Física Estadística I
Tarea 02: Mecánica Estadística Clásica

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Nombre del Estudiante: ______________________________

Problema 1 *N three-dimensional harmonic oscillators*

For a collection of N three-dimensional quantum harmonic oscillators of frequency ω and total energy E, find that the number of microstates Ω, entropy S, and the temperature T are given by:

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\begin{aligned}
\Omega(E,N) &= \frac{(E/\hbar\omega + 3N/2 - 1)!}{(3N-1)!\,(E/\hbar\omega - 3N/2)!},\\
S(E,N) &= Nk_B\left[-3\ln 3 + \left(\frac{E}{N\hbar\omega}+\frac{3}{2}\right)\ln\left(\frac{E}{N\hbar\omega}+\frac{3}{2}\right) - \left(\frac{E}{N\hbar\omega}-\frac{3}{2}\right)\ln\left(\frac{E}{N\hbar\omega}-\frac{3}{2}\right)\right],\\
T &= \frac{\hbar\omega}{k_B}\left[\ln\frac{(E/N\hbar\omega + 3/2)}{(E/N\hbar\omega - 3/2)}\right]^{-1}.
\end{aligned}
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Problema 2 *Classical spin system*

1. We have a system of three classical non-interacting spins that can be aligned up $\uparrow$, or down $\downarrow$. The spins are under the influence of an applied magnetic field towards the down direction. Such field gives an ϵ energy for the $\uparrow$ configuration, and an $-\epsilon$ energy for the $\downarrow$ configuration. Using the microcanonical ensemble, obtain the probability of the following configurations,

   (a) ($\downarrow\uparrow\uparrow$), if the total energy is ϵ.

   (b) ($\downarrow\downarrow\downarrow$), if the total energy is ϵ.

   (c) ($\downarrow\downarrow\downarrow$), if the total energy is -3ϵ.

   Where the probability is defined as:

   $$P = \frac{\text{possible cases}}{\text{total cases}}.$$

2. Now, using the canonical ensemble, find the probability of two configurations: ($\uparrow\uparrow\uparrow$) and ($\downarrow\downarrow\downarrow$), which we are calling $P_{\uparrow\uparrow\uparrow}$ and $P_{\downarrow\downarrow\downarrow}$, respectively. Analyze the ratio $P_{\uparrow\uparrow\uparrow}/P_{\downarrow\downarrow\downarrow}$ on the following cases,

(a) $T = \epsilon/k_B$,
(b) $T = 0$,
(c) $T \to \infty$.

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Problema 3 *Zipper problem*

A zipper has N links, each link has a state in which it is closed with energy 0 and a state in which it is open with energy ϵ. We require that the zipper only unzip from one side (say from the left) and that the n link can only open if all links to the left of it $(1, 2, \ldots, n-1)$ are already open.

1. Find that the canonical partition function is:
$$Z(T, V, N) = \frac{1 - e^{-\beta\epsilon(N+1)}}{1 - e^{-\beta\epsilon}}.$$
2. Show that the average number of open links $\langle n_a \rangle$ is given by:
$$\langle n_a \rangle = \frac{e^{-\beta\epsilon}}{1 - e^{-\beta\epsilon}} - \frac{(N+1)e^{-\beta\epsilon(N+1)}}{1 - e^{-\beta\epsilon(N+1)}}.$$
3. Obtain $\langle n_a \rangle$ for low-temperature ($k_B T \ll \epsilon$) and high-temperature ($k_B T \gg \epsilon$) limits:
$$\begin{aligned} &\text{if} \quad k_B T \ll \epsilon \quad \Rightarrow \quad \langle n_a \rangle \approx e^{-\beta\epsilon}, \\ &\text{if} \quad k_B T \gg \epsilon \quad \Rightarrow \quad \langle n_a \rangle \approx N/2. \end{aligned}$$

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Problema 4 *N harmonic oscillators in $1D$*

For a collection of N harmonic oscillators in $1D$ of frequency ω, discussing the system:

1. Classically, find that the canonical partition function, and the entropy are given by:
$$\begin{aligned} Z(T, V, N) &= \left(\frac{k_B T}{\hbar\omega}\right)^N, \\ S(T, V, N) &= N k_B \left[\ln\left(\frac{k_B T}{\hbar\omega}\right) + 1\right], \\ S(E, V, N) &= N k_B \left[\ln\left(\frac{E}{N\hbar\omega}\right) + 1\right]. \end{aligned}$$
2. Quantum mechanically, obtain also the canonical partition function, and the entropy, described as:
$$\begin{aligned} Z(T, V, N) &= \left[\frac{1}{2\mathrm{Sinh}\left(\hbar\omega/2k_B T\right)}\right]^N, \\ S(T, V, N) &= N k_B \left[\frac{\hbar\omega/k_B T}{e^{\hbar\omega/k_B T} - 1} - \ln\left(1 - e^{-\hbar\omega/k_B T}\right)\right], \\ S(E, V, N) &= N k_B \left[\left(\frac{E}{N\hbar\omega} + \frac{1}{2}\right)\ln\left(\frac{E}{N\hbar\omega} + \frac{1}{2}\right) - \left(\frac{E}{N\hbar\omega} - \frac{1}{2}\right)\ln\left(\frac{E}{N\hbar\omega} - \frac{1}{2}\right)\right]. \end{aligned}$$

