Problem 1:

Consider a magnetic system whose free energy, near the critical point, scales as $\lambda^5 g(\epsilon, B) = g(\lambda^2\epsilon, \lambda^3 B)$. Compute the following critical exponents for this system: $\beta, \delta, \gamma, \alpha$.

$$\lambda^5 g(\varepsilon, B) = g(\lambda^2\varepsilon, \lambda^3 B) \qquad \lambda^5 = \mu \qquad \lambda = \mu^{1/5}$$

$$g(\varepsilon, B) = \mu^{-1}\, g(\mu^{2/5}\varepsilon, \mu^{3/5} B)$$

$$C \sim \frac{\partial^2 g}{\partial \varepsilon^2} = \mu^{-1/5}\, g(\mu^{2/5}\varepsilon, \mu^{3/5} B)$$

$$M \sim \frac{\partial g}{\partial B} = \mu^{-2/5}\, g(\mu^{2/5}\varepsilon, \mu^{3/5} B)$$

$$\chi \sim \frac{\partial^2 g}{\partial B^2} = \mu^{1/5}\, g(\mu^{2/5}\varepsilon, \mu^{3/5} B)$$

$$\boxed{\text{set} \quad \mu^{2/5}\varepsilon = 1 \rightarrow \mu\varepsilon^{5/2} = 1}$$

$$C\big|_{B=0} = \varepsilon^{1/2} g(1,0) \longrightarrow \boxed{\alpha = -1/2}$$

$$M\big|_{B=0} = \varepsilon\, g(1,0) \longrightarrow \boxed{\beta = 1}$$

$$\chi\big|_{B=0} = \varepsilon^{-1/2} g(1,0) \longrightarrow \boxed{\gamma = 1/2}$$

set $\mu^{3/5} B = 1 \rightarrow \mu B^{5/3} = 1 \qquad \mu = B^{-5/3}$

$$M\big|_{\varepsilon=0} = B^{2/3} g(0,1) \longrightarrow \boxed{\delta = 3/2}$$

Problem 2:

A system consists of N noninteracting, distinguishable two-level atoms. Each atom can exist in one of two energy states, $E_0 = 0$ or $E_1 = \varepsilon$. The number of atoms in energy level E_0 is n_0, and the number of atoms in energy level E_1 is n_1. The internal energy is given by $U = E_0 n_0 + E_1 n_1$. Calculate

- the number of microscopic states $\rightarrow$ $\boxed{\Omega(U) = \frac{N!}{n_0!\,n_1!} = \frac{N!}{(N-n_1)!\,n_1!}}$
- the entropy as a function of internal energy
- the temperature
- the heat capacity

- $U = n_1 \varepsilon \rightarrow S = k \ln \Omega(U) = k \ln \frac{N!}{(N-n_1)!\,n_1!}$

$$S = k\left[N \ln N - (N-n_1)\ln(N-n_1) - n_1 \ln n_1\right]$$

$$\boxed{S = k\left[N \ln N - \left(N - \frac{U}{\varepsilon}\right)\ln\left(N - \frac{U}{\varepsilon}\right) - \frac{U}{\varepsilon}\ln\frac{U}{\varepsilon}\right]}$$

- $\frac{1}{T} = \frac{\partial S}{\partial U} = \frac{1}{\varepsilon}\frac{\partial S}{\partial n_1} = \frac{k}{\varepsilon}\left[\ln(N-n_1) + 1 - \ln n_1 - 1\right]$

$$\boxed{\frac{1}{T} = \frac{k}{\varepsilon}\ln\left[\frac{N-n_1}{n_1}\right]}$$

- $C = \frac{\partial U}{\partial T} \Rightarrow \exp\left(\frac{\varepsilon}{kT}\right) = \frac{N\varepsilon - U}{U}$

$$U = \frac{N\varepsilon}{\left(1+\exp\left(\frac{\varepsilon}{kT}\right)\right)}$$

$$\boxed{C = \frac{\partial U}{\partial T} = -\frac{N\varepsilon}{\left(1+\exp\left(\frac{\varepsilon}{kT}\right)\right)}\left(-\frac{\varepsilon}{kT^2}\right) = \frac{N\varepsilon^2}{kT^2\left(1+\exp\left(\frac{\varepsilon}{kT}\right)\right)}}$$

Sackur-Tetrode: $S = \frac{5}{2}Nk + Nk \ln\left[\frac{N_0}{V_0 T_0^{3/2}} \frac{VT^{3/2}}{N}\right]$

Problem 3:

The entropy of an ideal gas consisting of N atoms is given by the Sackur-Tetrode equation. The equation of state is $PV = NkT$.

