Azterketa egiteko baldintzak

(i) ez dago elkarrekintzarik

(ii) gas ez-endekatua da $\frac{n}{n_Q} \lll 1$ $\nRightarrow$ gas boltzmanndarra

"Kanonikoan"!!

$$\left[\; Q_N(V,T) = \frac{1}{N!}\left[Q_1(T,V)\right]^N \right.$$

$$\left[\; Q_1(T,V) = \left[\frac{V}{\lambda_T^3}\right]\cdot\left[j(T)\right] \rightarrow \right.$$

$$\boxed{j(T) = \sum_i g_i\, e^{-\varepsilon_i/k_B T}}$$

"klasikoki" ordezten dugu ez dugu ondo zenbatu behar

barneko askatasun-graduekin "partikula" bakar batenak lotutako partizio-funtzioa definituz

⇓ termodinamika

$$F_{barne} = -N\,(k_B T)\,\ln\left[j(T)\right]$$

$$\mu_{barne} = -(k_B T)\,\ln\left[j(T)\right]$$

$$S_{barne} = N\,(k_B)\left\{\ln j(T) + T\frac{\partial}{\partial T}\ln j(T)\right\}$$

$$U_{barne} = N\,k_B T^2\,\frac{\partial}{\partial T}\ln j(T)$$

$$C_{V\,barne} = N\,k_B\,\frac{\partial}{\partial T}\left\{T^2\frac{\partial}{\partial T}\ln j(T)\right\}$$

molekulen barneko egoera

nukleoak, elektroiak	] barnekoak	Mono
molekula bera, konfigurazioa	< bibrazioak, biraketak	↓ poli

poli

(a) independenteak : $j(T) = \boxed{j_{ele}(T)\cdot j_{nu}(T)}\cdot j_{bib}(T)\cdot j_{bir}(T)$ (Mono)

(b) akoplatuta daude : $j_{ele}(T)\cdot j_{nuk-bir}(T)\cdot j_{bib}(T)$

Barne-higidura duten molekulez osatutako gas-sistema

ez dago "partikulen" arteko elkarrekintzarik

$$\frac{nh^3}{(2\pi mkT)^{3/2}} \ll 1$$

$$Q_N(V,T) = \frac{1}{N!}\left[Q_1(V,T)\right]^N$$

$$Q_1(V,T) = \left\{\frac{V}{h^3}2\pi mkT)^{3/2} j(T)\right\}$$

$$j(T) = \sum_i g_i e^{-\epsilon_i/kT}$$

$$A_{\text{barne}} = -NkT \ln j$$

$$\mu_{\text{barne}} = -kT \ln j$$

$$S_{\text{barne}} = NkT \left(\ln j + T \frac{\partial}{\partial T} \ln j \right)$$

$$U_{\text{barne}} = NkT^2 \frac{\partial}{\partial T} \ln j$$

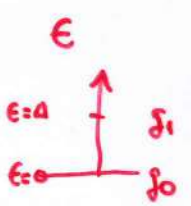
$$(C_V)_{\text{barne}} = Nk \frac{\partial}{\partial T} \left\{ T^2 \frac{\partial}{\partial T} \ln j \right\}$$

$$j(T) = j_{\text{elek}}(T)\,\boxed{j_{\text{nukl}}(T)}\,j_{\text{bibr}}(T)\,j_{\text{bira}}(T) \qquad \phi$$

$$\left[\; j(T) = \quad j_{bib}(T)\cdot j_{bir}(T)\cdot j_{bb}(T) \;\right]_{\text{ARINETA}}$$

$$j(T) = j_{\text{elek}}(T)\,\boxed{j_{\text{nukl-bira}}(T)}\,j_{\text{bibr}}(T) \qquad \phi$$

(41) $j_{elek}(T) = g_0 + g_1 e^{-\frac{\Delta}{k_B T}}$



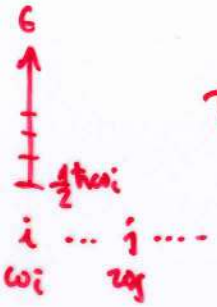
$T_e \equiv \frac{\Delta}{k_B}$

(46) $j_{bira}(T) = \sum_{l=0}^{\infty} (2l+1)\, e^{-l(l+1)\frac{\hbar^2}{2I k_B T}}$

$T_{bir} \equiv \frac{\hbar^2}{2I k_B}$

(47) $T \gg$
(20) $T \approx T_{bir}$
(22) $T \ll$

(43) $j_{bib}(T) = \prod_i \frac{e^{-\frac{\hbar\omega_i}{2k_B T}}}{1 - e^{-\frac{\hbar\omega_i}{k_B T}}}$



$T^i_{bib} \equiv \frac{\hbar\omega_i}{k_B}$