s}}{\beta d E} \right]_{s=-1}^{s=1} =$$

$$= 2\pi \frac{e^{\beta d E} - e^{-\beta d E}}{\beta d E} = 4\pi \frac{\operatorname{sh}(\beta d E)}{\beta d E}$$

$$\bar{U} = -\bar{d}_z \cdot E = -\frac{\partial}{\partial \beta} \ln Z = -\frac{\partial}{\partial \beta} \left( \ln \operatorname{sh}(\beta d E) - \ln(\beta d E) \right) =$$

$$= -\left( \frac{\operatorname{ch}(\beta d E)}{\operatorname{sh}(\beta d E)} d \cdot E - \frac{1}{\beta \cdot d E} \cdot d E \right)$$

$$\bar{d}_z = d \left( \operatorname{cth}(\beta d E) - \frac{1}{\beta d E} \right)$$

$\beta d E \gg 1 \qquad \bar{d}_z \simeq d$

$\beta d E \ll 1 \qquad \bar{d}_z \simeq d \cdot \frac{\beta d E}{3} = \frac{d^2}{3 k_B T} E$

$x \gg 1 \qquad \operatorname{cth} x \simeq 1$

$x \ll 1 \qquad \operatorname{cth} x \simeq \frac{1}{x} + \frac{x}{3} + \ldots$

dielettronica suscettibilità : $\frac{d^2}{3 k_B T}$

kanonikus eloszlás: $P(E_n) = \frac{1}{Z} e^{-\beta E_n}$

$\rightarrow$ klasszikusan: $\sim e^{-\beta \mathcal{H}(p,q)}$

1 atom gázban (T hőm.)

$$\mathcal{P}(p, d^3p) = C e^{-\beta \frac{p^2}{2m}} d^3p = C e^{-\beta \frac{p_x^2 + p_y^2 + p_z^2}{2m}} d^3p =$$

$$= m^3 C e^{-\beta \frac{m v^2}{2}} d^3v \qquad p_x = m v_x \qquad d^3p = m^3 d^3v$$

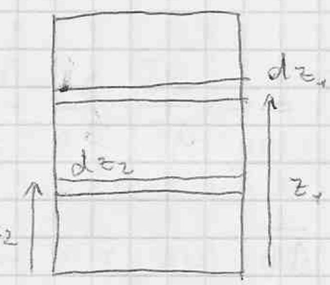
nehézségi erőtér: $\mathcal{H}(p,z) = \frac{p^2}{2m} + mgz$

$$\mathcal{P}(p, d^3p, z, dz) = C e^{-\beta\left(\frac{p^2}{2m} + mgz\right)} d^3p\, dz$$

$p$ és $z$ független valószínűségi változók

$$\mathcal{P}(z, dz) \sim e^{-\frac{mgz}{k_B T}} dz$$

$$\mathcal{P}(z, dz) = \frac{N(z, dz)}{N}$$




$$\frac{N(z_1, dz_1)}{N(z_2, dz_2)} = e^{-\frac{mg(z_1 - z_2)}{k_B T}}$$

Perrin (1908)

gumigutti részecskékkel: $r = 3 \cdot 10^{-5}$ cm

$m = 2{,}17 \cdot 10^{-14}$ g

$$P(E_n) = \frac{1}{Z} e^{-\beta E_n} \quad (T \text{ hő környezetben})$$

$$Z = \sum_n e^{-\beta E_n} \quad \text{állapotösszeg}$$

$$\bar{E} = \frac{\sum_n E_n e^{-\beta E_n}}{\sum_n e^{-\beta E_n}} = -\frac{1}{Z}\frac{\partial Z}{\partial \beta}$$

$$\frac{\partial \bar{E}}{\partial \beta} = \underbrace{-\frac{1}{Z}\frac{\partial^2 Z}{\partial \beta^2}}_{\frac{1}{Z}\sum_n (-E_n)^2 e^{-\beta E_n} = \overline{E^2}} + \frac{1}{Z^2}\left(\frac{\partial Z}{\partial \beta}\right)^2 = -\overline{E^2} + \bar{E}^2 = -\overline{\Delta E^2}$$

$$\overline{\Delta E^2} = \overline{(E-\bar{E})^2} = \overline{E^2} - \bar{E}^2 = -\frac{\partial \bar{E}}{\partial \beta} = -\frac{\partial \bar{E}}{\partial T}\cdot\frac{\partial T}{\partial \beta}$$

$$\beta = \frac{1}{k_B T} \qquad T = \frac{1}{k_B \beta} \qquad \frac{\partial T}{\partial \beta} = -\frac{1}{k_B \beta^2} = -\frac{(k_B T)^2}{k_B} = -k_B T^2$$

$$\overline{\Delta E^2} = -\frac{\partial \bar{E}}{\partial T}\cdot\frac{\partial T}{\partial \beta} = k_B T^2 \cdot \frac{\partial \bar{E}}{\partial T} = k_B T^2 \cdot C$$

$$\left.\begin{aligned} \overline{\Delta E^2} &= k_B T^2 C \sim N \\ \bar{E} &\sim N \end{aligned}\right\} \quad \frac{\sqrt{\overline{\Delta E^2}}}{\bar{E}} \sim \frac{\sqrt{N}}{N} = \frac{1}{\sqrt{N}}$$

makroszkópikus rendszer $\quad N \sim N_A = 6\cdot 10^{23}$

$$\frac{1}{\sqrt{N}} \sim 10^{-12}$$

makroszkopikus rendszer: legvalószínűbb $E \to E^*$

$$P(E) = \frac{1}{Z} e^{-\beta E} \cdot g(E,N) = \max \qquad \beta = \frac{1}{k_B T}$$

$$-\beta E + \ln g(E,N) = \max$$

$$-\beta + \frac{\partial}{\partial E} \ln g(E,N) = 0$$

$$\frac{1}{T} = k_B \frac{\partial}{\partial E} \ln g(E,N) = \underbrace{\frac{\partial}{\partial E} S(E,N)}_{\frac{1}{T_{\text{rendszer}}}}$$

