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

$$I^2 = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} dx\,dy\; e^{-(x^2+y^2)} = \int_0^{\infty} dr \int_0^{2\pi} d\varphi\; r\cdot e^{-r^2} =$$

$$x = r\cos\varphi \qquad u = r^2$$

$$y = r\sin\varphi \qquad du = 2r\,dr$$

$$= 2\pi \int_0^{\infty} \frac{du}{2}\cdot e^{-u} = \pi\left[\frac{e^{-u}}{-1}\right]_0^{\infty} = \pi$$

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

Gamma fv.

$$\Gamma(z) = \int_0^{\infty} t^{z-1}\cdot e^{-t}\,dt \qquad \mathrm{Re}\{z\} > 0$$

$$\Gamma(x) = \int_0^{\infty} t^{x-1}\cdot e^{-t}\,dt$$

dll: $\Gamma(x+1) = x\cdot\Gamma(x)$

$$\Gamma(x+1) = \int_0^{\infty} t^x\cdot e^{-t} = \underbrace{\left[t^x\cdot(-e^{-t})\right]_0^{\infty}}_{0} + \underbrace{\int_0^{\infty} x\,t^{x-1}\cdot e^{-t}\,dt}_{x\,\Gamma(x)}$$

per. int

$$\Gamma(1) = \int_0^\infty e^{-t}\,dt = \left[-e^{-t}\right]_0^\infty = 1$$

$$\Gamma(2) = \Gamma(1+1) = 1\cdot\Gamma(1) = 1$$

$$\Gamma(3) = \Gamma(2+1) = 2\cdot\Gamma(2) = 2$$

$$\Gamma(4) = \Gamma(3+1) = 3\cdot\Gamma(3) = 3\cdot 2$$

$$\Gamma(5) = \Gamma(4+1) = 4\cdot\Gamma(4) = 4\cdot 3\cdot 2$$

$$\boxed{\Gamma(n) = (n-1)!} \qquad \text{ha } n \text{ egész}$$

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

$$u = \sqrt{t} \qquad du = \frac{1}{2\sqrt{t}}\,dt$$

$$2\,du = \frac{dt}{\sqrt{t}}$$

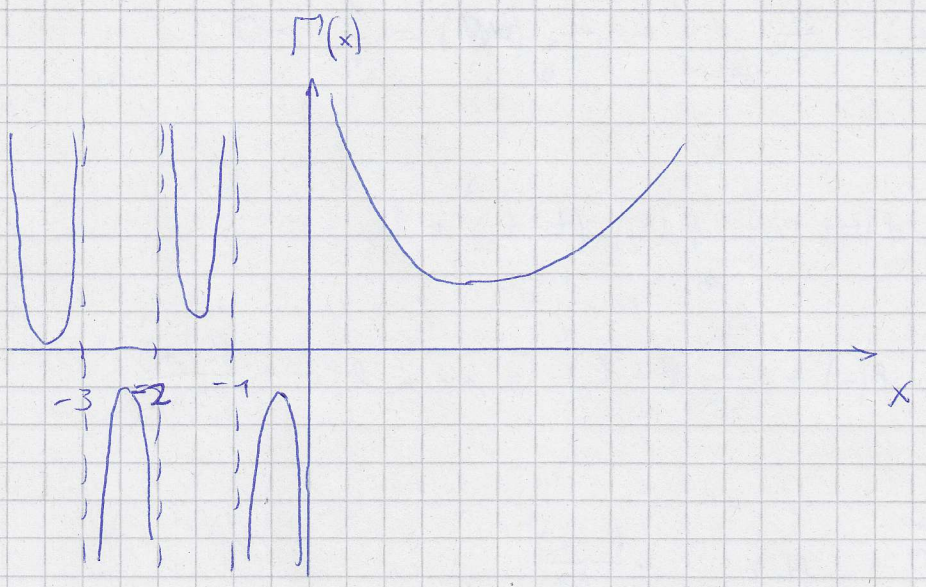
$$= 2\int_0^\infty e^{-u^2}\,du = \int_{-\infty}^{+\infty} e^{-u^2}\,du = \sqrt{\pi}$$

$$\Gamma\left(\tfrac{3}{2}\right) = \Gamma\left(\tfrac{1}{2}+1\right) = \frac{1}{2}\cdot\Gamma\left(\tfrac{1}{2}\right) = \frac{1}{2}\sqrt{\pi}$$

HF: $$\int_0^\infty x^{2\gamma}\cdot e^{-ax^2}\,dx = \frac{1}{2a^{\gamma+\frac{1}{2}}}\left(\gamma-\tfrac{1}{2}\right)!$$

faktoriális kiterjesztése: $n! = \Gamma(n+1)$

$$\int_0^\infty e^{-x^4}\,dx = \Gamma\left(\frac{1}{4}\right)$$

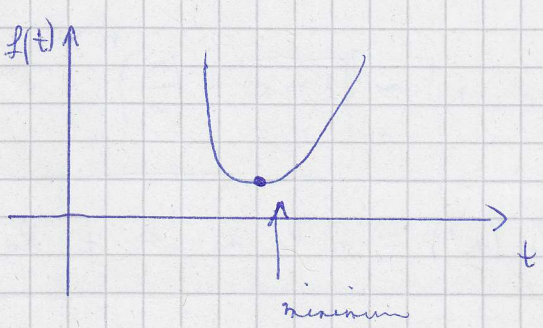


Stirling-formula

$$n! \overset{?}{=} \quad , \text{ ha } n \gg 1$$

$$n! = \Gamma(n+1) = \int_0^\infty t^n \cdot e^{-t}\,dt = \int_0^\infty e^{-t+n\ln t}\,dt =$$

$$= \int_0^\infty e^{-f(t)}\,dt \qquad f(t) = -n\ln t + t$$



minimum környékén sorfejtünk

$$f'(t) = 1 - n \cdot \frac{1}{t} = 0 \quad \Rightarrow \quad t_0 = n$$

$$f'(t_0) = 0$$

$$f''(t_0) = \left.\frac{n}{t^2}\right|_{t=t_0} = \frac{n}{t_0^2} = \frac{1}{n} > 0$$

$$f(t) \simeq f(t_0) + \frac{1}{2} f''(t_0) \cdot (t - t_0)^2 + \dots$$

$$= f(n) + \frac{1}{2n} (t - t_0)^2 = n - n \ln n + \frac{(t-n)^2}{2n}$$

$$n! \simeq \int_0^\infty e^{-f(n)} \cdot e^{-\frac{(t-n)^2}{2n}} \, dt =$$

$$= e^{n \ln n - n} \cdot \int_{-\infty}^{\infty} e^{-\frac{(t-n)^2}{2n}} \, dt \simeq e^{n \ln n - n} \cdot \int_{-\infty}^{+\infty} e^{-\frac{(t-n)^2}{2n}} \, dt$$

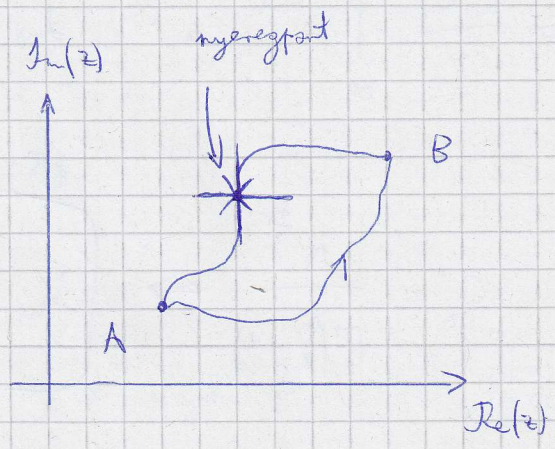
$$= e^{n \ln n - n} \cdot \sqrt{\frac{\pi}{\frac{1}{2n}}} = \underbrace{e^{n \ln n - n}}_{\left(\frac{n}{e}\right)^n} \cdot \sqrt{2\pi n}$$

$$n! \simeq \sqrt{2\pi n} \cdot \left(\frac{n}{e}\right)^n$$

$$\boxed{\ln(n!) = n \ln n - n + \ln \sqrt{2\pi n}}$$

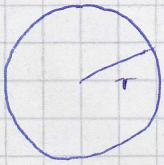
Nyeregponti integrál

$$\int_A^B e^{-f(z)}\, dz$$



n dim gömb térfogata

$$x_1^2 + \dots + x_n^2 = r^2$$



$$V_n = C_n \cdot r^n$$

gömbhéj térf. $dV_n = n\, C_n\, r^{n-1} \cdot dr$

$$\pi^{\frac{n}{2}} = \left[\int_{-\infty}^{+\infty} e^{-x^2}\, dx\right]^n = \int_{-\infty}^{+\infty} e^{\underbrace{-\left(x_1^2 + \dots + x_n^2\right)}_{r^2}} \underbrace{dx_1\, dx_2 \dots dx_n}_{n \cdot C_n\, r^{n-1}\, dr}$$

$$= \int_0^\infty e^{-r^2} \cdot n \cdot C_n \cdot r^{n-1}\, dr =$$

$$= n \cdot C_n \cdot \int_0^\infty r^{n-1} \cdot e^{-r^2}\, dr = n \cdot C_n \cdot \int_0^\infty e^{-u} \cdot u^{\frac{n-1}{2}} \cdot \frac{1}{2} u^{-\frac{1}{2}}\, du$$

$$u = r^2 \longrightarrow r = u^{\frac{1}{2}}$$

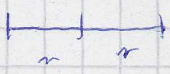
$$du = 2r\, dr \rightsquigarrow dr = \frac{du}{2r} = \frac{du}{2u^{1/2}}$$

$$= \frac{n \cdot C_n}{2} \int_0^\infty e^{-u} \cdot u^{\frac{n}{2}-1} \, du = \frac{n}{2} C_n \cdot \Gamma\left(\frac{n}{2}\right) = C_n \cdot \Gamma\left(\frac{n}{2}+1\right)$$

$$C_n = \frac{\pi^{\frac{n}{2}}}{\Gamma\left(\frac{n}{2}+1\right)} \Rightarrow \boxed{V_n = \frac{\pi^{\frac{n}{2}}}{\Gamma\left(\frac{n}{2}+1\right)} \cdot r^n}$$