- Compute the enthalpy for this system and express it in terms of its natural variables.
- Compute also the chemical potential of this system.

enthalpy: $H = E + PV \rightarrow dH = TdS + VdP (+\mu dN)$

- easy answer: $E = \frac{3}{2}NkT$ (ideal gas)

$H = E + PV = \frac{5}{2}NkT$

using Sackur-Tetrode:

assume constant pressure ⇒ $dH = TdS$

constant N ⇒?

invert Sackur-Tetrode eq'n (using $PV = NkT$)

$T = \frac{P}{A_0'} \exp\left[\frac{2S}{5Nk} - 1\right]$ $\qquad A_0' = \frac{N_0 k}{V_0 T_0^{3/2}}$

$dH = \frac{P}{A_0'} \exp\left[\frac{2S}{5Nk} - 1\right] \rightarrow H = \frac{5Nk}{2} \frac{P}{A_0'} \exp\left[\frac{2S}{5Nk} - 1\right]$

$H = \frac{5NkT}{2}$

- chemical potential:

$\mu = \left.\frac{\partial H}{\partial N}\right)_{S,P}$ $\qquad H = \frac{5}{2}Nk\frac{P}{A_0'} \exp\left[\frac{2S}{5Nk} - 1\right]$ (S, P fixed!)

$\frac{\partial H}{\partial N} = \frac{5}{2}k\frac{P}{A_0'} \exp\left[\frac{2S}{5Nk} - 1\right] + \frac{5}{2}\frac{NkP}{A_0'} \exp\left[\frac{2S}{5Nk} - 1\right]\left(-\frac{2S}{5N^2k}\right)$

$= \frac{5}{2}kT + \frac{5}{2}kT\left(-\frac{2S}{5Nk}\right) = \frac{5}{2}kT - T\frac{S}{N}$

$= T\left(\frac{5}{2}k - \frac{S}{N}\right)$

Problem 4:

A system has three distinguishable molecules at rest, each with a quantized magnetic moment that can have z compoments $\pm 1/2\mu$. Find an expression for the distribution function f_i (i denotes the ith configuration), which maximizes entropy subject to the conditions $\sum_i f_i = 1$ and $\sum_i M_{i,z} = \gamma\mu$, where $M_{i,z}$ is the magnetic moment of the system in the ith configuration. For the case $\gamma = 1/2$, compute the entropy and compute f_i.

$S = -\sum_i f_i \ln f_i$ (k = 1 for simplicity)

confs.:

$\uparrow\uparrow\uparrow$ degeneracy: 1 $M_i = \frac{3}{2}\mu \rightarrow f_1$

$\uparrow\uparrow\downarrow$ degeneracy: 3 $M_i = \frac{1}{2}\mu \rightarrow f_2$

$\downarrow\downarrow\uparrow$ degeneracy: 3 $M_i = -\frac{1}{2}\mu \rightarrow f_3$

$\downarrow\downarrow\downarrow$ degeneracy: 1 $M_i = -\frac{3}{2}\mu \rightarrow f_4$

$$M_i = \frac{3}{2}\mu f_1 + \frac{3}{2}\mu f_2 - \frac{3}{2}\mu f_3 - \frac{3}{2}\mu f_4$$
$$= \frac{3}{2}\mu(f_1 + f_2 - f_3 - f_4)$$

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optimize S with constraints $\frac{3}{2}(f_1 + f_2 - f_3 - f_4) = \gamma$

Normalization: $(f_1 + 3f_2 + 3f_3 + f_4) = 1$

Result: $\Rightarrow f_1 = x^3$ $f_2 = x$ $f_3 = x^{-1}$ $f_4 = x^{-3}$

$$\frac{3}{2}\left[\frac{x^3 + x - x^{-1} - x^{-3}}{x^3 + 3x + 3x^{-1} + x^{-3}}\right] = \gamma \Rightarrow$$ to solve for x,