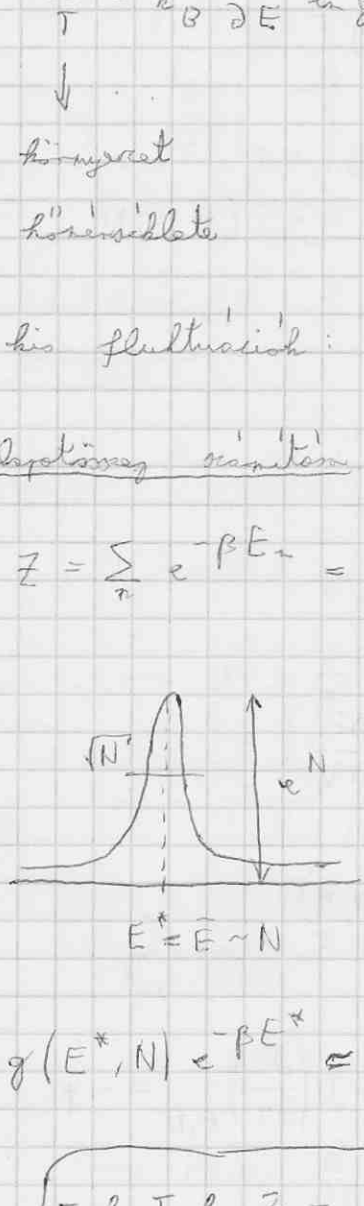
$\downarrow$

környezet hőmérséklete

kis fluktuációk: $E^* = \bar{E}$

állapotösszeg számítása

$$Z = \sum_n e^{-\beta E_n} = \sum_E \underbrace{g(E,N)\, e^{-\beta E}}_{P(E)\cdot Z} \simeq e^{-\beta E^*} e^{\frac{1}{k_B} S(E^*,N)} \cdot \sqrt{N}$$




$$\ln Z = -\beta E^* + \frac{1}{k_B} S(E^*,N) + O(\ln N)$$

$$= -\beta \bar{E} + \frac{1}{k_B} S(\bar{E},N) + O(\ln N)$$

$$g(E^*,N)\, e^{-\beta E^*} \simeq e^{-\beta E^*} e^{\frac{1}{k_B} S(E^*,N)} \sim e^{\alpha N}$$

$$\boxed{-k_B T \ln Z = \bar{E} - T S(\bar{E},N) = F}$$ szabadenergia

$$F(T,V,N) = \bar{E}(T,V,N) - TS\left(\bar{E}(T,V,N), V, N\right)$$

$$Z \longrightarrow \bar{E} = -\frac{\partial}{\partial \beta} \ln Z$$

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

$$\longrightarrow F = \bar{E} - TS$$

$$\left(\frac{\partial F}{\partial T}\right)_{V,N} = \underbrace{\left(1 - T \frac{\partial S}{\partial E}\Big|_{\bar{E}}\right)}_{0} \frac{\partial \bar{E}}{\partial T} - S(E,V,N)$$

$$\Rightarrow \frac{\partial F}{\partial T} = -S(E,V,N)$$

$$\bar{E} \simeq E^* \quad \frac{\partial S}{\partial E}\Big|_{E^*} = \frac{1}{T}$$

$$\left(\frac{\partial F}{\partial V}\right)_{T,N} = -k_B T \frac{\partial}{\partial V} \ln Z = -k_B T \cdot \frac{1}{Z} \frac{\partial Z}{\partial V}$$

$$Z = \sum_n e^{-\beta E_n(V,N)}$$

$$\left(\frac{\partial F}{\partial V}\right)_{T,N} = -k_B T \frac{1}{Z} \sum_n e^{-\beta E_n(V,N)} \left(-\beta \frac{\partial E_n}{\partial V}\right) =$$

$$= \frac{1}{Z} \sum_n e^{-\beta E_n} \cdot \frac{\partial E_n}{\partial V} = -p(T,V,N)$$

$$\frac{\partial F}{\partial V} = \frac{\partial}{\partial V}\left(\bar{E} - TS\right) = \underbrace{\left(1 - T \frac{\partial S}{\partial E}\Big|_{\bar{E}}\right)}_{0} \frac{\partial \bar{E}}{\partial V} - T\left(\frac{\partial S}{\partial V}\right)_{E,N} = -p$$

$$p = T\left(\frac{\partial S}{\partial V}\right)_{E,N}$$

$$dF = \underbrace{\left(\frac{\partial F}{\partial T}\right)_{V,N}}_{-S} \cdot dT + \underbrace{\left(\frac{\partial F}{\partial V}\right)_{T,N}}_{-p} \cdot dV + \underbrace{\left(\frac{\partial F}{\partial N}\right)_{T,V}}_{\mu} dN$$

$$\boxed{dF = -S\,dT - p\,dV + \mu\,dN}$$ fundamentális összefüggés

$$S = k_B \ln g(E,V,N)$$

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right)_{V,N}\Bigg|_{\bar{E}} \qquad p = T\left(\frac{\partial S}{\partial V}\right)_{E,N}\Bigg|_{\bar{E}} \qquad \mu = -T\left(\frac{\partial S}{\partial N}\right)_{E,V}\Bigg|_{\bar{E}}$$

$$\boxed{dS = \frac{1}{T}dE + \frac{p}{T}dV - \frac{\mu}{T}dN}$$

mikrokanonikus eloszlás (sokaság): izolált, makroszkopikus rendszer

multiplicitás: $g(E,V,N) \rightarrow S = k_B \ln g(E,V,N)$

$$\rightarrow dS = \frac{1}{T}dE + \frac{p}{T}dV - \frac{\mu}{T}dN$$

kanonikus eloszlás (sokaság): makroszkopikus rendszer $T$ hőm. környezetben

állapotösszeg: $Z = \sum_n e^{-\beta E_n} \rightarrow F = -k_B T \ln Z$

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

$$\rightarrow \bar{E} = -\frac{\partial}{\partial \beta}\ln Z = F + T\cdot S$$

A rendszer: $E_{A,n}$ $\quad Z_A = \sum_n e^{-\beta E_{A,n}}$.

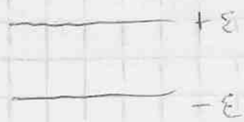
B rendszer: $E_{B,m}$ $\quad Z_B = \sum_m e^{-\beta E_{B,m}}$

$(A+B)$: $E_{A,n} + E_{B,m}$ $\quad Z_{A+B} = \sum_n \sum_m \underbrace{e^{-\beta(E_{A,n}+E_{B,m})}}_{e^{-\beta E_{A,n}} \cdot e^{-\beta E_{B,m}}} =$

$$= \underbrace{\sum_n e^{-\beta E_{A,n}}}_{Z_A} \cdot \underbrace{\sum_m e^{-\beta E_{B,m}}}_{Z_B}$$

$$\boxed{Z_{A+B} = Z_A \cdot Z_B}$$

N db bináris atom:




1 db: $Z_1 = e^{-\beta\varepsilon} + e^{\beta\varepsilon} = 2\,\mathrm{ch}\,\beta\varepsilon$

N db: $Z = Z_1^N = (2\,\mathrm{ch}(\beta\varepsilon))^N$

$$F = -k_B T \ln Z = -k_B T \cdot N \ln(2\,\mathrm{ch}(\beta\varepsilon))$$

$$S = -\frac{\partial F}{\partial T} = k_B N \ln(2\,\mathrm{ch}(\beta\varepsilon)) + k_B T N \frac{2\,\mathrm{sh}(\beta\varepsilon)}{2\,\mathrm{ch}(\beta\varepsilon)} \varepsilon \left(-\frac{1}{k_B T^2}\right) =$$

$$S = k_B N \ln(2\,\mathrm{ch}(\beta\varepsilon)) - \frac{\varepsilon}{T} N \cdot \mathrm{th}(\beta\varepsilon)$$

$$\bar{E} = -\frac{\partial}{\partial\beta}(\ln Z) = -N\varepsilon\,\mathrm{th}\,\beta\varepsilon$$

$$S = -\frac{F}{T} + \frac{\bar{E}}{T} \Rightarrow F = \bar{E} - TS$$

$\varepsilon \ll k_B T \qquad \beta \varepsilon \ll 1$

$$S \simeq N k_B \ln 2 = k_B \ln\left(2^N\right) \qquad \bar{E} \simeq 0$$

$\varepsilon \gg k_B T \qquad \beta \varepsilon \gg 1$

$$\bar{E} \simeq -N\varepsilon \qquad S \simeq N k_B \beta \varepsilon - \frac{N\varepsilon}{T} = 0$$