Spez.: $n=1$ $\quad C_1 = \frac{\pi^{\frac{1}{2}}}{\Gamma\left(\frac{3}{2}\right)} = \frac{\sqrt{\pi}}{\frac{1}{2}\Gamma\left(\frac{1}{2}\right)} = \frac{\sqrt{\pi}}{\frac{1}{2}\sqrt{\pi}} = 2$

$\Rightarrow V_1 = 2r$



$n=2$ $\quad C_2 = \frac{\pi}{\Gamma(2)} = \pi \qquad V_2 = \pi \cdot r^2$

$n=3$ $\quad C_3 = \frac{\pi^{\frac{3}{2}}}{\Gamma\left(\frac{5}{2}\right)} = \frac{\pi^{\frac{3}{2}}}{\frac{3}{2}\Gamma\left(\frac{3}{2}\right)} = \frac{\pi\sqrt{\pi}}{\frac{3}{4}\sqrt{\pi}} = \frac{4}{3}\pi$

$$V_3 = \frac{4\pi}{3} r^3$$

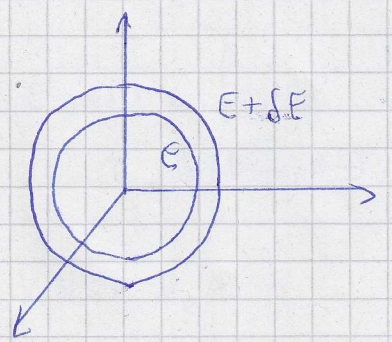
$n=4$ $\quad C_4 = \frac{\pi^2}{\Gamma(3)} = \frac{\pi^2}{2} \Rightarrow V_4 = \frac{\pi^2}{2} r^4$

1.d. g $\quad H = \sum_{i=1}^{3N} \frac{\vec{p}_i^{\,2}}{2m}$

Mikrokanonikus sokaság

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

$$S = k_B \ln \Omega$$



$$E = \sum_{i=1}^{3N} \frac{\vec{p}_i^{\,2}}{2m}$$

$$\left(\sqrt{2mE}\right)^2 = \sum_{i=1}^{3N} p_i^2$$

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

$$\Omega_0(E, V, N) = \frac{V^N}{N!\, h^{3N}} \int_{H<E} d^{3N}p = \frac{V^N}{N!\, h^{3N}} \cdot \frac{\pi^{\frac{3N}{2}}}{\left(\frac{3N}{2}\right)!} \left(\left(2mE\right)^{\frac{1}{2}}\right)^{3N} =$$

$$= \frac{V^N}{N!\, h^{3N}} \cdot \frac{\pi^{\frac{3N}{2}}}{\left(\frac{3N}{2}\right)!} (2mE)^{\frac{3N}{2}}$$

$$\Omega(E, V, N, \delta E) = \frac{d\Omega_0}{dE} \cdot \delta E = \frac{V^N}{N!\, h^{3N}} \cdot \frac{\pi^{\frac{3N}{2}}}{\left(\frac{3N}{2}\right)!} (2m)^{\frac{3N}{2}} \cdot$$

$$\cdot E^{\frac{3N}{2}-1} \cdot \frac{3N}{2} \cdot \delta E$$

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

$$\uparrow$$

$$\frac{3N}{2} \gg 1 \qquad \frac{3N}{2} \ln E \gg \ln \delta E$$

$$S = k_B \left[N \ln V + \frac{3N}{2} \ln E + \text{const}(N) \right]$$

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

$$\frac{1}{T} = \left.\frac{\partial S}{\partial E}\right|_{V,N} = \frac{3N}{2} k_B \frac{1}{E} \quad \Rightarrow \quad E = \frac{3}{2} N k_B T$$

$$E = \text{const} \\ N = \text{const} \quad \Rightarrow \quad 0 = T\,dS - p\,dV \qquad \frac{p}{T} = \left.\frac{\partial S}{\partial V}\right|_{E,N}$$

$$\frac{p}{T} = k_B N \cdot \frac{1}{V} \quad \Rightarrow \quad pV = k_B N T$$

$$\mu = ?$$

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

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

$$f(x,y,z) = 0$$

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

Termodinamika

Mikro

Izolált E, V, N rögzített

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

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

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

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

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

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

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

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

Kanonikus

Állandó: T, V, N rögzített

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

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

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

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

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

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

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

Př.: ideální plyn (nikoho)

$$S = N k_B \left[\ln \frac{V}{N} + \ln \underbrace{\left[\left(\frac{2\pi m}{h^2} \right)^{\frac{3}{2}} e^{\frac{5}{2}} \right]}_{C} + \frac{3}{2} \ln \frac{2E}{3N} \right]$$

$$\frac{1}{T} = \left. \frac{\partial S}{\partial E} \right|_{V,N} = N k_B \cdot \frac{3}{2} \cdot \frac{1}{E} \quad \Rightarrow \quad E = \frac{3}{2} N k_B T$$

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

$$\mu = -T \cdot \left. \frac{\partial S}{\partial N} \right|_{E,V} = -k_B T \cdot \frac{\partial}{\partial N} \left[\underbrace{N \ln \frac{V}{N}}_{\downarrow} + \frac{3}{2} N \ln \left(\frac{2E}{3N} \right) + N \ln C \right]$$

$$N \ln V - N \ln N$$

$$= -k_B T \left[\ln V - \ln N - N \cdot \frac{1}{N} + \frac{3}{2} \ln \left(\frac{2E}{3N} \right) + \underbrace{\frac{3}{2} N \cdot \frac{1}{\frac{2E}{3N}} \cdot \frac{2E}{3} \left(-\frac{1}{N^2} \right)}_{-\frac{3}{2}} + \ln C \right]$$

$$= -k_B T \left[\ln \frac{V}{N} - \frac{5}{2} + \frac{3}{2} \ln \frac{2E}{3N} + \underbrace{\ln C}_{\downarrow} \right]$$

$$\ln \left(\frac{2\pi m}{h^2} \right)^{\frac{3}{2}} + \frac{5}{2}$$

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

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

id. g., kanonikus

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

$$= \frac{V^N}{h^{3N} \cdot N!} \underbrace{\left[\int dp_x \, dp_y \, dp_z \cdot e^{-\beta \frac{p_x^2 + p_y^2 + p_z^2}{2m}} \right]^N}_{Z_1} =$$

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

$$Z_1 = \left(\int_{-\infty}^{+\infty} dp \cdot e^{-\beta \frac{p^2}{2m}} \right)^3 = \left(\sqrt{\frac{\pi}{\frac{\beta}{2m}}} \right)^3 = \left(\frac{2\pi m}{\beta} \right)^{\frac{3}{2}}$$

$$F = -k_B T \cdot \ln Z$$

$$= -k_B T \ln \left(\frac{V^N}{h^{3N} \cdot N!} \cdot Z_1^N \right)$$

$$E = -\frac{\partial (\ln Z)}{\partial \beta} = -N \frac{\partial (\ln Z_1)}{\partial \beta} = -N \cdot \left(-\frac{3}{2} \cdot \frac{1}{\beta} \right) = N \cdot \frac{3}{2} k_B T$$

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

$$\mu = \left. \frac{\partial F}{\partial N} \right|_{T,V} = -k_B T \cdot \frac{\partial}{\partial N} \left[\ln \left(\frac{V^N}{h^{3N} \cdot N!} \cdot Z_1^N \right) \right] =$$

$$= -k_B T \frac{\partial}{\partial N} \left(N \ln V - 3N \ln h - \ln N! + N \ln Z_1 \right)$$

