IFP
TU Wien

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2. Übung QFT für Vielteilchen-Systeme

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1. Bose-distribution function

1+3 Punkte

Consider a system of N non-interacting harmonic oscillators with frequencies ω_i, i.e.,

$$\hat{\mathcal{H}} = \sum_{i=1}^{N} \hat{\mathcal{H}}_i = \sum_{i=1}^{N} \hbar\omega_i(\hat{n}_i + \frac{1}{2}) \quad \hat{n}_i = \hat{a}_i^\dagger \hat{a}. \tag{1}$$

a) Z, the so called partition function ("Zustandssumme"), is defined as $Z = \mathrm{Tr}\left(e^{-\beta\hat{\mathcal{H}}}\right)$. Show that the total energy of a system, given as $\langle\hat{\mathcal{H}}\rangle$ (see exercise 1), can be calculated as

$$E = \langle\hat{\mathcal{H}}\rangle = -\frac{\partial \ln Z}{\partial \beta}. \tag{2}$$

b) Calculate the partition function Z for the Hamiltonian of Eq. (1) and show that the total energy can be written as

$$E = E_0 + \sum_{i=1}^{N} \hbar\omega_i b(\omega_i), \tag{3}$$

where b is the Bose-distribution function

$$b(\omega_i) = \frac{1}{e^{\beta\hbar\omega_i} - 1}, \tag{4}$$

and E_0 is the zero-point energy of N harmonic oscillators.
Hints: Since the oscillators are non-interacting the eigenstates of the system (which one uses for calculating the trace), can be written as the product of one-oscillator eigenstates, i.e., $|\{n_i\}\rangle = |n_1\rangle \otimes \ldots \otimes |n_N\rangle$, where $n_i = 0 \ldots \infty$ is the occupation of the i-th oscillator.

2. Fermi-distribution function

3+3=6 Punkte*

The entropy S of a system with total energy E and N particles is given by

$$S(E,N) = -\ln W(E,N), \tag{5}$$

where (for a discrete system) $W(E,N)$ is the number of configurations for given values of E and N.
The (discrete) one-particle energy-levels ε_i (non interacting) of the system are g_i-fold degenerate ($g_i \gg 1$). For large systems ($N \gg 1$) W can be approximated by

$$W = \prod_i w_i, \tag{6}$$

where w_i is the number of possible configurations of $\bar{n}_i$ identical fermions in g_i degenerate states. Here, $\bar{n}_i$ is the (still unknown!) most probable occupation of the (g_i-fold degenerate) energy level

ε_i and $g_i > \bar{n}_i$. The $\bar{n}_i$ can be computed by finding the extremum of the entropy with respect to $\bar{n}_i$ considering the constraints

$$E = \sum_i \varepsilon_i \bar{n}_i \tag{7}$$

$$N = \sum_i \bar{n}_i. \tag{8}$$

a) Calculate w_i for a given (integer) number $\bar{n}_i$ of fermions and degeneracy g_i ($> \bar{n}_i$) of the energy level ε_i. Hint: Start considering $g_i = 2, 3, 4, \ldots$. How many possible configurations exist for $\bar{n}_i = 1, 2, 3, \ldots$ independent fermions? Finally, calculate the number of configurations for a general g_i and $\bar{n}_i$.

b) Calculate the extremum of the entropy $S = -\ln W$, with W as given in Eq. (6) with respect to $\bar{n}_i$. In order to include the constraints (7) and (8) use the Lagrange multipliers β for the energy and α for the particle number.
Hints: Make use of the Stirling formula for the factorial of a large number N:

$$\ln N! \sim N(\ln N - 1). \tag{9}$$

For further information see also Ref. 1.

[1] Kerson Huang, "Statistical Mechanics", chapter 4.3 and chapter 7.

* Bonuspoints