1 részecske: $\varepsilon_0, \varepsilon_1, \varepsilon_2, \dots, \varepsilon_l, \dots$

$$\varsigma = \sum_l e^{-\beta \varepsilon_l}$$

$p_x^2 + p_y^2 + p_z^2$

Klasszikusan: $\mathcal{H}_1 = \frac{p^2}{2m} \qquad \varsigma = \frac{1}{h^3}\int d^3r \, d^3p \, e^{-\beta \frac{p^2}{2m}} =$

$$= \frac{V}{h^3}\left(\int_{-\infty}^{+\infty} dp_x \, e^{-\beta \frac{p_x^2}{2m}}\right)^3 = \frac{V}{h^3}\left(\sqrt{\frac{\pi}{\beta/2m}}\right)^3 =$$

$$= \frac{V}{h^3}\left(2\pi m k_B T\right)^{\frac{3}{2}} = V\left(\frac{2\pi m k_B T}{h^2}\right)^{\frac{3}{2}}$$

<u>N részecske</u>: kölcsönhatás nélkül

(ideális gáz)

$$Z = \varsigma \cdot \varsigma \cdot \ldots \cdot \varsigma = \varsigma^N$$

id. gáz

$$F = -k_B T \ln Z = -N k_B T \ln \varsigma = -N k_B T \ln\left[V\left(\frac{2\pi m k_B T}{h^2}\right)^{\frac{3}{2}}\right]$$

$$F = \bar{E} - T S(\bar{E})$$

nem extenzív!

$$N \phi\left(\frac{V}{N}, T\right)$$

azonos részecskék megkülönböztethetetlensége $\rightarrow \frac{1}{N!}$

$$Z = \frac{1}{N!} \zeta^N$$

$$F = -k_B T \ln Z = -N k_B T \ln \zeta + k_B T \underbrace{\ln N!}_{N \ln N - N + \cancel{O(\ln N)}}$$

$$= -N k_B T \ln \frac{\zeta}{N} - N k_B T$$

$$= -N k_B T \left( \ln \frac{\zeta}{N} + 1 \right) \quad \text{extenzív!}$$

$$E = -\frac{\partial (\ln Z)}{\partial \beta} = -\frac{\partial}{\partial \beta} \left( N \ln \zeta - \ln N! \right) = -N \frac{\partial \ln \zeta}{\partial \beta} =$$

$$= \frac{3}{2} N k_B T$$

$$p = -\frac{\partial F}{\partial V} = +N k_B T \frac{\partial}{\partial V} \ln \left[ V \left( \frac{2\pi m k_B T}{h^2} \right)^{\frac{3}{2}} \right] = \frac{N k_B T}{V}$$

$$S = -\frac{\partial F}{\partial T} = N k_B \ln \frac{\zeta}{N} + N k_B T \frac{\partial}{\partial T} \ln \frac{\zeta}{N}$$

$$\ln \frac{\zeta}{N} = \ln \left[ \frac{V}{N} \left( \frac{2\pi m k_B T}{h^2} \right)^{\frac{3}{2}} \right] = \frac{3}{2} \ln T + \ln \left[ \frac{V}{N} \left( \frac{2\pi m k_B}{h^2} \right)^{\frac{3}{2}} \right]$$

$$\frac{\partial}{\partial T} \ln \frac{\zeta}{N} = \frac{3}{2} \frac{1}{T}$$

$$S = N k_B \left( \ln \frac{\zeta}{N} + \frac{5}{2} \right) = N k_B \left( \ln \frac{V}{N} \left( \frac{2\pi m k_B T}{h^2} \right)^{\frac{3}{2}} + \frac{5}{2} \right) =$$

$$= N k_B \left( \ln \left[ \frac{V}{N} \left( \frac{2\pi m}{h^2} \cdot \frac{2E}{3N} \right)^{\frac{3}{2}} \right] + \frac{5}{2} \right) = k_B \ln g(E, N, V)$$

$$k_B T = \frac{2E}{3N}$$

$$\mu = \frac{\partial F}{\partial N} = -k_B T \ln \frac{\varsigma}{N} \cancel{- k_B T - N k_B T \left(-\frac{1}{N}\right)}$$

$$\mu = -k_B T \ln \frac{\varsigma}{N} \qquad \frac{\varsigma}{N} = \frac{V}{N} \left(\frac{2\pi m k_B T}{h^2}\right)^{\frac{3}{2}} = e^{-\frac{\mu}{k_B T}}$$

$$F: \quad -k_B T \ln N!$$

$$\ln Z: \quad -\ln N!$$

részecske: hullámcsomag

$$\left.\begin{matrix} \Delta x \\ \Delta p \end{matrix}\right\} \text{ pontossággal ismerjük } x, p\text{-t}$$

$V$ térfogatban $N$ részecske

átlagos távolság: $\left(\frac{V}{N}\right)^{\frac{1}{3}} = R$

$$R \gg \Delta x > \frac{h}{\Delta p} \gg \frac{h}{p_T} \qquad p_T: \text{ jellemző impulzus}$$

határozatlansági reláció: $\Delta x \, \Delta p > h$

$$\frac{p_T^2}{2m} = k_B T \qquad p_T = \sqrt{2 m k_B T}$$

$$R \gg \frac{h}{p_T} = \frac{h}{\sqrt{2 m k_B T}} = \lambda_T$$

termikus de Broglie-hullámhossz

$$\frac{V}{N} = R^3 \gg \frac{h^3}{(2 m k_B T)^{\frac{3}{2}}} = \left(\frac{h^2}{2 m k_B T}\right)^{\frac{3}{2}}$$

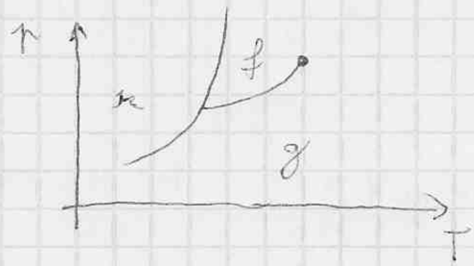
$$\frac{V}{N}\left(\frac{2 m k_B T}{h^2}\right)^{\frac{3}{2}} \gg 1$$

klasszikus gáz $\left\{ \begin{array}{l} \text{nagy hőmérséklet} \\ \text{kis sűrűség} \end{array} \right.$