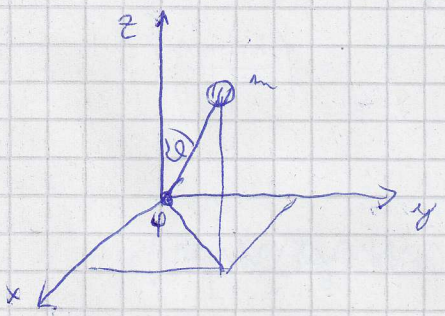
$$\ln N! \simeq N \ln N - N$$

$$\frac{\partial}{\partial N} \ln N! = \ln N + N \cdot \frac{1}{N} - 1 = \ln N$$

$$\mu = -k_B T \left[\ln V - \ln N - \frac{3}{2} \ln k^2 + \ln Z_1 \right]$$

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

Klassisker rotator



$$x = r \sin\vartheta \cos\varphi$$

$$y = r \sin\vartheta \cdot \sin\varphi$$

$$z = r \cos\vartheta$$

$$\dot{x} = r \cos\vartheta \cdot \cos\varphi \cdot \dot{\vartheta} + r \sin\vartheta (-\sin\varphi) \cdot \dot{\varphi}$$

$$\dot{y} = r \cos\vartheta \cdot \sin\varphi \cdot \dot{\vartheta} + r \sin\vartheta \cdot (\cos\varphi) \cdot \dot{\varphi}$$

$$\dot{z} = -r \cdot \sin\vartheta \cdot \dot{\vartheta}$$

$$T = \frac{1}{2} m \left(\dot{x}^2 + \dot{y}^2 + \dot{z}^2 \right) = \frac{1}{2} m r^2 \left[\cos^2\vartheta \cdot \dot{\vartheta}^2 + \sin^2\vartheta \cdot \dot{\varphi}^2 + \sin^2\vartheta \cdot \dot{\vartheta}^2 \right]$$

$$= \frac{1}{2} m r^2 \left[\dot{\vartheta}^2 + \sin^2\vartheta \cdot \dot{\varphi}^2 \right] = \frac{1}{2} \Theta \cdot \left(\dot{\vartheta}^2 + \sin^2\vartheta \cdot \dot{\varphi}^2 \right)$$

$$\Theta = m r^2$$

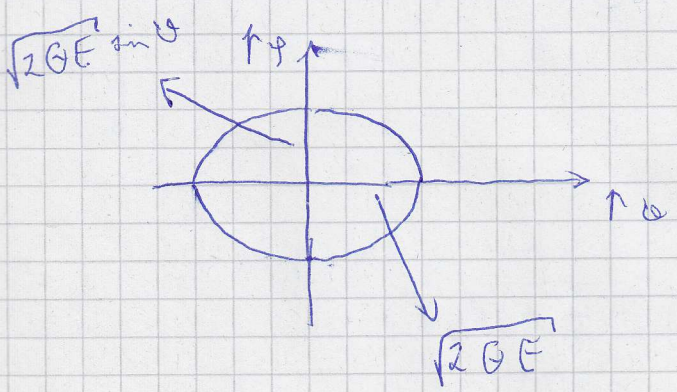
$$L = T$$

$$\uparrow_\vartheta = \frac{\partial L}{\partial \dot\vartheta} = \Theta \cdot \dot\vartheta \longrightarrow \dot\vartheta = \frac{\uparrow_\vartheta}{\Theta}$$

$$\uparrow_\varphi = \frac{\partial L}{\partial \dot\varphi} = \Theta \cdot \sin^2\vartheta \cdot \dot\varphi \longrightarrow \dot\varphi = \frac{\uparrow_\varphi}{\Theta \sin^2\vartheta}$$

$$H = T = \frac{1}{2}\Theta\left[\left(\frac{\uparrow_\vartheta}{\Theta}\right)^2 + \frac{\uparrow_\varphi^2}{\Theta^2 \sin^2\vartheta}\right] = \frac{1}{2\Theta}\left(\uparrow_\vartheta^2 + \frac{\uparrow_\varphi^2}{\sin^2\vartheta}\right)$$

$$\Omega_0(E) = \frac{1}{k^2}\int_{\mathcal{H}<E} d\varphi\, d\vartheta\, d\uparrow_\varphi\, d\uparrow_\vartheta =$$



$$E = \frac{1}{2\Theta}\left(\uparrow_\vartheta^2 + \frac{\uparrow_\varphi^2}{\sin^2\vartheta}\right)$$

$$1 = \left(\frac{\uparrow_\vartheta}{\sqrt{2\Theta E}}\right)^2 + \left(\frac{\uparrow_\varphi}{\sqrt{2\Theta E}\sin\vartheta}\right)^2$$

ellipszis

$$= \frac{1}{k^2}\int d\varphi\, d\vartheta \cdot \pi \sqrt{2\Theta E}\cdot\sqrt{2\Theta E}\sin\vartheta =$$

$$= \frac{2\pi\Theta E}{k^2}\underbrace{\int_0^{2\pi} d\varphi \int_0^{\pi} d\vartheta \sin\vartheta}_{4\pi \text{ teljes térszög}} = \frac{8\pi^2\Theta E}{k^2} = \frac{2\Theta E}{k^2}$$

Kanonikus, rotátor: súlytalan gömbirga

$$\mathcal{H} = \frac{1}{2\Theta}\left(p_\vartheta^2 + \frac{p_\varphi^2}{\sin^2\vartheta}\right)$$

$$Z = \frac{1}{h^2}\int d\varphi\, d\vartheta\, dp_\varphi\, dp_\vartheta \cdot e^{-\frac{\beta}{2\Theta}\left(p_\vartheta^2 + \frac{p_\varphi^2}{\sin^2\vartheta}\right)} =$$

↑ Gauss-int.

$$= \frac{1}{h^2}\int d\vartheta\, d\varphi \sqrt{\frac{\pi}{\frac{\beta}{2\Theta}}} \sqrt{\frac{\pi}{\frac{\beta}{2\Theta\sin\vartheta}}} = \frac{1}{h^2}\cdot\frac{2\Theta\cdot\pi}{\beta}\underbrace{\iint \sin\vartheta\, d\vartheta\, d\varphi}_{4\pi}$$

$$= \frac{8\pi^2\Theta}{h^2\beta} = \frac{2\Theta}{h^2\beta}$$

$$E = -\frac{\partial \ln Z}{\partial\beta} = -\frac{\partial}{\partial\beta}(-\ln\beta) = \frac{1}{\beta} = k_B T$$

Parabolikus potenciálú ion rendszer, kanonikus

$$H = \frac{p_x^2 + p_y^2}{2m} + \frac{1}{2}m\omega^2(x^2+y^2)$$

$$Z_1 = \frac{1}{h^2}\int dp_x\, dp_y\, dx\, dy\; e^{-\beta\left(\frac{p_x^2}{2m} + \frac{p_\vartheta^2}{2m} + \frac{1}{2}m\omega^2(x^2+y^2)\right)} =$$

$$= \frac{1}{h^2}\left(\sqrt{\frac{\pi}{\frac{\beta}{2m}}}\right)^2 \cdot \left(\sqrt{\frac{\pi}{\beta\frac{1}{2}m\omega^2}}\right)^2 = \frac{1}{h^2}\cdot\frac{\pi^2}{\beta^2}\cdot 4\cdot\frac{1}{\omega^2} = \frac{1}{h^2\beta^2\omega^2}$$

$Z_N = Z_1^N$ (figyelem)

↑ figyelem részrendszerek esetén:

$A, B \rightarrow A+B$ $\qquad Z_{A+B} = Z_A \cdot Z_B$

$$E = -\frac{\partial}{\partial \beta} \ln Z_N = -N \frac{\partial}{\partial \beta} \ln Z_1 = -N \cdot \frac{\partial}{\partial \beta}\left(-\ln \beta^2\right) =$$

$$= 2N \cdot \frac{1}{\beta} = 2N \cdot k_B T$$

$$\langle r^2 \rangle = \langle x^2 + y^2 \rangle = ?$$

$$\langle r^2 \rangle = \int r^2 \cdot \underbrace{\frac{e^{-\beta \mathcal{H}}}{Z_1}}_{\rho} d\Gamma = \frac{1}{Z_1} \int r^2 e^{-\beta\left(\frac{p_x^2 + p_y^2}{2m} + \frac{1}{2} m\omega^2 r^2\right)}$$

$$\frac{1}{h^2} \cdot dp_x \cdot dp_y \cdot \underbrace{r\, d\varphi\, dr}_{\uparrow \; dx\, dy}$$

$$Z_1 = \int \frac{dp_x\, dp_y\, dx\, dy}{h^2} e^{-\beta\left[\frac{p_x^2 + p_y^2}{2m} + \frac{1}{2} m\omega^2 (x^2 + y^2)\right]}$$

$$\frac{\partial Z_1}{\partial \omega^2} = \int \frac{dp_x\, dp_y\, dx\, dy}{h^2} \cdot e^{-\beta\left(\frac{p_x^2 + p_y^2}{2m} + \frac{1}{2} m\omega^2 (x^2 + y^2)\right)} \left(-\beta\right) \frac{1}{2} m r^2$$

$$\langle r^2 \rangle = \frac{1}{Z_1} \underbrace{\int \frac{dp_x\, dp_y\, dx\, dy}{h^2} e^{-\beta \mathcal{H}} \cdot r^2}_{-\frac{2}{m\beta} \cdot \frac{\partial Z_1}{\partial \omega^2}}$$

$$\langle x^2 \rangle = -\frac{2}{m\beta} \cdot \frac{1}{Z_1} \cdot \frac{\partial Z_1}{\partial \omega^2} = -\frac{2}{m\beta} \cdot \frac{\partial (\ln Z_1)}{\partial \omega^2} =$$

$$= \frac{2}{m\beta} \underbrace{\frac{\partial}{\partial \omega^2} \left(\ln \omega^2 \right)}_{\frac{1}{\omega^2}} = \frac{2}{m\beta\omega^2} = \frac{2 k_B T}{m \omega^2}$$

1d. g. Nagykanonikus

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

$$\downarrow$$

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

$$\downarrow$$

Euler

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

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

$$Z_1 = \int \frac{d^3 p \, d^3 q}{h^3} e^{-\beta \frac{p_x^2 + p_y^2 + p_z^2}{2m}} = \frac{V}{h^3} \left(\sqrt{\frac{\pi}{\frac{\beta}{2m}}} \right)^3 =$$

