$\boxed{03.23.}$ Statfiz gyak előadás helyett

ZH:

① $$Q = \sum_{N=0}^{\infty} \int \frac{d\Gamma_N}{h^{3N} N!} e^{-\beta(\mathcal{H}-\mu N)} = \sum_{N=0}^{\infty} \frac{Z_1^N}{N!} e^{\beta\mu N} =$$

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

$$= \sum_{N=0}^{\infty} \frac{(Z_1 e^{\beta\mu})^N}{N!} = e^{Z_1 e^{\beta\mu}}$$

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

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

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

$$= \cancel{k_B T} Z_1 \cancel{\beta} e^{\beta\mu} = Z_1 e^{\beta\mu}$$

$$\mu = \frac{1}{\beta} \ln \frac{N}{Z_1} = k_B T \ln \frac{N}{Z_1}$$

$$Z_1 = \frac{1}{h^3} \int d^3p\, d^3q\, e^{-\beta \frac{p_x^2 + p_y^2 + p_z^2}{2m}} = \frac{V}{h^3} \left(\frac{\pi}{\beta \frac{1}{2m}}\right)^{3/2} =$$

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

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

② $0, \varepsilon, \varepsilon$

$$Z_1 = 1 + 2e^{-\beta\varepsilon}$$

$Z = Z_1^N$ független részecskék ($\cancel{N!}$)

$$= (1 + 2e^{-\beta\varepsilon})^N$$

$$E = -\frac{\partial \ln Z}{\partial \beta} = -N \frac{\partial \ln(1 + 2e^{-\beta\varepsilon})}{\partial \beta} = -N \frac{2e^{-\beta\varepsilon}(-\varepsilon)}{1 + 2e^{-\beta\varepsilon}} =$$

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

$T \to 0$
$\beta \to \infty$ $\quad E(T) = 2N\varepsilon e^{-\beta\varepsilon}$

$T \to \infty$
$\beta \to 0$ $\quad E(T) = \frac{2}{3} N\varepsilon$

$$S = -\frac{\partial F}{\partial T}\Big|_{V,N} \qquad F = -k_B T \ln Z$$

$$S = N k_B \left[\ln(1 + 2e^{-\beta\varepsilon}) + 2\varepsilon\beta \frac{1}{e^{\beta\varepsilon}+2} \right]$$

$T \to 0$
$\beta \to \infty$ $\quad S = N k_B \left[2e^{-\beta\varepsilon} + 2\varepsilon\beta\, e^{-\beta\varepsilon} \right] =$

$$= N k_B\, e^{-\beta\varepsilon}\, 2\left[1 + \varepsilon\beta\right] \to 0$$

$T \to \infty$
$\beta \to 0$ $\quad S = N k_B \left[\ln 3 + \frac{2}{3}\varepsilon\beta \right] \to N k_B \ln 3$

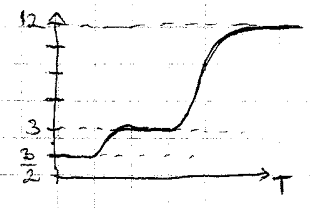
3. CH_4 $\quad n = 5 \quad$ tr: $3 \frac{1}{2} k_B T$

forg: $3 \frac{1}{2} k_B T$

rezgés: $3n - 6 = 9$ [redacted] módus $9 \cdot 2 \cdot \frac{1}{2} k_B T$

$$24 \cdot \frac{1}{2} k_B T = 12 k_B T = E$$

$c_V = 12 k_B$



4. $$\mathcal{H} = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + a(x^n + y^n + z^n)$$

$$E = -\frac{\partial \ln Z}{\partial \beta}, \qquad Z = \frac{Z_1^N}{N!},$$

$$Z_1 = \int \frac{d^3p\, d^3q}{h^3} e^{-\beta \mathcal{H}} = \left(\frac{2m\pi}{\beta}\right)^{3/2} \frac{1}{h^3} \Big(\underbrace{\int_{-\infty}^{\infty} dx\, e^{-\beta a x^n}}_{I} \Big)^3$$

$$I = 2\int_0^\infty dx\, e^{-\beta a x^n}$$

$$u = \beta a x^n \qquad x = \left(\frac{u}{\beta a}\right)^{1/n} = u^{1/n} (\beta a)^{-\frac{1}{n}}$$

$$du = n\beta a x^{n-1}\, dx = n(\beta a)\, u^{\frac{n-1}{n}} (\beta a)^{-\frac{n-1}{n}}\, dx =$$

$$= n(\beta a)^{\frac{1}{n}}\, u^{1-\frac{1}{n}}$$

$$dx = \frac{du}{n} (\beta a)^{-\frac{1}{n}}\, u^{\frac{1}{n}-1}\, du$$

$$I = 2\int_0^\infty \frac{1}{n}(\beta a)^{-\frac{1}{n}}\, u^{\frac{1}{n}-1} e^{-u}\, du = (\beta a)^{-\frac{1}{n}} \underbrace{\frac{1}{n}\Gamma\left(\frac{1}{n}\right)}_{\Gamma\left(1+\frac{1}{n}\right)}$$