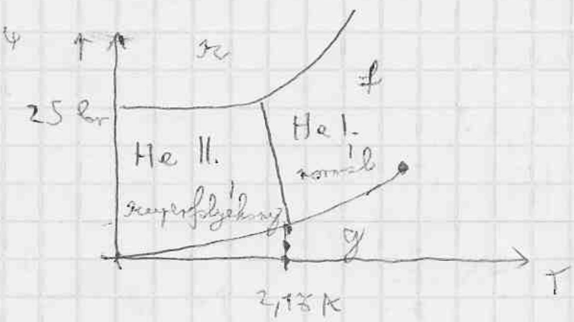
$He^3$  2p  1n  2e  fermion

$He^4$  2p  2n  2e  bozon

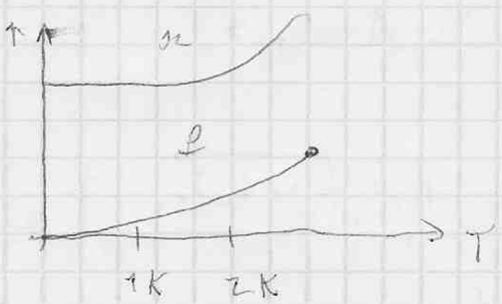
közönséges gáz (víz, $CO_2$, stb.)

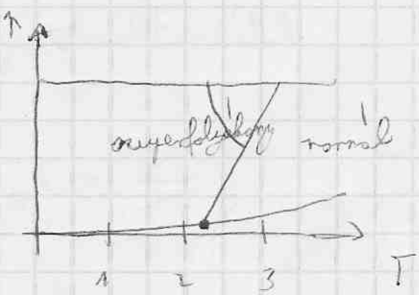



$He^4$




$He^3$




ideális kvantumgázok – azonos részecskék

- fermion  félegész spin
- bozon  egész spin

1 részecske  $\varepsilon_0, \varepsilon_1, \varepsilon_2, \ldots, \varepsilon_\ell, \ldots$ egyrészecske energiaszintek


N részecske: betöltési szám: $n_\ell$

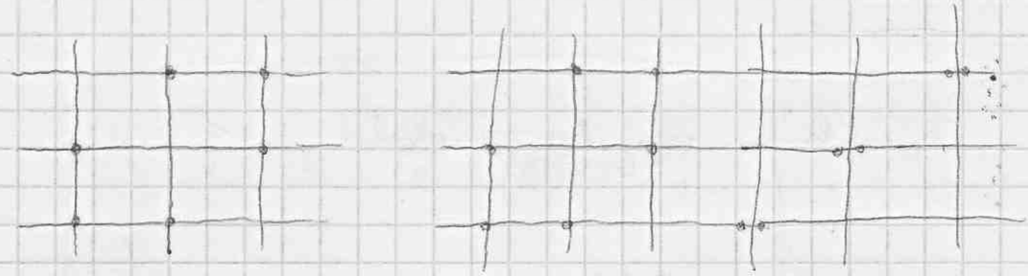
$n_\ell$ db $\varepsilon_\ell$ energiájú részecske

$$N = \sum_\ell n_\ell \qquad E = \sum_\ell \varepsilon_\ell n_\ell$$

fermion: $n_\ell = 0, 1$

bozon: $n_\ell = 0, 1, 2, \ldots$

2 db részecske, 3 állapot

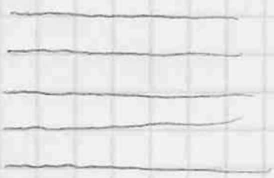


fermion  bozon

3 állapot  6 állapot

megkülönböztethető részecskék: $3^2 = 9$ állapot

N fermion



$p_i(N)$ : annak a valószínűsége, hogy i-edik állapotban $n_i = 1$

$1 - p_i(N)$ : ------ $n_i = 0$

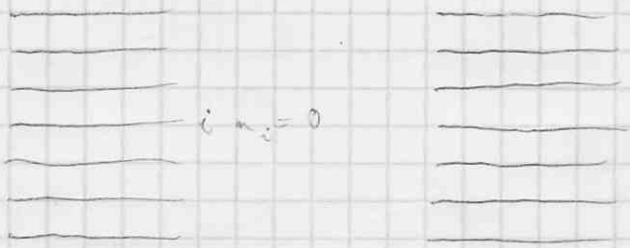
$$\bar{n}_i = 1 \cdot p_i(N) + 0 \cdot (1 - p_i(N)) = p_i(N)$$

$$p_i(N) = \sum_{\ell \in \mathcal{A}(N)} \frac{1}{Z} e^{-\beta E_\ell(N)} = 1 - \sum_{\ell \in \mathcal{B}(N)} \frac{1}{Z} e^{-\beta E_\ell(N)}$$

$\mathcal{A}(N) = \{$ összes olyan állapot, amelyben $n_i = 1 \}$

$\mathcal{B}(N) = \{$ összes olyan állapot, amelyben $n_i = 0 \}$

$\mathcal{B}(N)$ N részecske N+1 részecske $\mathcal{A}(N+1)$




egyértelműen egymáshoz rendelhetők

$$p_i(N) = 1 - \sum_{\ell \in \mathcal{B}(N)} \frac{1}{Z_N} e^{-\beta E_\ell(N)} = 1 - \sum_{\ell \in \mathcal{A}(N+1)} \frac{1}{Z_N} e^{-\beta (E_\ell(N+1) - \varepsilon_i)}$$

$$= 1 - \frac{Z_{N+1}}{Z_N} \underbrace{\sum_{\ell \in \mathcal{A}(N+1)} \left( \frac{1}{Z_{N+1}} e^{-\beta E_\ell(N+1)} \right)}_{p_i(N+1)} e^{\beta \varepsilon_i}$$

$$F_N = -k_B T \ln Z_N \qquad Z_N = e^{-\frac{F_N}{k_B T}}$$

$$Z_{N+1} = e^{-\frac{F_{N+1}}{k_B T}}$$

$$\frac{Z_{N+1}}{Z_N} = e^{-\frac{F_{N+1}-F_N}{k_B T}}$$

$$n_i(N) = 1 - n_i(N+1)\, e^{\beta \varepsilon_i}\, e^{-\frac{F_{N+1}-F_N}{k_B T}} =$$

$$= 1 - n_i(N+1)\, e^{\beta(\varepsilon_i - \mu)}$$

$\underline{N \to \infty}$ $\qquad n_i(N) \simeq n_i(N+1)$

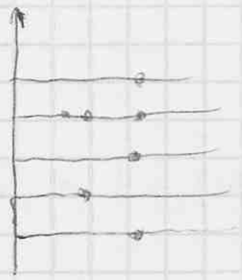
$$F_{N+1} - F_N = \frac{\partial F}{\partial N}(N+1-N) = \mu$$

$$n_i = 1 - n_i\, e^{\beta(\varepsilon_i - \mu)} \qquad \boxed{n_i = \frac{1}{e^{\beta(\varepsilon_i-\mu)}+1}}$$

$$\boxed{\begin{aligned} N &= \sum_l \bar{n}_l = \sum_l \frac{1}{e^{\beta(\varepsilon_l-\mu)}+1} \\ \bar{E} &= \sum_l \varepsilon_l \bar{n}_l = \sum_l \frac{\varepsilon_l}{e^{\beta(\varepsilon_l-\mu)}+1} \end{aligned}}$$