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

$$Q = \sum_{N=0}^{\infty} \frac{Z_1^N \cdot e^{\beta \mu N}}{N!} = \sum_{N=0}^{\infty} \frac{\left(Z_1 \cdot e^{\beta \mu} \right)^N}{N!} = \exp\left(Z_1 \cdot e^{\beta \mu} \right)$$

$$\Phi = -kT \ln Q = -kT \cdot Z_1 \cdot e^{\beta \mu}$$

$$N = -\left.\frac{\partial \Phi}{\partial \mu}\right|_{T,V} = kT \cdot Z_1 \cdot e^{\beta\mu} \cdot \beta = Z_1 \cdot e^{\beta\mu}$$

$$\mu = \frac{1}{\beta} \ln\left(\frac{N}{Z_1}\right) = kT \cdot \ln \frac{N}{V \cdot \left(\frac{2\pi m}{\beta \hbar^2}\right)^{\frac{3}{2}}} =$$

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

$$\Phi = -pV = -kT \cdot \underbrace{Z_1 \cdot e^{\beta\mu}}_{N} \Rightarrow pV = NkT$$

$$S = -\left.\frac{\partial \Phi}{\partial T}\right|_{V,\mu} = +\frac{\partial}{\partial T}\left(kT \cdot Z_1 \cdot e^{\beta\mu}\right)\Big|_{V,\mu} = \dots =$$

$$= \frac{5}{2} Nk + Nk \ln \frac{V}{N} + Nk \ln\left(\frac{2\pi m kT}{\hbar^2}\right)^{\frac{3}{2}}$$

$S(T,V,N)$

$$E = TS - pV + \mu N = \frac{3}{2} NkT$$

$$C_V = T \cdot \left.\frac{\partial S}{\partial T}\right|_{V,N} \qquad C_p = T \cdot \left.\frac{\partial S}{\partial T}\right|_{p,N}$$

T - p ensemble

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

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

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

↑ Euler

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

$$Y = \int_V \left(\int \frac{d^{3N}p\, d^{3N}q}{h^{3N} N!}\, e^{-\beta(\mathcal{H} + pV)} \right) dV$$

$$= \int_0^\infty \frac{V^N}{N!} \cdot \left(\frac{2\pi m kT}{h^2} \right)^{\frac{3N}{2}} \cdot e^{-\beta p V}\, dV$$

$$t = \beta p V \rightarrow dt = \beta p\, dV$$

$$= \frac{1}{\beta p} \int \frac{dt}{N!}\, e^{-t} \left(\frac{t}{\beta p} \right)^N \cdot \left(\frac{2\pi m kT}{h^2} \right)^{\frac{3N}{2}}$$

$$= \frac{1}{(\beta p)^{N+1}} \cdot \frac{1}{N!} \left(\frac{2\pi m kT}{h^2} \right)^{\frac{3N}{2}} \int_0^\infty t^N e^{-t}\, dt$$

$$\Gamma(N+1) = N!$$

$$= \left(\frac{kT}{p} \right)^{N+1} \cdot \left(\frac{2\pi m kT}{h^2} \right)^{\frac{3N}{2}}$$

$$G(T,p,N) = -kT \ln Y = -kT\left[(N+1)\ln\frac{kT}{p} + \frac{3N}{2}\ln\left(\frac{2\pi m kT}{h^2}\right)\right]$$

$$V = \left.\frac{\partial G}{\partial p}\right|_{T,N} = \left.\frac{\partial}{\partial p}\left(NkT\ln p\right)\right|_{T,N} = \frac{NkT}{p}$$

$$S = -\left.\frac{\partial G}{\partial T}\right|_{p,N} = -\left.\frac{\partial(\mu N)}{\partial T}\right|_{p,N} =$$

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

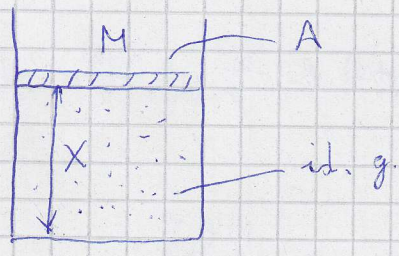
$$\mu = \frac{G}{N} = -\frac{kT}{N}\ln\left[\left(\frac{kT}{p}\right)^{N}\cdot\left(\frac{2\pi m kT}{h^2}\right)^{\frac{3N}{2}}\right]$$

$$\frac{kT}{p} \uparrow \frac{V}{N}$$

$$= -kT\left(\ln\frac{V}{N} + \ln\left(\frac{2\pi m kT}{h^2}\right)^{\frac{3}{2}}\right)$$

$$S = -N\frac{\partial}{\partial T}\left\{kT\left[\ln\frac{p}{kT} - \ln\left(\frac{2\pi m kT}{h^2}\right)^{\frac{3}{2}}\right]\right\}\Bigg|_{p,N}$$

$$E = T\cdot S - p\cdot V + \mu\cdot N = \ldots = \frac{3}{2}NkT$$



(T)

a) $E = \langle \mathcal{H} \rangle = ?$

b) $\langle X \rangle = ?$

$$\mathcal{H} = \frac{p^2}{2M} + Mg X + \sum_i \frac{1_i^2}{2m} \qquad 0 < x_i < X$$

$$0 \le y_i, z_i \le L \qquad L^2 = A$$

$$Z = \int e^{-\beta \mathcal{H}} \frac{\prod_{i=1}^{N} d^3 r_i \, d^3 q_i}{h^{3N} \cdot N!} \cdot \frac{dP \cdot dX}{h} =$$

$$= \frac{1}{h^{3N+1} N!} \cdot \left(\frac{2\pi m}{\beta}\right)^{\frac{3N}{2}} \cdot \left(\frac{2\pi M}{\beta}\right)^{\frac{1}{2}} \cdot A^N \cdot \int X^N \cdot e^{-\beta M g X} \, dX$$

$$\prod_{i=1}^{N} \int_0^L \int_0^L dy_i \, dz_i \qquad \prod_{i=1}^{N} \int_0^X dx_i$$

$$u = \beta M g X$$

$$= \frac{1}{h^{3N+1} \cdot N!} \left(\frac{2\pi m}{\beta}\right)^{\frac{3N}{2}} \cdot \left(\frac{2\pi M}{\beta}\right)^{\frac{1}{2}} \cdot A^N \cdot (\beta M g)^{-(N+1)} \int_0^\infty u^N \cdot e^{-u} \, du$$

$$M(N+1) = N!$$

$$\ln Z = -\left(\frac{3N}{2} + \frac{1}{2} + N + 1\right) \ln \beta + \text{konst}$$

$$E = \langle \mathcal{H} \rangle = -\frac{\partial \ln Z}{\partial \beta} = \left(\frac{3N}{2} + \frac{1}{2} + 1 + N\right) kT = \underbrace{\frac{5N}{2} kT}_{C_V}$$

$\langle X \rangle = ?$ $\quad pV = NkT \Rightarrow \frac{Mg}{A} A \langle X \rangle = NkT$

$$\langle X \rangle = \frac{NkT}{Mg}$$

Másik megoldás:

$$E = \langle \mathcal{H} \rangle = \left\langle \frac{p^2}{2M} \right\rangle + Mg\langle X \rangle + \sum_i \frac{\langle p_i^2 \rangle}{2m}$$

$$= \frac{1}{2} kT + Mg\langle X \rangle + \frac{3N}{2} kT = \frac{5N}{2} kT$$

$$\langle X \rangle = \frac{NkT}{Mg}$$

Harmadik megoldás:

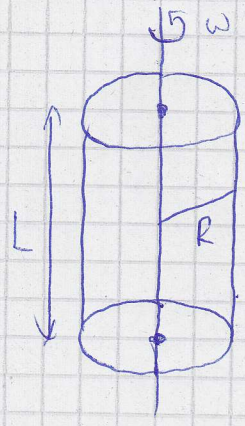
$$\langle X \rangle = \frac{\int X e^{-\beta \mathcal{H}} \, d\Gamma}{\underbrace{\int e^{-\beta \mathcal{H}} \, d\Gamma}_{Z}} = -\frac{1}{\beta} \cdot \frac{1}{Z} \frac{\partial}{\partial (Mg)} \underbrace{\int e^{-\beta \mathcal{H}} \, d\Gamma}_{Z}$$

$$= -kT \cdot \frac{1}{Z} \frac{\partial Z}{\partial (Mg)} = -kT \frac{\partial}{\partial (Mg)} (\ln Z)$$

$$= \frac{\partial F}{\partial (Mg)}$$

I-1

$$Y = \iint e^{-\beta (\mathcal{H}(r) + pV)} \, d\Gamma \, dV$$



$$\mathcal{H} = \sum_{i=1}^{N} \left(\frac{\vec{p}_i^{\,2}}{2m} - \frac{1}{2} m\omega^2 r_i^2 \right)$$

$$F = m\omega^2 r \longrightarrow U(r) = -\frac{1}{2} m\omega^2 r^2 =$$

$$= -\frac{1}{2} m\omega^2 (x^2 + y^2)$$

$$Z = \frac{Z_1^N}{N!}$$

$$Z_1 = \frac{1}{h^3} \int \underbrace{dx\,dy\,dz}_{2\pi r\,dr}\, d^3p \cdot e^{-\beta \left(\frac{\vec{p}^{\,2}}{2m} + \frac{1}{2} m\omega^2 \underbrace{(x^2+y^2)}_{\Downarrow r^2} \right)} =$$