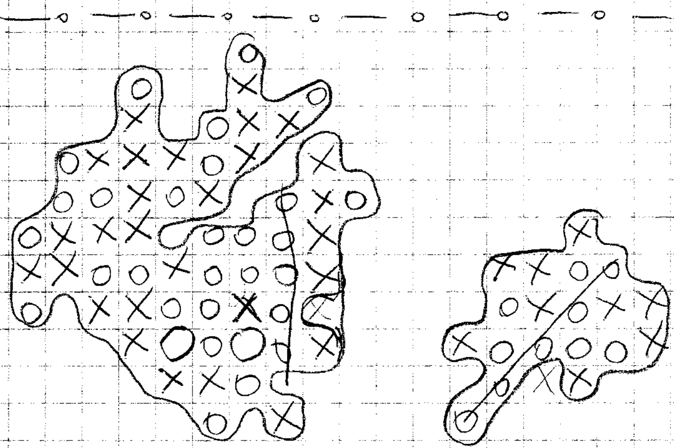
$$Z = \frac{1}{N!} Z_1^N = \frac{1}{N!}\, \beta^{-\frac{3N}{2}}\, \beta^{-\frac{3N}{n}} \cdot A$$

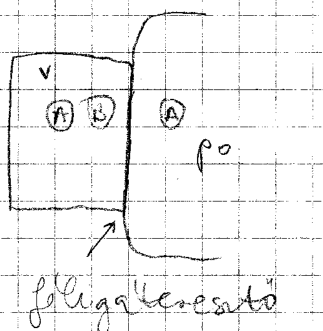
↑ nem függ β-tól

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

$$S = -\frac{\partial F}{\partial T}\bigg|_{N,V} = \frac{\partial (k_B T \ln Z)}{\partial T} = \ldots$$

$$= N k_B \left[\frac{5}{2} + \frac{3}{n} + \ln \frac{Z_1}{N}\right]$$





Vegyes sokaság

B kanonikus

A nagykanonikus

$$Z = \left(\frac{1}{N_B!} Z_{1B}^{N_B}\right)\left(\sum_{N_A=0}^{\infty} \frac{1}{N_A!} Z_{1A}^{N_A} e^{\beta \mu_A N_A}\right) =$$

↑ kanonikus ↑ nagykan.

$$= \frac{1}{N_B!} V^{N_B} \left(\frac{2\pi m_B k_B T}{h^2}\right)^{\frac{3N_B}{2}} \exp\left(\left(e^{\beta\mu_A}\right) V \left(\frac{2\pi m_A k_B T}{h^2}\right)^{3/2}\right)$$

$$Z_{1B} = V \cdot \left(\frac{2\pi m_B k_B T}{h^2}\right)^{3/2} \qquad \left(Z_{1A} = \dots \; m_A\right)$$

$$F(T, V, N_B, \mu_A) = - k_B T \cdot \ln Z$$

$$dF = - S dT - p dV + \mu_B dN_B - N_A \, d\mu_A$$

$$\langle N_A \rangle = - \left.\frac{\partial F}{\partial \mu_A}\right|_{T, V, N_B} = \cancel{\beta k_B T} \cdot e^{\beta\mu_A} \cdot V \left(\frac{2\pi m_A k_B T}{h^2}\right)^{3/2}$$

$$p = - \left.\frac{\partial F}{\partial V}\right|_{T, N_B, \mu_A} = k_B T \left(N_B \cdot \frac{1}{V} + e^{\beta\mu_A} \left(\frac{2\pi m_A k_B T}{h^2}\right)^{3/2}\right) =$$

$$= k_B T \left(\frac{N_B}{V} + \frac{\langle N_A \rangle}{V}\right) = \frac{\left(\langle N_A \rangle + N_B\right) k_B T}{V}$$

külső rész $\rightarrow$ ideális gáz p_0 nyomáson

$$\frac{N_k}{V_k} = \frac{p_0}{k_B T} = e^{\beta\mu_A} \left(\frac{2\pi m_A k_B T}{h^2}\right)^{3/2} = \frac{\langle N_A \rangle}{V}$$

$$\langle N_A \rangle = \frac{p_0 \cdot V}{k_B T}$$

$$p = p_0 + \frac{N_B k_B T}{V}$$

<u>2. mo.</u>: $\mu_A = - k_B T \left[\ln \frac{V}{N_A} + \frac{3}{2} \ln \left(\frac{2\pi m k_B T}{h^2}\right)\right] = - k_B T \left[\ln \frac{V_k}{N_k} + \frac{3}{2} \ln \frac{2\pi m_A k_B T}{h^2}\right.$

$$\cancel{\ln} \frac{V}{N_A} = \cancel{\ln} \frac{V_k}{N_k} = \left(\frac{p_0}{k_B T}\right)^{-1} \Rightarrow N_A = \frac{p_0 \cdot V}{k_B T}$$