## ideális gázok

egyrészecske állapotok | betöltési számok



$\varepsilon_0 = 0$

$$E = \sum_i \varepsilon_i \cdot n_i$$

$$N = \sum_i n_i$$

Fermi-Dirac-statisztika → fermion félegész spin $n_i = 0, 1$

Bose-Einstein-statisztika → bozon egész spin $n_i = 0, 1, 2, \ldots$

Maxwell-Boltzmann-statisztika → $n_i = 0, 1, 2, \ldots$

(megkülönböztethető rész., $1/N!$)

Fermi-Dirac: $$\bar{n}_i = \frac{1}{e^{\beta(\varepsilon_i - \mu)} + 1}$$

Bose-Einstein: $$\bar{n}_i = \frac{1}{e^{\beta(\varepsilon_i - \mu)} - 1} \qquad (\mu < 0)$$

$$\left( \bar{n}_{\varepsilon_i = 0} = \frac{1}{e^{-\beta\mu} - 1} > 0 \right)$$

Maxwell-Boltzmann:

$$p(n_i) = \left( \frac{e^{-\beta\varepsilon_i}}{\zeta} \right)^{n_i} \cdot \left( 1 - \frac{e^{-\beta\varepsilon_i}}{\zeta} \right)^{N - n_i} \cdot \binom{N}{n_i}$$

binomiális alakú

$$\zeta = \sum_i e^{-\beta\varepsilon_i}$$

$$\bar{n}_i = N \frac{e^{-\beta \varepsilon_i}}{\varsigma}$$

$$Z = \frac{1}{N!} \cdot \varsigma^N \qquad F = -k_B T \ln Z = -k_B T N \left[ \ln \frac{\varsigma}{N} + 1 \right]$$

$$\mu = \frac{\partial F}{\partial N} = -k_B T \ln \frac{\varsigma}{N}$$

$$\frac{\varsigma}{N} = e^{-\beta\mu} \implies \bar{n}_i = e^{-\beta(\varepsilon_i - \mu)}$$

statisztikák különbsége eltűnik, ha $e^{\beta(\varepsilon_i - \mu)} \gg 1$

$$e^{\beta(\varepsilon_i - \mu)} > e^{\beta(\varepsilon_0 - \mu)} = e^{-\beta\mu} \gg 1$$

$$\boxed{e^{\beta\mu} \ll 1} \qquad (\text{ekkor } \mu < 0)$$

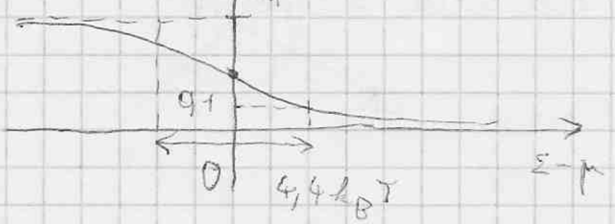
$$\boxed{\bar{n}_i \ll 1}$$

klasszikus határeset

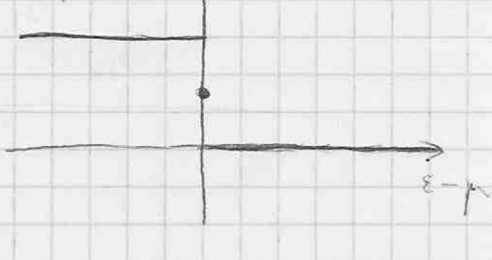
$$e^{\beta\mu} = \frac{N}{\varsigma} = \frac{N}{V} \left( \frac{h^2}{2\pi m k_B T} \right)^{\frac{3}{2}} \ll 1$$

<u>Fermi-statisztika</u>

$$\bar{n}(\varepsilon) = \frac{1}{e^{\beta(\varepsilon - \mu)} + 1}$$




$$\xrightarrow[\beta \to \infty]{T \to 0}$$



$$\lim_{\beta\to\infty} \bar{n}(\varepsilon) = \begin{cases} 1 & \varepsilon < \mu \\ 0 & \varepsilon > \mu \end{cases}$$

$T = 0$ : alapállapot : $\varepsilon < \mu$ állapotok betöltve

$$\beta(\varepsilon - \mu) = u$$

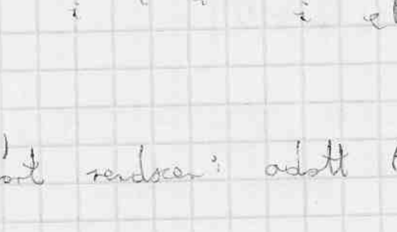
$$\frac{1}{e^{u}+1} = 0{,}1 \qquad e^{u} = 9 \qquad u = \ln 9 = 2{,}2$$

$$N = \sum_i \bar{n}_i = \sum_i \frac{1}{e^{\beta(\varepsilon_i - \mu)} + 1} \qquad N = N(\beta, \mu)$$

$$\bar{E} = \sum_i \varepsilon_i \bar{n}_i = \sum_i \frac{\varepsilon_i}{e^{\beta(\varepsilon_i - \mu)} + 1} \qquad \bar{E} = \bar{E}(\beta, \mu)$$

- zárt rendszer: adott $E, N \longrightarrow \mu, \beta = \frac{1}{k_B T}$
- kanonikus sokaság: adott $\beta, N \longrightarrow \mu, \bar{E}$
  (hőtartály)
- nagykanonikus sokaság: $\beta, \mu \longrightarrow N, \bar{E}$

kvázi klasszikus számolás




$\Delta x \cdot \Delta p = h$

1 fáziscella = 1 állapot

energia: $\frac{p^2}{2m}$

térbeli mozgás: fáziscella $\Delta x \Delta y \Delta z \Delta p_x \Delta p_y \Delta p_z = h^3 \to 1$ állapot

$$N = \frac{1}{h^3} \int d^3 r \int d^3 p \, \frac{1}{e^{\beta(\varepsilon(p) - \mu)} + 1} \qquad \varepsilon(p) = \frac{p^2}{2m}$$

$$N = \frac{V}{h^3} \int d^3 p \, \frac{1}{e^{\beta(\varepsilon(p) - \mu)} + 1}$$

$$E = \frac{V}{h^3} \int d^3 p \, \frac{\varepsilon(p)}{e^{\beta(\varepsilon(p) - \mu)} + 1}$$