$$= \frac{1}{h^3} \left(\frac{2\pi m}{\beta} \right)^{\frac{3}{2}} \cdot L \cdot \int_0^R 2\pi r\,dr \cdot e^{+\beta \frac{1}{2} m\omega^2 r^2}$$

$$u = \beta \frac{m\omega^2}{2} r^2 \qquad du = \beta \frac{m\omega^2}{2} 2r\,dr$$

$$= \frac{1}{h^3} \left(\frac{2\pi m}{\beta} \right)^{\frac{3}{2}} \cdot L \cdot \frac{2\pi}{\beta m\omega^2} \int_0^{u(R)} du \cdot e^u = \dots =$$

$$= \left(\frac{2\pi m}{\beta h^2} \right)^{\frac{3}{2}} \cdot \frac{2\pi L}{\beta m\omega^2} \left(e^{\beta \frac{m\omega^2 R^2}{2}} - 1 \right)$$

$$Z = \frac{Z_1^N}{N!}$$

$$E = \langle \mathcal{H} \rangle = -\frac{\partial \ln Z}{\partial \beta} = -\frac{\partial}{\partial \beta} \left(N \ln Z_1 - \underbrace{\ln N!}_{N \ln N - N} \right) =$$

$$= -\frac{\partial}{\partial \beta} N \left[\ln \beta^{-\frac{5}{2}} + \ln \left(e^{\beta \frac{m\omega^2 R^2}{2}} - 1 \right) \right] =$$

$$= \frac{5N}{2} k_B T - N \cdot \frac{\frac{m\omega^2 R^2}{2} e^{\beta \frac{m\omega^2 R^2}{2}} + \beta \frac{m\omega^2 R^2}{2}}{e^{\beta \frac{m\omega^2 R^2}{2}} - 1}$$

$$F = -k_B T \ln Z = -N k_B T \ln Z_1 + N k_B T (\ln N - 1)$$

Tetőlapra ható erő:

$$-\frac{\partial F}{\partial L} = \frac{\partial}{\partial L}\left[k_B T N \ln L + \dots\right] = \frac{k_B T N}{L}$$

Palástra ható erő:

$$\uparrow_R 2\pi R L = -\frac{\partial F}{\partial R} = \dots = N k_B T \frac{\beta m\omega^2 R e^{-\beta \frac{m\omega^2 R^2}{2}}}{e^{\beta \frac{m\omega^2 R^2}{2}} - 1}$$

$$\uparrow_R = \frac{N m\omega^2 e^{\beta \frac{m\omega^2 R^2}{2}}}{2\pi L \left(e^{\beta \frac{m\omega^2 R^2}{2}} - 1\right)}$$

Sűrűségeloszlás:

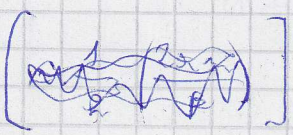
$$n(r) = N \cdot \frac{e^{\beta \frac{m\omega^2 r^2}{2}}}{\int_0^L \int_0^R e^{\beta \frac{m\omega^2 r^2}{2}} \cdot 2\pi r \, dr \, dz} =$$

$$= \frac{N}{2\pi L} \cdot \frac{\beta m\omega^2 e^{\beta \frac{m\omega^2 r^2}{2}}}{e^{\beta \frac{m\omega^2 R^2}{2}} - 1} \rightarrow \uparrow(R) = n(R) k_B T$$

$$\uparrow(r) = n(r) k_B T$$

Megj: tetőlapra ható erő

$$\int_0^R p(r)\, 2\pi r\, dr = k_B T \int_0^R n(r)\, 2\pi r\, dr =$$

$$\left[\text{  } \right] = k_B T \cdot \frac{N}{2}$$

Közelítések: $\omega \to 0$ $\frac{1}{2} m \omega^2 R^2 \ll k_B T$ (nagyon fontos)

$$E = \langle \mathcal{H} \rangle = \dots = \frac{3N}{2} k T - N k T \left(1 + \beta \frac{m \omega^2 R^2}{2}\right)$$

$$= \frac{3}{2} N k T - N \frac{m \omega^2 R^2}{2}$$

$$e^x \approx 1 + x \qquad x = \frac{\beta m \omega^2 R^2}{2} \ll 1$$

$$\omega \to \infty \qquad E = \frac{3N}{2} k T - N \frac{m \omega^2 R^2}{2} \approx -N \frac{m \omega^2 R^2}{2}$$

$$F_{Cor} = -2m \underline{\omega} \times \underline{v}$$

$$F_{cf} = m \omega^2 r$$

forgó $\quad L = m \frac{v^2}{2} + m (\underline{\omega} \times \underline{r})\, \underline{v} - U(r) \qquad U(r) = -\frac{1}{2} m \omega^2 r^2$

$$p_i = \frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial \underline{v}_i} = m v_i + m (\underline{\omega} \times \underline{r}_i)$$

$$\dot{p}_i = \frac{\partial L}{\partial \underline{r}_i} = -m (\underline{\omega} \times \underline{v})_i - \text{grad}_i\, U$$

$$m\dot{\underline{v}} = -2m\,\underline{\omega}\times\underline{v} - \operatorname{grad} U$$

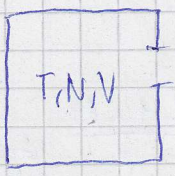
F_{Cor} , F_{φ}

$$H = \sum_i \underline{p}_i \underline{v}_i - L = \sum_i \frac{\left(\underline{p} - m\underline{\omega}\times\underline{r}\right)^2}{2m} + U(r)$$

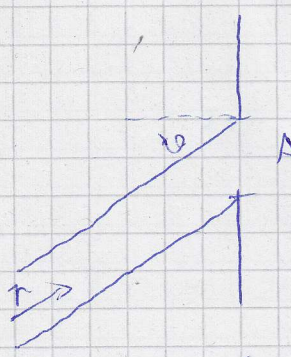
$$\underline{P} = \underline{p} - m\underline{\omega}\times\underline{r}$$

I. ZH: Március 23 Kedd $12^{\frac{15}{}}$ -

(1.)



1 fea alatt hány részecske jut ki a lyukon?



$$P_{ki} = \int d\Gamma \cdot \frac{e^{-\beta H}}{Z}\,\Theta(\text{eltűnik})$$

$$\Theta(x) = \begin{cases} 1 & , \text{ha } x \geq 0 \\ 0 & , \text{ha } x < 0 \end{cases}$$

$$d\ell = v\cos\vartheta \cdot d\tau$$

$$v = \frac{p}{m}$$

$$d\Gamma \Rightarrow \int dx\,dy\,dz = A \cdot \frac{p}{m}\cos\vartheta\,d\tau$$

$$0 < \vartheta < \frac{\pi}{2}$$

$$\frac{\pi}{2} < \vartheta < \pi$$

$$P_{hi} = \frac{\int_0^{\infty} r^2\,dr \int_0^{2\pi} d\varphi \int_0^{\frac{\pi}{2}} d\vartheta \sin\vartheta \cdot A \cdot \frac{r}{m}\cos\vartheta \cdot \delta\tau \cdot e^{-\beta\frac{r^2}{2m}}}{V\int_0^{\infty} 4\pi r^2\,dr \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\vartheta\,d\vartheta \cdot e^{-\beta\frac{r^2}{2m}}}$$

$$N_{hi} = N \cdot P_{hi}$$

$$\frac{dN_{hi}}{d\tau} = N \cdot \frac{A}{V} \cdot \frac{1}{m} \cdot \frac{2\pi \int_0^{\frac{\pi}{2}} d\vartheta \sin\vartheta\cos\vartheta \int_0^{\infty} r^3\,dr\, e^{-\beta\frac{r^2}{2m}}}{2\pi \int_0^{\infty} dr \int_0^{\pi} d\vartheta \sin\vartheta \cdot e^{-\beta\frac{r^2}{2m}}}$$

$$\int_0^{\frac{\pi}{2}} \frac{1}{2}\sin 2\vartheta\,d\vartheta = \frac{1}{2}\left[-\frac{\cos(2\vartheta)}{2}\right]_0^{\frac{\pi}{2}} = -\frac{1}{2}\frac{(-1-1)}{2} = \frac{1}{2}$$

$$\frac{dN_{hi}}{d\tau} = N \cdot \frac{A}{V} \cdot \frac{1}{m} \cdot \frac{\frac{1}{2}\int_0^{\infty} r^3\,dr \cdot e^{-\beta\frac{r^2}{2m}}}{2\int_0^{\infty} dr \cdot r^2 \cdot e^{-\beta\frac{r^2}{2m}}} =$$

$$u = \beta \cdot \frac{r^2}{2m} \qquad du = \beta \cdot \frac{2r\,dr}{2m}$$

$$= N \cdot \frac{A}{V} \cdot \frac{1}{m} \cdot \frac{1}{4} \cdot \frac{\frac{m}{\beta}\int_0^{\infty} \left(\frac{2m}{\beta}\right) u \cdot e^{-u}\,du}{\sqrt{\frac{2m}{\beta}}\int_0^{\infty} u^{\frac{1}{2}} e^{-u}\,du} =$$

$$= N \cdot \frac{A}{nV} \sqrt{\frac{m}{\beta}} \frac{1}{2\sqrt{2}} \frac{\Gamma(2)}{\Gamma\left(\frac{3}{2}\right)} = \dots = N \cdot \frac{A}{V} \sqrt{\frac{h^2 \beta}{2\pi m}} =$$

