

近独立子组成的系统：把系统分成不同的子系（粒子，粒子的某个自由度，元激发）

单原子气体 $\hat{H} = \sum_i \frac{p_i^2}{2m}$ 多原子分子气体： $\hat{H} = \sum_i (\frac{p_i^2}{2M} + \frac{I_i^2}{2I} + \hbar \omega)$ 声子： $\hat{H} = E_0 + \sum_k \hbar \omega_k \times \text{制}$

注：从单粒子态到系统态时需考虑粒子全同性

Boltzmann 统计：

$W_{\text{bol}}(\{a_i\}) = \frac{N!}{\prod_i a_i!} \prod_i w_i^{a_i}$ 最可几分布 $\delta(\ln \Omega - \beta \delta E - \alpha \delta N) = 0$

$a_i = w_i e^{-\alpha - \beta \epsilon_i} = \frac{N}{Z_1} w_i e^{-\beta \epsilon_i} = N \frac{w_i e^{-\beta \epsilon_i}}{\sum_i w_i e^{-\beta \epsilon_i}}$ $N = \sum_i a_i = \frac{N}{Z_1} \sum_i w_i e^{-\beta \epsilon_i}$

→ 引入 Z ，求解系统宏观参量（ α 难求但 N 易知）

$Z = Z_1^N$ 无相互作用的定域粒子 $\Leftrightarrow Z = Z_1^N / N!$ 无相互作用的非定域粒子（无相互作用的经典粒子）

$U = - \left(\frac{\partial \ln Z}{\partial \beta} \right)_V = \sum_i a_i \epsilon_i = \sum_i w_i e^{-\alpha - \beta \epsilon_i} \epsilon_i = \frac{N}{Z_1} \sum_i w_i \epsilon_i e^{-\beta \epsilon_i}$

$S = k_B \ln Z + \frac{U}{T} - k_B \ln N!$

$F = - \frac{1}{\beta} (\ln Z - \ln N!)$ > 非定域性 $p = \frac{1}{\beta} \left(\frac{\partial \ln Z}{\partial V} \right)_\beta$ $\mu = \left(\frac{\partial F}{\partial N} \right)_{\beta, V}$

Fermion 统计：

$W_F(\{a_i\}) = \prod_i \frac{w_i!}{a_i! (w_i - a_i)!}$

$a_i = w_i / (e^{\alpha + \beta \epsilon_i} + 1)$ $\alpha = -\beta \mu$

→ 引入 Ξ ，求解系统宏观参量（ α, β 需要知道）

$\Xi = \prod_i (1 + e^{-\alpha - \beta \epsilon_i}) w_i$

$U = - \left(\frac{\partial \ln \Xi}{\partial \beta} \right)_{\alpha, V} = k_B T^2 \left(\frac{\partial \ln \Xi}{\partial T} \right)_{\alpha, V} + N \mu$

$S = k_B (\ln \Xi + \alpha N + \beta U)$

$N = - \left(\frac{\partial \ln \Xi}{\partial \alpha} \right)_{\beta, V}$

$p = \frac{1}{\beta} \left(\frac{\partial \ln \Xi}{\partial V} \right)_{\alpha, \beta}$

Boson 统计：

$W_B(\{a_i\}) = \prod_i \frac{(a_i + w_i - 1)!}{a_i! (w_i - 1)!}$

$a_i = w_i / (e^{-\alpha - \beta \epsilon_i} - 1)$

$\Xi = \prod_i (1 - e^{-\alpha - \beta \epsilon_i})^{-w_i}$

双原子气体 $\hat{H} = \frac{p_c^2}{2m} - \frac{\hbar^2}{2\mu} \alpha^2 + \frac{1}{2} \mu \omega^2 x^2 + V_0 - \frac{\hbar^2}{2I} \left[\left(\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \right)^2 + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right]$ 转动：与全同性有关

$Z_t = V \left(\frac{2\pi m}{\beta h^2} \right)^{3/2}$ $Z_v = \sum_{n=0}^{\infty} e^{-\beta \hbar \omega (n + 1/2)}$ $Z_r = \begin{cases} w_s \sum_{l=0}^{\infty} (2l+1) e^{-\beta \frac{l(l+1)\hbar^2}{2I}} & \text{(非全同, 无近似)} \\ w_s (1 + 3e^{-\frac{2\theta_r}{T}}) & \text{(非全同, 低温取前两项)} \\ w_s \int_0^{\infty} e^{-\frac{\theta_r k(k+1)}{T}} d[k(k+1)] & \text{(非全同, 高温变积分)} \\ \sum_{l=1,3,\dots} 3(2l+1) e^{-\frac{\theta_r l(l+1)}{T}} & \text{(全同, 正数)} \\ \sum_{l=0,2,\dots} 1(2l+1) e^{-\frac{\theta_r l(l+1)}{T}} & \text{(全同, 半整数)} \end{cases}$

简并划分： $\lambda \ll 1 \Rightarrow$ 弱简并，全同性不重要

$\lambda \sim 1 \Rightarrow$ 玻色强简并

$\lambda > 1 \Rightarrow$ 费米强简并

弱简并理想气体： $\ln \Xi = Z_1(T, V) F_{5/2}^{(\mp)}(\lambda)$ $\begin{cases} \text{上: Fermion} \\ \text{下: Boson} \end{cases}$

w_s ：对光子： $w_s=2$ ，对电子： $w_s=2s+1=2$

$N = Z_1(T, V) \left[\frac{\partial}{\partial \lambda} F_{5/2}^{(\mp)}(\lambda) \right] \triangleq y \quad (y = \frac{N}{Z_1(T, V)} \text{ 已知})$