elemi kvantálás


$p$ impulzus

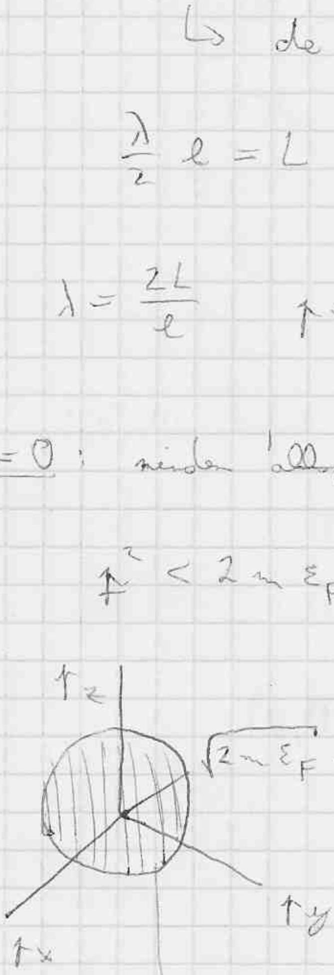
↳ de Broglie-hullámhossz: $\lambda = \frac{h}{p}$

$$\frac{\lambda}{2} l = L \qquad l = 1, 2, \ldots$$

$$\lambda = \frac{2L}{l} \qquad p = \frac{h}{\lambda} = \frac{h}{2L} \cdot l$$

$\underline{T = 0}$: minden állapot betöltve: $\varepsilon(p) = \frac{p^2}{2m} < \mu = \varepsilon_F$

$p^2 < 2m\varepsilon_F$ (Fermi-energia)




$\sqrt{2m\varepsilon_F} = p_F$ (Fermi-impulzus)

$$N = \frac{V}{h^3} \int d^3 p \cdot 1 = \frac{V}{h^3} \frac{4\pi}{3} p_F^3$$

$$|p| < p_F$$

Fermi-gömb

spin $\Rightarrow$ minden hop egy $(2s+1)$ marcót

$$N = \frac{V}{h^3} \cdot \frac{4\pi}{3} \cdot (2s+1) \left(2m\,\varepsilon_F\right)^{\frac{3}{2}}$$

$$\bar{E} = \frac{V}{h^3} (2s+1) \int d^3p \, \frac{p^2}{2m} = \frac{V}{h^3} \frac{2s+1}{2m} \underbrace{\int_0^{p_F} dp \cdot 4\pi p^2 \cdot p^2}_{4\pi \cdot \frac{1}{5} p_F^5} =$$

$$\left.\begin{aligned} \bar{E} &= \frac{V}{h^3} (2s+1) \frac{4\pi}{2m} \frac{p_F^5}{5} \\ N &= \frac{V}{h^3} (2s+1) \frac{4\pi}{3} p_F^3 \end{aligned}\right\} \quad p_F = \sqrt{2m\,\varepsilon_F}$$

$$\frac{\bar{E}}{N} = \frac{3}{5} \cdot \frac{p_F^2}{2m} = \frac{3}{5} \varepsilon_F$$

$$p_F^3 = \frac{N}{V} \frac{3h^3}{4\pi(2s+1)}$$

$$\frac{\bar{E}}{N} = \frac{3}{5} \cdot \frac{1}{2m} \left( \frac{N}{V} \frac{3h^3}{4\pi(2s+1)} \right)^{\frac{2}{3}}$$

$P$ nyomás:

$$P = -\frac{\partial F}{\partial V} \qquad F = E - T \cdot S$$

$$T = 0 \qquad F(T=0, N, V) = E(T=0, N, V)$$

$$P = -\frac{\partial E}{\partial V} \qquad E = C \cdot V^{-\frac{2}{3}}$$

$$\frac{\partial E}{\partial V} = -\frac{2}{3} C V^{-\frac{2}{3}-1} = -\frac{2}{3}\frac{E}{V}$$

$$\boxed{P = \frac{2}{3}\frac{E}{V}}$$

Bernoulli-formula: $P \cdot V = \frac{2}{3} N \cdot \frac{E}{N}$

N állandó: $P = A \cdot V^{-\frac{5}{3}}$ $\qquad P \cdot V^{\frac{5}{3}} =$ állandó

<u>Cu:</u> vezetési elektronok sűrűsége

$$n = \frac{N}{V} = 8{,}4 \cdot 10^{22} \frac{1}{cm^3} = 8{,}4 \cdot 10^{28} \frac{1}{m^3}$$

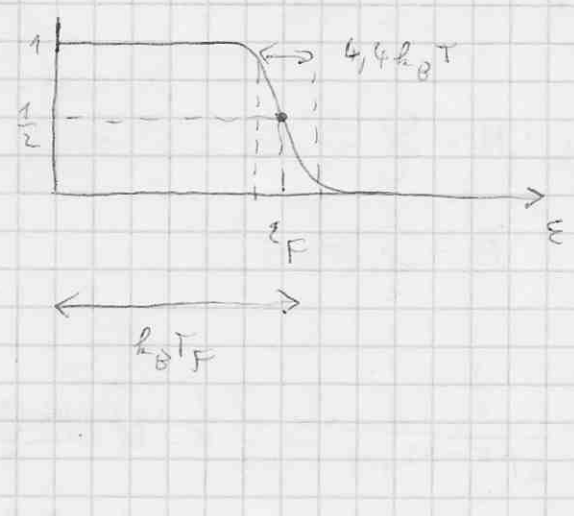
$$m_e = 9{,}1 \cdot 10^{-31}\ kg \qquad h = 6{,}6 \cdot 10^{-34}\ Js$$

$$2s+1 = 2 \quad \left(s = \frac{1}{2}\right) \qquad \varepsilon_F = 11 \cdot 10^{-19}\ J$$

$$k_B T_F = \varepsilon_F \Rightarrow T_F = 8 \cdot 10^4\ K$$

Fermi-hőmérséklet

$$1{,}6 \cdot 10^{-19}\ J = 1\ eV \qquad \varepsilon_F \doteq 6{,}9\ eV$$



heurisztikus érvelés $T \ll T_F$

gerjesztett részecskék száma $N_{eff}$

$$\frac{N_{eff}}{N} = \frac{T}{T_F}$$

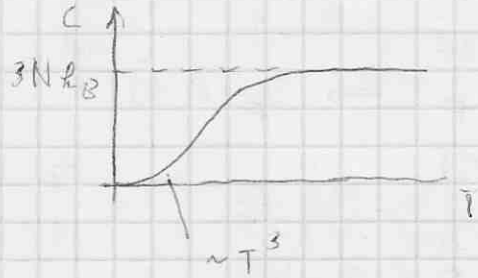
(ekvipartíció) klasszikus leírás:

$$E - E(T=0) \approx N_{eff}\, k_B T \approx N k_B \frac{T^2}{T_F} = N \frac{(k_B T)^2}{\varepsilon_F}$$

$$C = \frac{\partial E}{\partial T} \approx N k_B \cdot \frac{k_B T}{\varepsilon_F} \cdot 2$$