$\Gamma(2) = 1! = 1$

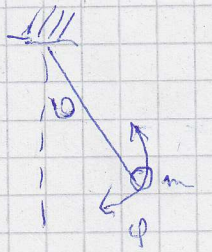
$\Gamma\left(\frac{3}{2}\right) = \frac{1}{2}\sqrt{\pi}$

$$= \frac{N}{V} \cdot A \sqrt{\frac{V}{N} \frac{h^2}{2\pi m}}$$

② Gömbinga

$$H = \frac{1}{2ml^2} \left(p_\vartheta^2 + \frac{p_\varphi^2}{\sin^2 \vartheta} \right) + mgl(1 - \cos\vartheta)$$

$\Theta = ml^2$



$$Z = \frac{1}{h^2} \int dr_\varphi \, dr_\vartheta \, d\varphi \, d\vartheta \, \sin\vartheta \, e^{-\beta H} =$$

$$= \frac{2\pi}{h^2} \int_0^\pi d\vartheta \sqrt{\frac{\pi}{\beta \cdot \frac{1}{2ml^2}}} \cdot \sqrt{\frac{\pi}{\beta \cdot \frac{1}{2ml^2 \sin^2\vartheta}}} \cdot \sin\vartheta \, e^{-\beta mgl(1-\cos\vartheta)}$$

$$= \frac{2\pi}{h^2} \cdot \frac{\pi}{\beta} \cdot 2ml^2 \int_0^\pi d\vartheta \sin\vartheta \, e^{-\beta mgl(1-\cos\vartheta)}$$

$$= \left(\frac{2\pi}{h}\right)^2 \cdot \frac{ml^2}{\beta} \cdot \frac{1}{\beta mgl} \int_0^{2\beta mgl} du \cdot e^{-u} = \left(\frac{2\pi}{h}\right)^2 \cdot \frac{l}{\beta^2 g} \cdot \left[\frac{e^{-u}}{-1} \right]_0^{2\beta mgl}$$

$u = \beta mgl(1 - \cos\vartheta) \qquad du = \beta mgl \sin\vartheta \, d\vartheta$

$$Z = \frac{1}{h^2} \cdot \frac{2\pi l^2}{\beta} \cdot \frac{1 - e^{-2\beta m g l}}{\beta m g l}$$

$$E = -\frac{\partial(\ln Z)}{\partial \beta} = -\frac{\partial}{\partial \beta}\left[-2\ln\beta + \ln\left(1 - e^{-2\beta m g l}\right)\right] =$$

$$= \frac{2}{\beta} - \frac{2 m g l^2 \, e^{-2\beta m g l}}{1 - e^{-2\beta m g l}} =$$

$$= 2 k_B T - 2 m g l \frac{e^{-2\beta m g l}}{1 - e^{-2\beta m g l}}$$

a) $T \to 0$ $\quad \beta m g l \ll 1$

~~$E = 2 k_B T - 2 m g l$~~

$$Z = \frac{1}{h^2} \cdot \frac{2\pi l^2}{\beta} \cdot \frac{2\beta m g l}{\beta m g l} = \frac{1}{h^2} \frac{2\beta m g l}{\beta m g l} = \frac{1}{h^2} \cdot \frac{2\pi l^2}{\beta}$$

$$E = -\frac{\partial(\ln Z)}{\partial \beta} = \frac{1}{\beta} = k_B T \quad : \text{ rotator}$$

b) $T \to \infty$ $\quad \beta m g l \gg 1$

$$Z \approx \frac{1}{h^2} \frac{2\pi l^2}{\beta} \frac{1}{\beta m g l} = \frac{1}{h^2} \cdot \frac{l}{g} \cdot \frac{1}{\beta^2}$$

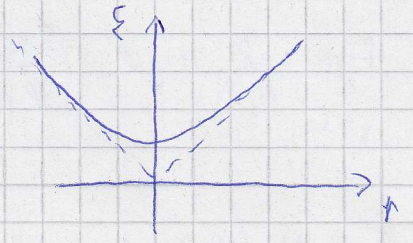
$$E = -\frac{\partial(\ln Z)}{\partial \beta} = 2 k_B T \quad \to \quad \omega = \sqrt{\frac{g}{l}}$$

Klassikus ultrarelativisztikus gáz állapotegyenlete

$$\varepsilon^2 = (m_0 c^2)^2 + (c \cdot p)^2$$

$$\downarrow$$

$$\approx 0 \quad \text{ultra}$$



$$\varepsilon = c \cdot p = c \cdot |\vec{p}|$$

$$= c \cdot \sqrt{p_x^2 + p_y^2 + p_z^2}$$

$$H = \sum_{i=1}^{N} c \cdot |\vec{p}_i| \longrightarrow Z_1 = \frac{1}{h^3} \int d^3p \, d^3r \, e^{-\beta c \sqrt{p_x^2 + p_y^2 + p_z^2}} =$$

$$= \frac{V}{h^3} 4\pi \int p^2 dp \cdot e^{-\beta p c} = \frac{4\pi V}{h^3} \int \frac{u^2}{(\beta c)^2} \cdot \frac{du}{\beta c} \cdot e^{-u} \rightarrow \Gamma(3)$$

$$u = \beta c p \qquad du = \beta c \, dp$$

$$= \frac{4\pi}{h^3} V \cdot \frac{\Gamma(3)^2}{(\beta c)^3} = \frac{8\pi V}{(h\beta c)^3} \longrightarrow Z = \frac{Z_1^N}{N!}$$

$$E = -\frac{\partial (\ln Z)}{\partial \beta} = -\frac{\partial}{\partial \beta} \left(N \ln Z_1 \right) = 3N \cdot \frac{1}{\beta} = 3N k_B T$$

$$\downarrow$$

$$\dots - 3 \ln \beta$$

$$F = -k_B T \ln Z$$

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

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

$$F = -k_B T \ln\left(\left(\frac{8\pi V}{(hpc)^3}\right)^N \cdot \frac{1}{N!}\right) =$$

$$= -k_B T \cdot N \cdot (\ln V + \dots)$$

$$p = -\left.\frac{\partial F}{\partial V}\right|_{T,N} = N \cdot k_B T \cdot \frac{1}{V}$$

$$\mu = \left.\frac{\partial F}{\partial N}\right|_{V,T} = \frac{\partial}{\partial N}\left(-k_B T \ln\left(\frac{Z_1^N}{N!}\right)\right) =$$

$$= -k_B T \cdot \frac{\partial(N \ln Z_1 - \ln N!)}{\partial N} \simeq -k_B T \ln(Z_1/N)$$

$$\ln N! = N \ln N - N$$

$$\frac{\partial}{\partial N}(\ln N!) = \ln N + N \cdot \frac{1}{N} - 1 = \ln N$$

<u>Ekvipartíció-tétel:</u>

$$\left\langle x_i \cdot \frac{\partial H}{\partial x_j} \right\rangle = k_B T \cdot \delta_{ij} \qquad x_1, x_2, \dots, x_{2f}$$

<u>Bizo.:</u>

$$\left\langle x_i \cdot \frac{\partial H}{\partial x_j} \right\rangle = \int x_i \cdot \frac{\partial H}{\partial x_j} \cdot \frac{e^{-\beta H}}{Z} \, d^{2f}x$$

parciális integrálás

$$Z = \int e^{-\beta H} \, d^{2f}x = \text{konst} \quad \rightarrow \text{ist klar}$$

$$\frac{\partial}{\partial x_j}\left(x_i \, e^{-\beta H}\right) = \delta_{ij} e^{-\beta H} + x_i \, e^{-\beta H} (-\beta) \cdot \frac{\partial H}{\partial x_j}$$

$$\int x_i \frac{\partial H}{\partial x_j} e^{-\beta H} \, dx_j = k_B T \cdot \delta_{ij} \int e^{-\beta H} \, dx_j -$$

$$- k_B T \left[x_i \cdot e^{-\beta H} \right]_{-\infty}^{+\infty}$$

$$\hookrightarrow \; e^{-\beta H}\Big|_{-\infty}^{+\infty} = 0$$

$$\Rightarrow \int x_i \frac{\partial H}{\partial x_j} e^{-\beta H} \, dx_j = k_B T \, \delta_{ij} \cdot \int e^{-\beta H} \, dx_j$$

$$\left\langle x_i \frac{\partial H}{\partial x_j} \right\rangle = \frac{1}{Z} \int x_i \frac{\partial H}{\partial x_j} e^{-\beta H} \, d^{2f}x = k_B T \cdot \delta_{ij} \, \frac{1}{Z} \cancel{\int e^{-\beta H} \, d^{2f}x}$$

$$= k_B T \cdot \delta_{ij} \cdot \qquad \square$$

Bsp.: $H = c\sqrt{p_x^2 + p_y^2 + p_z^2} = c \cdot \left(\sum_{j=1}^{3} p_j^2 \right)^{\frac{1}{2}}$

$$\left\langle p_i \frac{\partial H}{\partial p_i} \right\rangle = k_B T = \left\langle p_i \cdot c \cdot \frac{1}{2\sqrt{\cdots}} \sum_{j=1}^{3} 2 p_j \cdot \delta_{ij} \right\rangle =$$

$$= \left\langle c \cdot \frac{p_i^2}{\sqrt{\cdots}} \right\rangle = \left\langle c \cdot \frac{p_i^2}{p} \right\rangle$$

$$3 k_B T = \left\langle c \cdot \frac{p_x^2 + p_y^2 + p_z^2}{p} \right\rangle = c \cdot \langle |p| \rangle = \langle H \rangle$$

$U = \frac{1}{4} \alpha x^4$ potenciálban rezgő részecske energiája?

