DESY Theory Group, Hamburg

Tutorials for the Lecture

Quantum Mechanics II

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Prof. Dr. J. Reuter
(Bldg. 2a/304), 3895
P. Bredt/F. Fabry; B. Richard; S. van Thurenhout; T. Wening;

Tutorial 5

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Home Exercise 13 Bose and Fermi distributions

In the lecture it is shown that the density operator of the grand canonical ensemble is the one that maximizes the entropy functional for a quantum mechanical many-body system under the boundary condition of a given energy and particle number expectation value. The corresponding Lagrange multipliers are the (inverse) temperature, $\beta = 1/(k_B T)$, and the chemical potential, μ. The grand canonical density operator is:

$$\hat{\rho}_{\text{gc.}} = \frac{1}{\mathcal{Z}_{\text{gc.}}} \exp\left(-\beta \sum_j (\epsilon_j - \mu)\hat{n}_j\right), \qquad \mathcal{Z}_{\text{gc.}} = \text{Tr}\left[\exp\left(-\beta \sum_j (\epsilon_j - \mu)\hat{n}_j\right)\right] \qquad . \tag{1}$$

The trace, $\text{Tr} \equiv \text{Tr}_{\mathcal{F}}$ is a trace over the full Fock space, $\mathcal{F}$. The particle number operator $\hat{n}_j$ is the one for fermions or bosons, respectively:

$$\hat{n}_j = \hat{c}_j^\dagger \hat{c}_j \qquad \text{or} \qquad \hat{n}_j = \hat{b}_j^\dagger \hat{b}_j \tag{2}$$

with $\left[\hat{b}_i, \hat{b}_j^\dagger\right] = \delta_{ij}$, $\left\{\hat{c}_i, \hat{c}_j^\dagger\right\} = \delta_{ij}$, respectively. Not needed for this exercise, just for information: The quantum numbers are energies expressed by wave vectors (and spins for electrons as fermions),

$$\epsilon_j \longrightarrow \epsilon_{\vec{k},\sigma} = \frac{\hbar^2 \vec{k}^2}{2m^*} + \frac{1}{2} g^* \mu_B \sigma B \;\; \text{(electrons)} \qquad \epsilon_j \longrightarrow \epsilon_{\vec{k},\sigma} = \frac{\hbar^2 \vec{k}^2}{2m^*} \;\; \text{(bosons)}. \tag{3}$$

Wave vectors and hence energies can be assumed to be discrete, for electrons in solids in the inverse lattice, for bosons by using periodic boundary conditions in a finite volume of a box. m^* is the effective mass, μ_B the Bohr magneton, $\sigma = \pm$ the spin component of electrons, B the external magnetic field.

(a) Show that the grand canonical ensemble can be written (for electrons or bosons) as the product over (discrete) energy quantum numbers:

$$\hat{\rho}_{\text{gc.}} = \prod_j \frac{1}{\mathcal{Z}_j} \exp\left(-\beta(\epsilon_j - \mu)\hat{n}_j\right) \qquad . \tag{4}$$

(b) Determine the partition function for a single quantum number j, $\mathcal{Z}_j$ for the bosonic and fermionic case, and calculate the expectation value for the particle number in the grand canonical ensemble for the bosonic ($g_j \equiv \langle \hat{n}_j \rangle_{\hat{\rho}_{\text{gc.}}}$) and fermionic ($f_j \equiv \langle \hat{n}_j \rangle_{\hat{\rho}_{\text{gc.}}}$) cases, respectively. These are the Bose and Fermi distribution, respectively.

(c) For the fermionic case, give the total energy of the system (relatively trivial). Show that the entropy of the system, $S = -k_B \mathrm{Tr}\left[\hat{\rho_{\text{gc.}}} \ln \hat{\rho_{\text{gc.}}}\right] = -k_B \left\langle \ln \hat{\rho}_{\text{gc.}} \right\rangle$, can be expressed as

$$S = -k_B \sum_j \left[f_j \ln f_j + (1 - f_j) \ln(1 - f_j)\right] \quad . \tag{5}$$

Can you give an interpretation of the result for the entropy when you compare with its definition from information theory as $S = -k_B \sum_j p_j \ln p_j$, where p_j is the probability of state j.

(d) Show that $f(x) = \frac{1}{2}\left(1 - \tanh \frac{\beta x}{2}\right)$. Draw the Fermi distribution for $T = 0$, for finite T and for $T \to \infty$.

(e) The occupation probability for a one-particle energy level ϵ_j with energy distance to the ground state $\Delta\epsilon_j = \epsilon_j - \epsilon_0$ is given by

$$w_F(\Delta\epsilon_j; T) = f(\epsilon_j - \mu) = f(\Delta\epsilon_j - [\mu(T) - \epsilon_0]) \tag{6}$$

For the limit that the energy levels are very high, much higher than the average temperature, $\Delta\epsilon_j - [\mu(T) - \epsilon_0] = \epsilon_j - \mu \gg k_B T$, what is distribution in that limit?

(f) Calculate the energy expectation value and entropy for the case of the Bose distribution.

Repetition QM I Exercise 1 Density operator for Spin 1/2 system

Consider a system of a spin-$\frac{1}{2}$ particle. Choose a matrix representation such that the basis $\hat{\sigma}_z |\pm\rangle = \pm |\pm\rangle$, $\langle + | + \rangle = \langle - | - \rangle = 1$, $\langle + | - \rangle = 0$ given by the eigenkets of $\hat{\sigma}_z$ can be written as:

$$|+\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |-\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{7}$$

Investigate the two density operators

$$\hat{\rho}_a = \frac{1}{2}\Big(|+\rangle\langle +| + |-\rangle\langle -|\Big) \tag{8}$$

$$\hat{\rho}_b = \frac{1}{2}\Big(|+\rangle\langle +| + |-\rangle\langle -| + e^{-i\alpha}|+\rangle\langle -| + e^{i\alpha}|-\rangle\langle +|\Big). \tag{9}$$

a) Check whether the states represented by the two density operators $\hat{\rho}_a$ and $\hat{\rho}_b$ are pure or mixed. For the case a density operator describes a pure state $|\psi\rangle$ beschreibt, i.e. can be written in the form $\hat{\rho} = |\psi\rangle\langle\psi|$, find the corresponding state $|\psi\rangle$.

b) Calculate the expectation values of an arbitrary operator $\hat{A}$ for the two density operators, $\left\langle \hat{A} \right\rangle_{\hat{\rho}_a}$ and $\left\langle \hat{A} \right\rangle_{\hat{\rho}_b}$ and interpret the result

Hint: Express $\hat{A}$ the basis used above, $\hat{A} = A_{++}|+\rangle\langle +| + \ldots$, or alternatively as a matrix.