$\rightarrow$ x must satisfy this!

for $\gamma = \frac{1}{2}$

$$x^6 - 3x^4 - 4 = 0$$

Problem 5:

Calculate the density matrix for a free particle in a box. Assume that the wavefunction obeys periodic boundary conditions. Also take the limit of large box size.

$$\hat{H} = -\frac{\hbar^2}{2m}\partial_x^2 \qquad \text{box } L \qquad \Psi(\vec{r}) = \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}}$$

$$\hat{H}\Psi = \frac{\hbar^2 k^2}{2m}\Psi$$

$$\boxed{\rho(\vec{r};\vec{r}\,') = \sum_{\vec{k}} e^{-\beta\frac{\hbar^2 k^2}{2m}} \frac{e^{i\vec{k}(\vec{r}-\vec{r}\,')}}{V}}$$

large box size $\quad \sum_{\vec{k}} \to \frac{V}{(2\pi)^3}\int d\vec{k}$

$$\rho(\vec{r};\vec{r}\,') = \frac{\cancel{V}1}{(2\pi)^3}\int d\vec{k}\, e^{-\frac{\beta\hbar^2}{2m}k^2 + i\vec{k}\cdot(\vec{r}-\vec{r}\,')}$$

$$\boxed{\rho(\vec{r};\vec{r}\,') = \frac{1}{(2\pi)^3}\left(\frac{\pi 2m}{\beta\hbar^2}\right)^{3/2} \exp\left[-\frac{m}{2\beta\hbar^2}(\vec{r}-\vec{r}\,')^2\right]}$$

$$\int dk\, e^{-Ak^2+Bk} = \int dk\, e^{-A\left(k^2 - \frac{B}{A}k + \frac{B^2}{4A^2} - \frac{B^2}{4A^2}\right)}$$

$$= \sqrt{\frac{\pi}{A}}\, e^{\frac{B^2}{4A}}$$

Problem 6:

Consider a spin-1/2 particle in a magnetic field in the z-direction. The Hamiltonian of this system is given by $H = -\mu_B B \sigma_z$. In the representation in which σ_z is diagonal the Pauli matrices are given by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Calculate the density matrix in this representation ($\rho = \exp(-\beta H)/\mathrm{Tr}\exp(-\beta H)$). Also calculate the average $\langle \sigma_z \rangle$.

Evaluate also the density matrix in the representation which makes σ_x diagonal.

$$\boxed{\rho = \begin{pmatrix} \exp(-\beta B\mu_B) & 0 \\ 0 & \exp(\beta B\mu_B) \end{pmatrix} \frac{1}{2\cosh \beta B \mu_B}}$$

$$\boxed{\langle \sigma_z \rangle = -\frac{2\sinh(\beta B\mu_B)}{2\cosh(\beta B\mu_B)} = -\tanh(\beta B\mu_B)}$$

$$\langle \sigma_z \rangle = \mathrm{Tr}\, \rho\, \sigma_z = \frac{1}{2\cosh(\beta B\mu_B)} \begin{pmatrix} \exp(-\beta B\mu_B) & 0 \\ 0 & \exp(\beta B\mu_B) \end{pmatrix} * \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$= -\tanh(\beta B\mu_B)$$

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} A \\ B \end{pmatrix} \Rightarrow \begin{pmatrix} B \\ A \end{pmatrix} = \begin{pmatrix} A \\ B \end{pmatrix} \rightarrow \begin{pmatrix} A \\ B \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = -\begin{pmatrix} A \\ B \end{pmatrix} \Rightarrow \begin{pmatrix} B \\ A \end{pmatrix} = \begin{pmatrix} -A \\ -B \end{pmatrix} \rightarrow \begin{pmatrix} A \\ B \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$\text{matrix}: U = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix}$$

$$\rho \rightarrow U \rho U = \begin{pmatrix} \cosh \beta B\mu_B & -\sinh \beta B\mu_B \\ -\sinh \beta B\mu_B & \cosh \beta B\mu_B \end{pmatrix}$$