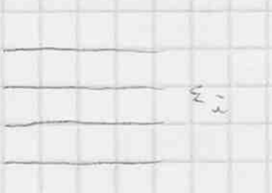
klasszikus gáz: $C = \frac{3}{2} N k_B$

rezgések fajhője




→ alacsony hőmérsékleten a vezetési $e^-$-ok dominálnak

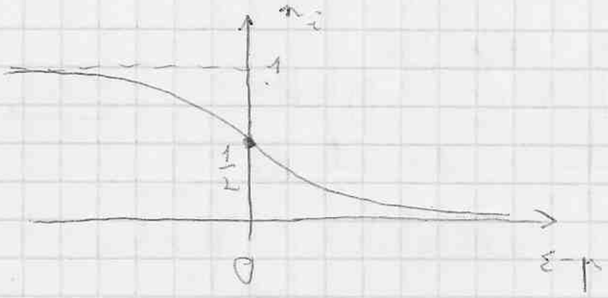
Fermi-gáz




$$N = \sum_i \bar{n}_i$$

$$\bar{E} = \sum_i \bar{n}_i \cdot \varepsilon_i$$

$$\bar{n}_i = \frac{1}{e^{\beta(\varepsilon_i - \mu)} + 1} = \frac{1}{2}\left(1 - \mathrm{th}\left(\frac{\beta(\varepsilon_i - \mu)}{2}\right)\right)$$




<u>egyrészecske állapotsűrűség</u>

$\Delta\varepsilon$-ban $\rightarrow D(\varepsilon)\,\Delta\varepsilon$ egyrészecske állapot

$\varepsilon_0 = 0$

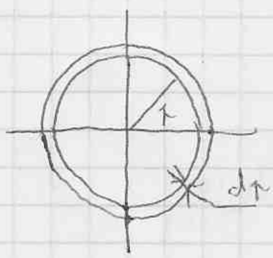
$$N = \sum_{\varepsilon} D(\varepsilon)\,\Delta\varepsilon \cdot \bar{n}(\varepsilon)$$

$$N = \int_0^\infty d\varepsilon\; D(\varepsilon)\, \bar{n}(\varepsilon) \qquad \bar{E} = \int_0^\infty d\varepsilon\; D(\varepsilon)\, \bar{n}(\varepsilon)\, \varepsilon$$

<u>$T=0$:</u>

$$N = \int_0^{\varepsilon_F} d\varepsilon\; D(\varepsilon) \qquad \bar{E} = \int_0^\infty d\varepsilon\; D(\varepsilon)\, \varepsilon$$

edényben szabadon mozgó részecskék



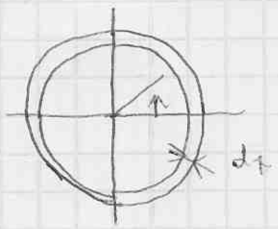

$$\varepsilon(p) = \frac{p^2}{2m} \qquad d\varepsilon = \frac{p}{m}\,dp$$

$$(2s+1)\,\frac{V}{h^3}\,4\pi p^2\,dp = (2s+1)\,\frac{V}{h^3}\,\overbrace{\sqrt{2m\varepsilon}}^{p}\cdot\overbrace{m\,d\varepsilon}^{p\,dp}\cdot 4\pi =$$

$$= D(\varepsilon)\cdot d\varepsilon$$

$$D(\varepsilon) = (2s+1)\,\frac{V}{h^3}\cdot 2\pi\cdot(2m)^{\frac{3}{2}}\cdot \varepsilon^{\frac{1}{2}}$$

síkban mozgó fermionok téglalap tartományban

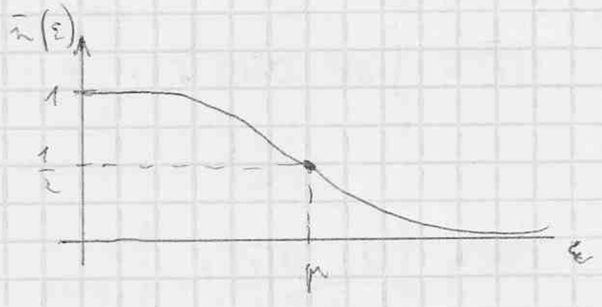



$$\varepsilon(p) = \frac{p^2}{2m} \qquad d\varepsilon = \frac{p}{m}\,dp$$

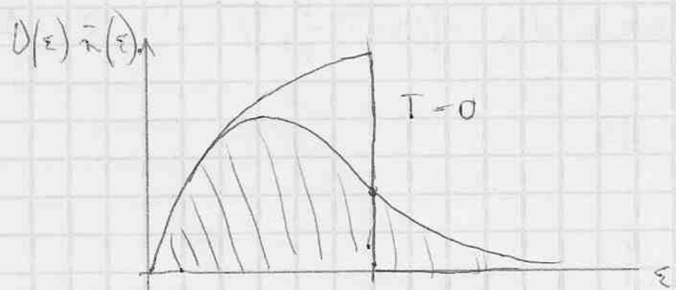
$$(2s+1)\cdot\frac{L^2}{h^3}\cdot 2\pi p\,dp = \underbrace{(2s+1)\,\frac{L^2}{h^3}\,2\pi m}_{D(\varepsilon)}\cdot d\varepsilon$$

$\Omega_0$: $\varepsilon$-nál kisebb energiájú állapotok száma

$$\Omega_0 = (2s+1)\,\frac{V}{h^3}\int\limits_{p<\sqrt{2m\varepsilon}} d^3p = (2s+1)\,\frac{V}{h^3}\cdot\frac{4\pi}{3}\cdot(2m\varepsilon)^{\frac{3}{2}} = \int_0^{\varepsilon} d\varepsilon'\,D(\varepsilon')$$








$\mu$ rögzített

$\Downarrow$

$N(T,\mu)$ $T$-nek növekvő fv.-e

$N$ rögzített

$\Downarrow$

$\mu$ $T$-nek csökkenő fv.-e

$\underline{\mu = 0}$ ?

$$N = (2s+1)\,\frac{V}{h^3}\cdot 2\pi\cdot(2m)^{\frac{3}{2}}\int_0^\infty d\varepsilon\cdot\varepsilon^{\frac{1}{2}}\cdot\frac{1}{e^{\beta\varepsilon}+1}$$

$$u = \beta\varepsilon \qquad du = \beta\, d\varepsilon$$

$$\int_0^\infty d\varepsilon\,\frac{\varepsilon^{\frac{1}{2}}}{e^{\beta\varepsilon}+1} = \frac{1}{\beta^{\frac{3}{2}}}\cdot\underbrace{\int_0^\infty du\,\frac{u^{\frac{1}{2}}}{e^{u}+1}}_{A \quad \text{szám}} = (k_B T)^{\frac{3}{2}}\cdot A$$

$$N = (2s+1)\,\frac{V}{h^3}\, 2\pi\cdot(2m)^{\frac{3}{2}}\cdot(k_B T)^{\frac{3}{2}}\cdot A$$

$$k_B T = \left(\frac{N}{V}\cdot\frac{h^3}{2s+1}\cdot\frac{1}{2\pi}\cdot\frac{1}{(2m)^{\frac{3}{2}}}\cdot\frac{1}{A}\right)^{\frac{2}{3}}$$

$$= \frac{h^2}{2m}\;\frac{N}{V}\left(\frac{1}{2\pi(2s+1)\cdot A}\right)^{\frac{2}{3}}$$

$$k_B T_F = \varepsilon_F = \frac{h^2}{2m}\left(\frac{N}{V}\;\frac{3}{4\pi(2s+1)}\right)^{\frac{2}{3}}$$