T hőmérsékleten 1 dim

$$H = \frac{p^2}{2m} + \frac{1}{4} \alpha x^4$$

a) $$Z = \frac{1}{h} \int dp\, dx\, e^{-\beta H} = \frac{1}{h} \int dp\, dx \cdot e^{-\beta \frac{p^2}{2m}} \cdot e^{-\beta \frac{1}{4} \alpha x^4} =$$

$$= \frac{1}{h} \cdot \sqrt{\frac{\pi}{\frac{\beta}{2m}}} \int_{-\infty}^{+\infty} dx\, e^{-\beta \frac{1}{4} \alpha x^4}$$

$$u = \beta \cdot \frac{1}{4} \alpha \cdot x^4 \qquad du = \beta \cdot \alpha \cdot x^3 \cdot dx \rightarrow dx = \frac{du}{\beta \cdot \alpha \cdot x^3}$$

$$dx = \frac{du}{\beta \cdot \alpha \cdot \left(\frac{4u}{\beta \alpha}\right)^{1/4}}$$

$$= \frac{1}{h} \cdot 2 \cdot \sqrt{\frac{2\pi m}{\beta}} \cdot (\beta \alpha)^{-\frac{1}{4}} \cdot (h)^{-\frac{3}{4}} \int_0^{\infty} u^{-\frac{3}{4}} e^{-u} du =$$

$$\Gamma\left(\frac{1}{4}\right)$$

$$= \dots = \left(\frac{2\pi m}{h^2 \beta}\right)^{1/2} \cdot \frac{1}{2} \cdot \left(\frac{4}{\beta \alpha}\right)^{\frac{1}{4}} \Gamma(1/4) \sim \beta^{-\frac{1}{2}} \beta^{-\frac{1}{4}} = \beta^{-\frac{3}{4}}$$

$$E = -\frac{\partial \ln Z}{\partial \beta} = \frac{3}{4} k_B T$$

$$\left\langle x \cdot \frac{\partial H}{\partial x} \right\rangle = k_B T = \left\langle x \cdot \alpha \cdot x^3 \right\rangle = \alpha \left\langle x^4 \right\rangle$$

$$\langle H \rangle = \left\langle \frac{p^2}{2m} \right\rangle + \frac{1}{4} \alpha \left\langle x^4 \right\rangle = \frac{1}{2} k_B T + \frac{1}{4} k_B T = \frac{3}{4} k_B T$$

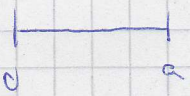
QM nikoli

$$\Omega_0(E) = \sum_{E_n < E} 1 = \sum_n \Theta(E - E_n)$$

klasicky

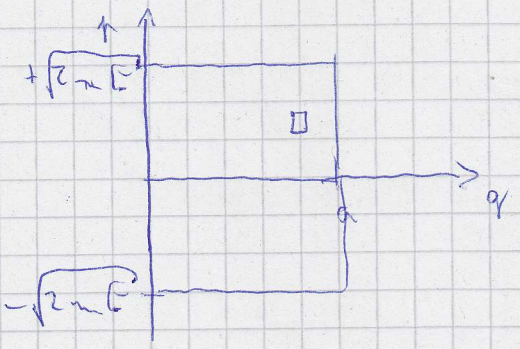
$$\Omega_0(E) = \int_{\mathcal{H}(p,q) \le E} d\Gamma \cdot 1$$

1 dim dobre



klass.

$$\mathcal{H} = \frac{p^2}{2m} \qquad p = \pm\sqrt{2mE} \qquad 0 < q < a$$



$$\Omega_0(E) = \frac{1}{R} \int_{\mathcal{H} < E} dp\, dq =$$

$$= \frac{1}{R} \cdot 2 \cdot \sqrt{2mE} \cdot a =$$

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

Isolierbox

Mikro. zeitl. r.

$E = \text{zeitl}$

$V = \text{zeitl}$

$N = \text{zeitl}$

Klass. $\Omega_0(E) = \frac{1}{h^{3N} N!} \int_{H(r,q)<E} d\Gamma \rightarrow \int d^{3N}r \, d^{3N}q$

Kv. $\Omega_0(E) = \sum_{E_n<E} 1$

$\frac{\partial \Omega_0}{\partial E} \delta E$

$S(E,V,N) = k_B \ln \Omega(E, \delta E)$ //

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

Kanonisch

$T = \text{zeitl}$

$V = \text{zeitl}$

$N = \text{zeitl}$

$Z = \frac{1}{h^{3N} N!} \int d\Gamma \, e^{-\beta H(r,q)}$ klassisch

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

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

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

Rotátor: $\mathcal{H} = \frac{1}{2\Theta}\left(\uparrow_\vartheta^2 + \frac{\uparrow_\varphi^2}{\sin^2\vartheta}\right)$

$$Z = \ldots = \frac{2\Theta}{\hbar^2\beta} \Rightarrow E = -\frac{\partial(\ln Z)}{\partial\beta} = \frac{1}{\beta} = k_B T$$

Kvantumos: $E_l = \frac{\hbar^2}{2\Theta}\cdot l(l+1) \leftarrow \hat{H} = \frac{\hat{L}^2}{2\Theta}$

$l = 0, 1, 2, \ldots$ és $\forall$ szint $2l+1$-szeresen degenerált

$m = -l, \ldots, +l$

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

$T \to 0$ alacsony hőm. / $\beta \to \infty$

$$Z \approx 1 + 3\cdot e^{-\beta\frac{\hbar^2}{2\Theta}\cdot 2}$$

$$\ln Z = \ln\left(1 + 3\cdot e^{-\beta\frac{\hbar^2}{\Theta}}\right) \approx 3\cdot e^{-\beta\frac{\hbar^2}{\Theta}}$$

$$\ln(1+x) \approx x$$

$$E = -\frac{\partial(\ln Z)}{\partial\beta} = 3\cdot e^{-\beta\frac{\hbar^2}{\Theta}}\cdot\frac{\hbar^2}{\Theta}$$

$$C = \frac{\partial E}{\partial T} = \ldots = 3\cdot\left(\frac{\hbar^2}{\Theta}\right)^2 e^{-\frac{\hbar^2}{\Theta k_B T}}\cdot\frac{1}{k_B T^2}$$

$\beta \to 0$, mogu $l^2 \gg 1$.

$$\beta \cdot \frac{\hbar^2}{2G} (l^*)^2 \approx 1$$

$$\uparrow$$

$$l(l+1)$$

$$Z \approx \sum_{l=0}^{l^*} (2l+1) \cdot 1 = (l^*+1)^2 \approx l^{*2} = \frac{1}{\beta \cdot \frac{\hbar^2}{2G}} =$$

$$= \frac{2G}{\hbar^2 \beta}$$

Lin. oscillator

$$H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2$$

Klas. $Z_1 \approx \frac{1}{h} \int dp\, dq \cdot e^{-\beta\left(\frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2\right)} =$

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

Kv. $H \psi_n = E_n \psi_n$

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \qquad n = 0, 1, 2, \ldots$$

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

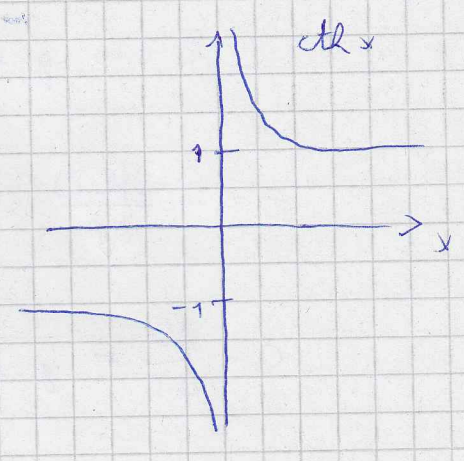
$$= e^{-\beta \frac{\hbar\omega}{2}} \sum_{n=0}^{\infty} \left(e^{-\beta\hbar\omega}\right)^n = e^{-\beta \frac{\hbar\omega}{2}} \cdot \frac{1}{1 - e^{-\beta\hbar\omega}} =$$

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

$$E = -\frac{\partial(\ln Z)}{\partial\beta} = \frac{\partial}{\partial\beta}\ln\left(2\,sh\,\frac{\beta\hbar\omega}{2}\right) =$$

$$= \frac{1}{2\cdot sh\frac{\beta\hbar\omega}{2}} \cdot 2\,ch\frac{\beta\hbar\omega}{2}\cdot\frac{\hbar\omega}{2} = \frac{\hbar\omega}{2}\,cth\,\frac{\beta\hbar\omega}{2} =$$

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



$T \to \infty,\ \beta \to 0$

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

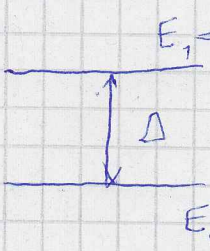
$$\frac{\hbar\omega}{\beta\hbar\omega} \sim \frac{1}{\beta} = k_B T \Rightarrow C = k_B$$

$$E = \frac{\hbar\omega}{2}\,cth\,\frac{\beta\hbar\omega}{2} \to C = \frac{\partial E}{\partial T} = k_B\left(\frac{\beta\hbar\omega}{2}\right)^2\cdot\frac{1}{sh^2\frac{\beta\hbar\omega}{2}}$$

