Física Estadística I
Tarea 03: Mecánica Estadística Cuántica

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Problema 1 *An electron in a magnetic field*

If we have an applied magnetic field $\mathbf{B} = B\hat{z}$ (z-direction), then the Hamiltonian of an electron−spin takes the following form:

$$\hat{H} = -\mu_B B \hat{\sigma}_z.$$

In the representation that makes $\hat{\sigma}_z$ diagonal:

$$\hat{\sigma}_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad \hat{\sigma}_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \qquad \hat{\sigma}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},$$

The density matrix $\hat{\rho}$ is given by:

$$\hat{\rho} = \frac{1}{e^{\beta\mu_B B} + e^{-\beta\mu_B B}} \begin{bmatrix} e^{\beta\mu_B B} & 0 \\ 0 & e^{-\beta\mu_B B} \end{bmatrix}.$$

1. Evaluate the density matrix $\hat{\rho}$ of the electron−spin in the representation that makes $\hat{\sigma}_x$ diagonal, and show that is given by:

$$\hat{\rho}' = \frac{1}{e^{\beta\mu_B B} + e^{-\beta\mu_B B}} \begin{bmatrix} \text{Cosh}\left(\beta\mu_B B\right) & \text{Senh}\left(\beta\mu_B B\right) \\ \text{Senh}\left(\beta\mu_B B\right) & \text{Cosh}\left(\beta\mu_B B\right). \end{bmatrix}$$

2. Show that the value $\langle \hat{\sigma}'_z \rangle$, resulting from this representation, is expressed as:

$$\left\langle \hat{\sigma}'_z \right\rangle = \text{Tgh}\left(\beta\mu_B B\right).$$

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Problema 2 *Free particle in the momentum representation*

A free particle in a box of volume $V = L^3$ and periodic boundary conditions, has a Hamiltonian given by:

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m}, \quad \text{where} \quad \hat{H}\left|\phi_{\mathbf{k}}\right\rangle = E_{\mathbf{k}}\left|\phi_{\mathbf{k}}\right\rangle \quad \forall \quad E_{\mathbf{k}} = \frac{\hbar^2\mathbf{k}^2}{2m},$$

and,

$$\phi_{\mathbf{k}} = \frac{1}{\sqrt{V}} \exp\left\{i\mathbf{k}\cdot\mathbf{r}\right\} \quad \forall \quad \left\langle \phi_{\mathbf{k}'} \middle| \phi_{\mathbf{k}} \right\rangle = \delta_{\mathbf{k}'\mathbf{k}}.$$

1. Demonstrate that the canonical density matrix in the momentum representation is given by:

$$\langle \phi_{\mathbf{k}'} | \hat{\rho} | \phi_{\mathbf{k}} \rangle = \frac{\lambda^3}{V} \exp\left\{ -\frac{\beta \hbar^2 \mathbf{k}^2}{2m} \right\} \delta_{\mathbf{k}'\mathbf{k}} \quad \forall \;\; \lambda = \left(\frac{h^2}{2m\pi k_B T} \right)^{1/2}.$$

2. Show that the average Hamiltonian for the system, in the momentum representation, using the definition $\langle \hat{H} \rangle = \mathrm{Tr}(\hat{\rho}\hat{H})$, is:

$$\langle \hat{H} \rangle = \frac{3}{2} k_B T.$$

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Problema 3 *Density matrix of a harmonic oscillator*

For an harmonic oscillator, with energy eigenvalues $E_n = \hbar\omega(n + 1/2)$, calculate the density matrix in the energy representation, and show that is:

$$\rho_{mn} = 2\mathrm{Senh}\left(1/2 \beta\hbar\omega\right) \exp\left\{ -\beta\hbar\omega \left(n + 1/2\right) \right\} \delta_{mn} \quad \forall \quad n = 0, 1, 2, \ldots.$$

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