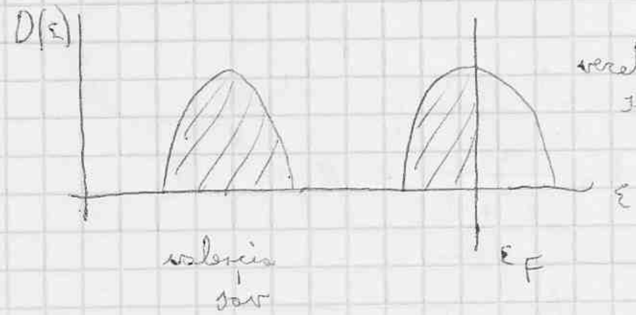
$T$ és $T_F$ azonos nagyságrendű

Klasszikus leírás feltétele:

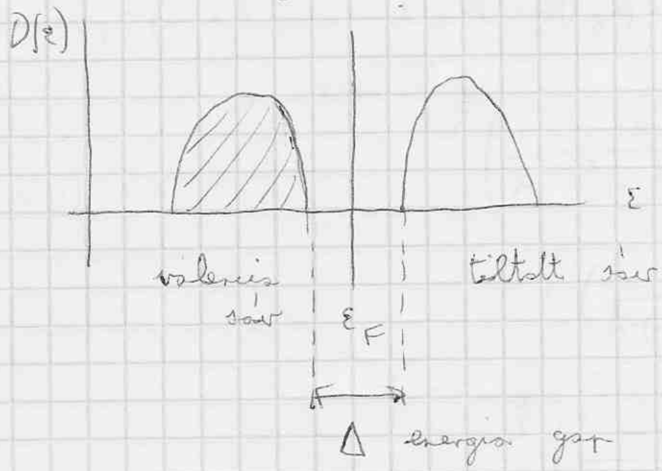
$$\frac{N}{V}\left(\frac{h^2}{2\pi m k_B T}\right)^{\frac{3}{2}} \ll 1$$

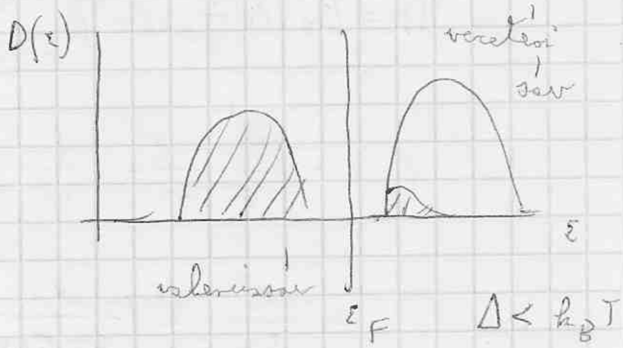
szilárdtest: elektronok

vezető

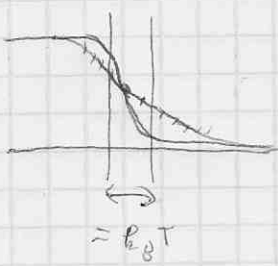



szigetelő - félvezető




hőkapacitás: $T << T_F$




$$E - E_0 \sim N_{eff} \cdot k_B T \sim N \frac{(k_B T)^2}{\varepsilon_F}$$

$$N_{eff} \sim N \frac{k_B T}{\varepsilon_F}$$

$$C \sim N k_B \cdot \underbrace{\frac{k_B T}{\varepsilon_F}}_{\frac{T}{T_F}}$$

szuszceptibilitás $\chi$

független 1/2 spinek

$$M = N m_0 \, \mathrm{th}\left(\frac{m_0 B}{k_B T}\right) \sim \frac{N m_0^2}{k_B T} B$$

mágn. mom. nagysága

$$\chi = \frac{\partial M}{\partial B} = N m_0 \cdot \frac{1}{\mathrm{ch}^2\left(\frac{m_0 B}{k_B T}\right)} \cdot \frac{m_0}{k_B T}$$

$$\chi \sim N_{eff} \cdot \frac{m_0^2}{k_B T} \sim N \frac{k_B T}{\varepsilon_F} \cdot \frac{m_0^2}{\cancel{k_B T}} = \frac{N m_0^2}{\varepsilon_F}$$ hőmérséklet független

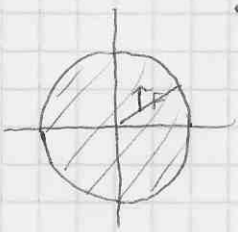
pontos számolás:

$$C = N k_B \frac{k_B T}{\varepsilon_F} \cdot \frac{\pi^2}{2}$$

$$\chi = \frac{N m_0^2}{\varepsilon_F} \cdot \frac{3}{2}$$

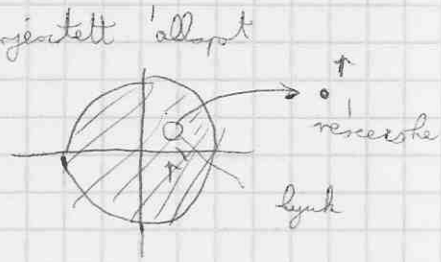
gerjesztések:

alapállapot




$p_F = \sqrt{2m\varepsilon_F}$

gerjesztett állapot



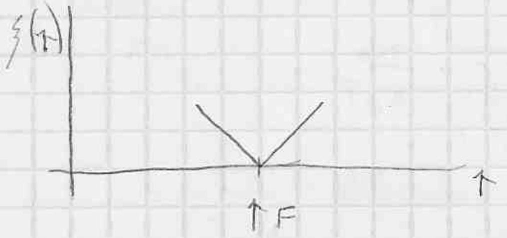

$$E - E_0 = \frac{p^2}{2m} - \frac{p'^2}{2m} = \underbrace{\frac{p^2}{2m} - \varepsilon_F}_{\text{részecske}} + \underbrace{\varepsilon_F - \frac{p'^2}{2m}}_{\text{lyuk}}$$

$$\varepsilon_F = \frac{p_F^2}{2m} \qquad \left.\begin{array}{l} p - p_F \\ p_F - p' \end{array}\right\} \text{kicsi}$$

$$p^2 - p_F^2 = 2p_F(p - p_F)$$

$$p_F^2 - p^2 = 2p_F(p_F - p)$$

$$\left.\begin{array}{ll} \text{részecske:} & \xi(p) = \frac{p_F}{m}(p - p_F) \\ \text{lyuk:} & \xi(p) = \frac{p_F}{m}(p_F - p) \end{array}\right\} \quad \xi(p) = \frac{p_F}{m}|p - p_F|$$




normál Fermi-folyadékok

más: szupravezető elektron-gáz