μ_A a két oldalon megegyezik

Perturbációs számítás

klassz: $\mathcal{H} = \mathcal{H}_0 + \lambda \cdot V$

$$Z = \int d\Gamma \cdot e^{-\beta\mathcal{H}} = \int e^{-\beta\mathcal{H}_0} \cdot \underset{\sim 1-\beta\lambda V}{e^{-\beta\lambda V}} \, d\Gamma = \int e^{-\beta\mathcal{H}_0}(1-\lambda\beta V)\, d\Gamma =$$

$$= Z_0 - \lambda\beta Z_0 \frac{\int V \cdot e^{-\beta\mathcal{H}_0} d\Gamma}{Z_0} = Z_0 - \lambda\beta Z_0 \cdot \langle V\rangle_0$$

$$\langle V\rangle_0 = \int V \cdot \frac{e^{-\beta\mathcal{H}_0}}{Z_0}\, d\Gamma$$

$$F = -k_B \cdot T \cdot \ln Z = -k_B T \ln Z_0 - k_B T \cdot \ln(1-\lambda\beta\langle V_0\rangle)$$

$$\approx k_B T \ln Z_0 + \lambda \langle V\rangle_0$$

$$\boxed{F = F_0 + \lambda\langle V\rangle_0}$$

kv.: $E_n = E_n^0 + \langle n|\lambda V|n\rangle$

$$Z = \sum_n e^{-\beta E_n} = \sum_n e^{-\beta E_n^0} \cdot e^{-\beta\lambda\langle n|V|n\rangle} \approx \sum_n e^{-\beta E_n^0}(1-\lambda\beta\langle n|V|n\rangle)$$

↘ sorfejtjük

$$= Z_0 - \lambda\beta\sum_n \langle n|V|n\rangle \cdot e^{-\beta E_n^0} = Z_0(1-\lambda\beta\langle V\rangle_0)$$

Pl $\mathcal{H}_0 = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$

$$\mathcal{H} = \mathcal{H}_0 + \lambda x^4$$

$$Z_0 = \frac{1}{h}\int dp\, dx\, e^{-\beta\mathcal{H}_0} = \frac{1}{h}\sqrt{\frac{\pi \cdot 2m}{\beta}}\sqrt{\frac{2\pi}{\beta m\omega^2}} = \frac{1}{\beta\hbar\omega}$$

$$\langle x^4\rangle_0 = \frac{\frac{1}{h}\int x^4 \cdot e^{-\beta\mathcal{H}_x} dx}{\frac{1}{h}\int e^{-\beta\mathcal{H}_x} dx} \qquad \mathcal{H}_x = \frac{1}{2} m\omega^2 x^2$$

$$u = \frac{\beta m\omega^2}{2}$$

$$\langle x^4\rangle_0 = \frac{\int x^4 e^{-ux^2} dx}{\int e^{-ux^2} dx} = \frac{\frac{\partial^2}{\partial u^2}\left(\int e^{-ux^2} dx\right)}{\int e^{-ux^2} dx} = \frac{\frac{\partial^2}{\partial u^2}\sqrt{\frac{\pi}{u}}}{\sqrt{\frac{\pi}{u}}} = \ldots$$

$$\ldots = \frac{3}{(\beta m \omega^2)^2}$$

$$Z = Z_0 (1 - \lambda\beta \langle V_{\#} \rangle_0) = Z_0 (1 - \beta\lambda \langle x^4 \rangle_0) = \frac{1}{\beta\hbar\omega}\left(1 - \lambda\beta \frac{3}{(\beta m \omega^2)^2}\right)$$

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

$$\ln Z \approx \ln Z_0 - \lambda\beta \langle x^4 \rangle_0 = \ldots$$

$$\cancel{E = \frac{1}{\beta} - \lambda \langle x^4 \rangle_0 = k_B T - \frac{3\lambda}{}}$$

$$\ldots \rightarrow E = k_B T - \frac{3\lambda}{m^2 \omega^4} (k_B T)^2$$

$$C_V = k_B - \frac{6\lambda}{m^2 \omega^4} k_B^2 \cdot T$$