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Problema 5 *Dipole interaction*

Consider a pair of dipoles $\boldsymbol{\mu}$ and $\boldsymbol{\mu}'$ (could be electric or magnetic), oriented on the directions (θ, ϕ) and (θ', ϕ'), respectively. The distance R between their centers is assumed fixed. Their potential energy in this orientation is given by,

$$U = -\frac{\mu\mu'}{R^3}\left[2\text{Cos}\theta\text{Cos}\theta' - \text{Sin}\theta\text{Sin}\theta'\text{Cos}(\phi - \phi')\right],$$

Now, consider this pair of dipoles to be in thermal equilibrium. Show that the magnitude of the mean force between these dipoles, at high temperature, is given by:

$$\langle F\rangle = \frac{2(\mu\mu')^2}{k_B T R^7}.$$

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Problema 6 *Megacanonical ensemble*

Consider a statistical ensemble, similar to the macrocanonical one, where we allow it to interchange energy and volume, instead of particles, and we call it *megacanonical* ensemble. The number of particles N is constant, and the total energy E_t as well as the total volume V_t are fixed.

1. Find that the probability expression $P_{r,s}$ and the corresponding partition function $\mathcal{W}$ on this particular ensemble are:

$$P_{r,s} = \frac{e^{-\beta(E_s + pV_r)}}{\sum_{r,s} e^{-\beta(E_s+pV_r)}}, \quad \mathcal{W} = \sum_{r,s} e^{-\beta(E_s+pV_r)}.$$

2. Identify that the thermodynamic potential with which our partition function relates is the Gibbs free-energy, and find that the relationship is given by:

$$G(T,p,N) = -k_B T \ln \mathcal{W}(T,p,N).$$

3. Obtain the expressions for the average volume $\langle V\rangle$ and the average energy $\langle E\rangle$ from the partition function:

$$\langle V\rangle = -\frac{1}{\beta}\frac{\partial}{\partial p}\ln\mathcal{W}\bigg|_{T,N}, \quad \langle E\rangle = -\frac{\partial}{\partial\beta}\ln\mathcal{W}\bigg|_{p,N} + \frac{p}{\beta}\frac{\partial}{\partial p}\ln\mathcal{W}\bigg|_{T,N}.$$

4. Calculate the volume fluctuation σ_V^2 and the energy fluctuation $\sigma_E^2 = \langle E^2\rangle - \langle E\rangle^2$:

$$\sigma_V^2 = \langle V^2\rangle - \langle V\rangle^2 = -k_B T\,\frac{\partial\langle V\rangle}{\partial p}\bigg|_{T,N} = k_B T V \kappa_T,$$

$$\sigma_E^2 = \langle E^2\rangle - \langle E\rangle^2 = k_B T^2\,\frac{\partial\langle E\rangle}{\partial T}\bigg|_{V,N} - k_B T\,\frac{\partial\langle V\rangle}{\partial p}\bigg|_{T,N}\left(\frac{\partial\langle E\rangle}{\partial V}\bigg|_{T,N}\right)^2,$$

$$= k_B T^2 C_V + k_B T V\kappa_T\left(\frac{\partial\langle E\rangle}{\partial V}\bigg|_{T,N}\right)^2,$$

and show that the relative fluctuations σ_V/V and σ_E/E are inversely proportional to the square root of the size of the system.

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Problema 7 *Surface absorption*

A classical ideal gas is contained in a box of fixed volume V whose walls have N_0 absorbing sites. Each of these sites can absorb at most two particles, the energy of each absorbed particle being $-\epsilon$. Use the macrocanonical ensemble to:

1. Obtain the equation of state of the gas in the presence of the absorbing walls:

$$p = e^{\beta\mu} \left(\frac{2\pi m}{h^2}\right)^{3/2} (k_B T)^{5/2}.$$

2. Calculate the average number of free and absorbed particles:

$$\langle N_{free} \rangle = e^{\beta\mu} V \left(\frac{2\pi m k_B T}{h^2}\right)^{3/2},$$
$$\langle N_{abs} \rangle = N_0 \frac{e^{\beta(\mu+\epsilon)} + 2e^{2\beta(\mu+\epsilon)}}{1 + e^{\beta(\mu+\epsilon)} + e^{2\beta(\mu+\epsilon)}}.$$

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