$\beta \to \infty,\ T \to 0$

$$E \approx \hbar\omega\left(\frac{1}{2} + e^{-\beta\hbar\omega}\right) = \frac{1}{2}\hbar\omega + \frac{1}{2}\hbar\omega\cdot e^{-\beta\hbar\omega}$$

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



$\longrightarrow$ g-szeresen degenerált

$$Z = \sum_n e^{-\beta E_n} = 1 + g e^{-\beta\Delta} + \dots$$

$$\ln Z = \ln\left(1 + g e^{-\beta\Delta}\right) \qquad T \to 0 \quad (\beta \to \infty)$$

$$\ln Z \approx g \cdot e^{-\beta\Delta}$$

$$E = -\frac{\partial(\ln Z)}{\partial \beta} = g \cdot e^{-\beta\Delta} \cdot \Delta = g \cdot \Delta \cdot e^{-\frac{\Delta}{k_B T}}$$

$$C = \frac{\partial E}{\partial T} = g \cdot \Delta \cdot e^{-\frac{\Delta}{k_B T}} \cdot \frac{\Delta}{k_B T^2} =$$

$$= k_B \, g \left(\frac{\Delta}{k_B T}\right)^2 \cdot e^{-\frac{\Delta}{k_B T}}$$

$S = ?$

$$S = -\frac{\partial F}{\partial T}$$

$$F = -k_B T \ln Z \approx -k_B T \cdot g \cdot e^{-\beta\Delta}$$

$$S = \dots = k_B g \cdot e^{-\frac{\Delta}{k_B T}} + \frac{\Delta}{T} g e^{-\frac{\Delta}{k_B T}}$$

$$C = T \cdot \frac{\partial S}{\partial T} = \dots$$

$$\left\langle \frac{\partial H_\lambda}{\partial \lambda} \right\rangle = -\frac{1}{\beta} \frac{\partial}{\partial \lambda} \ln Z = \frac{\partial F_\lambda}{\partial \lambda}$$

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

$\lambda = \frac{1}{2} m \omega^2 \qquad \left\langle \frac{\partial H}{\partial \lambda} \right\rangle = \langle x^2 \rangle = \dots$

$$\left\langle \frac{\partial H}{\partial \omega} \right\rangle = m \omega \langle x^2 \rangle$$

$$\left\langle \frac{\partial H}{\partial \omega} \right\rangle = -\frac{1}{\beta} \frac{\partial}{\partial \omega} \ln \left(\frac{1}{2 \operatorname{sh} \frac{\beta \hbar \omega}{2}} \right) =$$

$$= \frac{1}{\beta} \frac{\partial}{\partial \omega} \ln \left(2 \operatorname{sh} \left(\frac{\beta \hbar \omega}{2} \right) \right) =$$

$$= \frac{1}{\beta} \cdot \frac{1}{2 \operatorname{sh} \left(\frac{\beta \hbar \omega}{2} \right)} \cdot 2 \cdot \operatorname{ch} \left(\frac{\beta \hbar \omega}{2} \right) \cdot \frac{\beta \hbar}{2} =$$

$$= \frac{\hbar}{2} \cdot \operatorname{cth} \left(\frac{\beta \hbar \omega}{2} \right)$$

$$\frac{1}{2} m \omega^2 \cdot \langle x^2 \rangle = \frac{\hbar \omega}{4} \operatorname{cth} \left(\frac{\beta \hbar \omega}{2} \right)$$

a) klasse $\left\langle \frac{\partial H_\lambda}{\partial \lambda} \right\rangle = \frac{\frac{1}{h^n} \int d^n p \, d^n q \, e^{-\beta H_\lambda}}{Z} = \frac{-\frac{1}{\beta} \frac{\partial Z}{\partial \lambda}}{Z} =$

$$= \frac{\partial F_\lambda}{\partial \lambda}$$

$$Z = \frac{1}{h^n} \int d^n p \, d^n q \, e^{-\beta H_\lambda}$$

$$\uparrow$$

$$F_\lambda = -k_B T \cdot \ln Z_\lambda$$

b) kvantum

$$\left\langle \frac{\partial \hat{H}_\lambda}{\partial \lambda} \right\rangle = \sum_i \langle \varphi_i | \frac{\partial H_\lambda}{\partial \lambda} | \varphi_i \rangle \cdot \frac{e^{-\beta E_i}}{Z}$$

$$E_i = \langle \varphi_i | \hat{H}_\lambda | \varphi_i \rangle \qquad \langle \varphi_i | \varphi_i \rangle = 1$$

$$\frac{\partial E_i}{\partial \lambda} = \left\langle \frac{\partial \varphi_i}{\partial \lambda} \middle| \underbrace{H | \varphi_i \rangle}_{E_i | \varphi_i \rangle} \right. + \langle \varphi_i | \frac{\partial \hat{H}_\lambda}{\partial \lambda} | \varphi_i \rangle + \underbrace{\langle \varphi_i | \hat{H}_\lambda}_{\langle \varphi_i | \cdot E_i} \left| \frac{\partial \varphi_i}{\partial \lambda} \right\rangle$$

$$= E_i \underbrace{\left[\left\langle \frac{\partial \varphi_i}{\partial \lambda} \middle| \varphi_i \right\rangle + \left\langle \varphi_i \middle| \frac{\partial \varphi_i}{\partial \lambda} \right\rangle \right]}_{\frac{\partial}{\partial \lambda} \langle \varphi_i | \varphi_i \rangle = 0} + \langle \varphi_i | \frac{\partial \hat{H}_\lambda}{\partial \lambda} | \varphi_i \rangle$$

$$\boxed{\frac{\partial E_i}{\partial \lambda} = \langle \varphi_i | \frac{\partial \hat{H}_\lambda}{\partial \lambda} | \varphi_i \rangle}$$

Feynman - Hellmann tétel

$$\left\langle \frac{\partial \hat{H}_\lambda}{\partial \lambda} \right\rangle = \sum_i \frac{\partial E_i}{\partial \lambda} \cdot \frac{e^{-\beta E_i}}{Z} = \frac{1}{Z} \cdot \frac{1}{-\beta} \cdot \frac{\partial Z}{\partial \lambda} =$$

$$Z = \sum_i e^{-\beta E_i}$$

$$\frac{\partial Z}{\partial \lambda} = \sum_i (-\beta) \frac{\partial E_i}{\partial \lambda} \cdot e^{-\beta E_i}$$

$$= -\frac{1}{\beta} \frac{\partial}{\partial \lambda} \ln Z_\lambda = \frac{\partial F_\lambda}{\partial \lambda}$$

□

Kvazikémiai egyensúly



molekula → rögzítési a rácsszerkezet

rácsszerkezet:	0	1	2
energia:	0	$-U$	$-2V$
degeneráció:	1	2	1

$$Q = \sum_{N,e} e^{-\beta(H_e - \mu N)} = 1 + 2\cdot e^{-\beta(-U-\mu)} + e^{-\beta(-2V-\mu\cdot 2)}$$

$$= 1 + 2e^{\beta(U+\mu)} + e^{2\beta(V+\mu)}$$

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

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

$$N = -\left.\frac{\partial \Phi}{\partial \mu}\right|_{T,V} = +k_B T \cdot \frac{\partial \ln Q}{\partial \mu} =$$

$$= +k_B T \; \frac{2e^{\beta(U+\mu)}\cdot\beta + e^{2\beta(V+\mu)}\cdot 2\beta}{1 + 2e^{\beta(U+\mu)} + e^{2\beta(V+\mu)}} =$$

$$= \frac{2\left(e^{\beta(U+\mu)} + e^{2\beta(V+\mu)}\right)}{1 + 2e^{\beta(U+\mu)} + e^{2\beta(V+\mu)}}$$

$\mu = ?$ → kémiai potenciál: ism. g

id. gaz

$$Z \approx \frac{Z_1^N}{N!} \rightarrow \ln Z = N \ln Z_1 - N \ln N + N$$

$$F = -k_B T \ln Z = -k_B T N \ln Z_1 + k_B T (N \ln N - N)$$

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

$$\mu = \left.\frac{\partial F}{\partial N}\right|_{T,V} = -k_B T \ln Z_1 + k_B T \left(\ln N + N \cdot \frac{1}{N} - 1\right) =$$

$$= -k_B T \cdot \ln Z_1 + k_B T \ln N$$

$$\beta \cdot \mu = -\ln \frac{Z_1}{N} \Rightarrow \boxed{e^{-\beta\mu} = \frac{Z_1}{N}}$$

$$Z_1 = \frac{1}{h^3} \int d^3p\, d^3q\, e^{-\beta \frac{p_x^2 + p_y^2 + p_z^2}{2m}} =$$

$$= \frac{1}{h^3} \left(\sqrt{\frac{\pi}{\beta \cdot \frac{1}{2m}}}\right)^3 = \frac{V}{h^3} \cdot \left(\frac{2\pi m}{\beta}\right)^{\frac{3}{2}}$$

$$\boxed{e^{\beta\mu} = \frac{N}{Z_1} = \frac{N}{V} \cdot \left(\frac{2\pi m \cdot k_B T}{h^2}\right)^{\frac{3}{2}} = \frac{n}{k_B T} \left(\frac{2\pi m k_B T}{h^2}\right)^{\frac{3}{2}}}$$

$$pV = N k_B T$$

Hint: $p \rightarrow 0$

$p \rightarrow \infty \quad N \approx \frac{0+2}{0+0+1} = 2 \Leftarrow e^{\beta\mu} \rightarrow \infty$