BEC: $\ln \Xi = -Wg \ln(1 - e^{-\alpha}) - \int_0^\infty g(\epsilon) \ln[1 - e^{-\alpha - \beta \epsilon}] d\epsilon$

强简并玻色气体: $= -Wg \ln(1 - \lambda) + Z_1(T, V) F_{5/2}^{(T)}(\lambda)$

$N = \frac{Wg\lambda}{1-\lambda} + Z_1(T, V) F_{3/2}^{(T)}(\lambda)$ $\lambda_{max} = 1 \Rightarrow \mu = 0$

$= N_0 + N(T/T_c)$ $T = T_c$ 时 $N = Z_1(T_c, V) F_{3/2}^{(T)}(1)$

光子气体: $\mu = 0$ $\epsilon = cp$ $g(\epsilon) = 2 \int \delta(\epsilon - cp) \frac{d^3r \cdot d^3p}{h^3}$ 3D. $\frac{d^3x d^3p}{h^3}$ 1D.

$\ln \Xi = -\frac{V}{\pi^2 c^3} \int_0^\infty d\omega \omega^2 \ln(1 - e^{-\hbar\omega/\beta})$ 保留此形式, 不积分, 求 $U(T) = -(\frac{\partial \ln \Xi}{\partial \beta})_V$

强简并费米气体: $g(\epsilon) = \int \delta(\epsilon - \frac{p^2}{2m}) \frac{d^3r \cdot d^3p}{h^3}$ or other form

$\ln \Xi = 4\pi V (\frac{2m}{h^2})^{3/2} \int_0^\infty \sqrt{\epsilon} \ln(1 + e^{-\alpha - \beta \epsilon}) d\epsilon$

$= 4\pi V (\frac{2m}{h^2})^{3/2} \frac{2\beta}{3} \int_0^\infty \epsilon^{3/2} f(\epsilon) d\epsilon$

Sommerfeld 展开: $I = \int_0^\infty N(\epsilon) f(\epsilon) d\epsilon = \int_0^\mu N(\epsilon) d\epsilon + \frac{\pi^2}{6} (kT)^2 N'(\mu)$

Ising 平均场理论: $\hat{H} = -\frac{1}{2} \sum_{ij} J_{ij} \hat{S}_i \cdot \hat{S}_j - \sum_i g \mu_B H \hat{S}_i$

$= -\frac{1}{2} \sum_{ij} \hat{S}_i \hat{S}_j - g \mu_B H \sum_i \hat{S}_i$

令 $\sigma_i = \bar{\sigma} + \delta\sigma_i$ ($\bar{\sigma} = \langle \sigma_i \rangle$)

$\hat{H} = -JZ\bar{\sigma} \sum_i \sigma_i - g \mu_B H \sum_i \sigma_i + NJZ\bar{\sigma}^2/2$ Z 为最近邻格点数

$\bar{\sigma} = \tanh[\beta \mu_B g [H + JZ\bar{\sigma}/g \mu_B]]$

$\Xi = \sum_N e^{\beta \mu N} Z(\beta, N, V) = \sum_N e^{\beta \mu N} \sum_E \Omega(E, N, V) e^{-\beta E} = \sum_{N=0}^\infty \frac{1}{N!} e^{\beta \mu N} \int e^{-\beta \hat{H}} \frac{d^3r \cdot d^3p}{h^{3d}}$ (经典极限 非定域)

微正则系综的经典极限 $\Omega(E, N, V) = \begin{cases} \int \delta(E - \hat{H}) \frac{d^3r \cdot d^3p}{h^{3d}} & \text{定域} \\ \frac{1}{N!} \int \delta(E - \hat{H}) \frac{d^3r \cdot d^3p}{h^{3d}} & \text{非定域} \end{cases}$

$dS = \frac{dE}{T} + \frac{p}{T} dV - \frac{\mu}{T} dN$ 故 T, p, μ 由 S 的偏微分得到

正则系综 $Z(T, N, V) = \sum_N e^{-\beta E} = \sum_E \sum_{\{S_i | E_S = E\}} e^{-\beta E} = \sum_E \Omega(E, N, V) e^{-\beta E}$

经典极限 $Z(T, N, V) = \begin{cases} \int e^{-\beta \hat{H}} \frac{d^3r \cdot d^3p}{h^{3d}} & \text{定域} \\ \frac{1}{N!} \int e^{-\beta \hat{H}} \frac{d^3r \cdot d^3p}{h^{3d}} & \text{非定域} \end{cases}$

$\Delta N^2 = (\frac{\partial^2 \ln \Xi}{\partial \alpha^2})_{\beta, V}$

$\Delta E^2 = (\frac{\partial^2 \ln \Xi}{\partial \beta^2})_{\mu, V}$ (算 E^2)

$\bar{\alpha}_i = -\frac{\partial \ln Z}{\partial (\beta \epsilon_i)}$

$\bar{\alpha}_i = -\frac{\partial \ln \Xi}{\partial (\beta \epsilon_i)}$

$\Delta \alpha_i^2 = \frac{\partial^2 \ln \Xi}{\partial (\beta \epsilon_i)^2} = \frac{\partial^2 \ln Z}{\partial (\beta \epsilon_i)^2}$

Tips: 题目要求涨落 \Rightarrow 用系综

$N, T, V = \text{正则}$
{ 经典粒子: 几率法
{ 玻色子
{ 费米子 } 系综