Advanced statistical mechanics II

(SS 16, FU Berlin)

Problem sheet 6

Due date: June 7th, 2016

Problems

17. Review of second quantization – Fermions (1+1+1+1+1+1)

Given a single particle Hilbert space $\mathcal{H}$, the Hilbert space of n fermions is $S_- \, \mathcal{H}^{\otimes n}$ where $S_- \, \mathcal{H}^{\otimes n}$ is the image of the linear anti-symmetrization operator S_-. Recall that S_- is defined via

$$S_- \, |\psi_1\rangle \, |\psi_2\rangle \dots |\psi_n\rangle = \frac{1}{\sqrt{n!}} \sum_{\sigma \in S_n} \operatorname{sign}(\sigma) \, |\psi_{\sigma(1)}\rangle \, |\psi_{\sigma(2)}\rangle \dots |\psi_{\sigma(n)}\rangle \,, \tag{1}$$

where S_n is the symmetric group (permutations) and $\operatorname{sign}(\sigma) \in \{-1, 1\}$ is the signature of the permutation σ, i.e. $\operatorname{sign}(\sigma) = 1$ iff σ can be composed of an even number of transpositions. For example we have

$$\begin{aligned} S_- \, |\psi_1\rangle \, |\psi_2\rangle \, |\psi_3\rangle = \frac{1}{\sqrt{3!}} \big(& |\psi_1\rangle \, |\psi_2\rangle \, |\psi_3\rangle - |\psi_1\rangle \, |\psi_3\rangle \, |\psi_2\rangle + |\psi_2\rangle \, |\psi_3\rangle \, |\psi_1\rangle \\ & - |\psi_2\rangle \, |\psi_1\rangle \, |\psi_3\rangle + |\psi_3\rangle \, |\psi_1\rangle \, |\psi_2\rangle - |\psi_3\rangle \, |\psi_2\rangle \, |\psi_3\rangle \big) \,. \end{aligned}$$

Now we assume $\mathcal{H}$ to be m-dimensional. In this case one says that we have n Fermions in m *modes*. In order to be able to allow for a varying particle number we define the *(Fermionic) Fock space* by

$$\mathcal{F}_- = \bigoplus_{n=0}^{m} S_- \, \mathcal{H}^{\otimes n} \quad \text{with } S_- \mathcal{H}^{\otimes 0} := S_- \mathbb{C} := \mathbb{C}. \tag{2}$$

This space is a Hilbert space with the usual inner product, so that states from different *Fock layers*, i.e., from different components of the direct sum, are orthogonal. Let $(|j\rangle)_{j=1}^{m}$ be an orthonormal basis of $\mathcal{H}$. We define

$$|n_1, n_2, \dots, n_m\rangle := S_- \, |1\rangle^{\otimes n_1} \, |2\rangle^{\otimes n_2} \dots |m\rangle^{\otimes n_m} \tag{3}$$

which is a basis for $\mathcal{F}_-$, where due to Pauli's principle $n_j \in \{0, 1\}$. Moreover, we define the *annihilation operators* c_j via

$$c_j \, |n_1, n_2, \dots, n_j, \dots, n_m\rangle = \begin{cases} (-1)^{\sum_{k<j} n_k} \, |n_1, n_2, \dots, 0, \dots, n_m\rangle & \text{if } n_j = 1 \\ 0 & \text{otherwise.} \end{cases} \tag{4}$$

The *creation operators* are defined as the adjoints of the annihilation operators and denoted by $c_j^\dagger$.

Denoting the anti-commutator of operators A and B by $\{A, B\} := AB + BA$ and the commutator by $[A, B] := AB - BA$, show the following:

a) $c_j^\dagger \, |n_1, n_2, \dots, n_j, \dots, n_m\rangle = \begin{cases} (-1)^{\sum_{k<j} n_k} \, |n_1, n_2, \dots, 1, \dots, n_m\rangle & \text{if } n_j = 0 \\ 0 & \text{otherwise.} \end{cases}$

b) $c_j^2 = (c_j^\dagger)^2 = 0$

c) $\{c_j, c_k\} = \{c_j^\dagger, c_k^\dagger\} = 0$

d) $\{c_j, c_k^\dagger\} = \delta_{j,k}$

e) $c_j^\dagger c_j \,|n_1, n_2, \dots, n_j, \dots, n_m\rangle = n_j \,|n_1, n_2, \dots, n_j, \dots, n_m\rangle$
Remark: Therefore, $\hat{N}_j := c_j^\dagger c_j$ is called *particle number operator* of the j^{th} mode.

f) $[\hat{N}_j, \hat{N}_k] = 0$

18. Quantum statistics: bosonic and fermionic distributions (1+1+1+2+1+1+3+2+2)
In Problem 9 on the 3rd sheet we considered m independent random variables, i.e., observables $M^{(j)} : \Gamma \to \mathbb{R}$ that map from a finite sample space Γ to $\mathbb{R}$. We found that the probability distribution which maximizes the Shannon entropy under the constraints

$$\langle M^{(j)} \rangle = K^{(j)} \qquad j \in 1, \dots, m, \tag{5}$$

is given by

$$p_\gamma = \mathrm{e}^{-\psi}\, \mathrm{e}^{-\lambda \cdot M_\gamma}, \tag{6}$$

where $\lambda \cdot M_\gamma = \sum_{j=1}^m \lambda_j M_\gamma^{(j)}$, λ is a vector of Lagrange multipliers and the additional Lagrange multiplier ψ depends on the $K^{(j)}$ only indirectly because it is a function of λ.

a) Conclude that for the special case $m = 1$ with $M^{(1)} = H$ the energy functional, and $K^{(1)} = E$ the energy, Eq. (6) implies that the Shannon entropy is maximized by the canonical ensemble

$$p_\gamma = \mathrm{e}^{-\beta H_\gamma} / \sum_{\gamma' \in \Gamma} \mathrm{e}^{-\beta H_{\gamma'}} \quad \forall \gamma \in \Gamma. \tag{7}$$

How is the inverse temperature β related to the Lagrange parameters?

b) Which choice for m, the $M^{(j)}$, and $K^{(j)}$ gives the grand canonical ensemble? Write down the formula for the probability vector of the grand canonical ensemble. What is the relation between the inverse temperature, the chemical potential and the Lagrange parameters?

The quantum analog of the (Shannon) entropy maximization under constraints of the form (5) is the following: Find the density matrix $\rho \in \mathcal{S}(\mathcal{H})$ that maximizes the von Neumann entropy

$$S(\rho) := -\mathrm{Tr}[\rho \ln \rho] \tag{8}$$

and satisfies m constrains of the form

$$\mathrm{Tr}[\rho\, \hat{M}^{(j)}] = K^{(j)} \qquad j \in 1, \dots, m, \tag{9}$$

where $K^{(j)} \in \mathbb{R}$ and the $\hat{M}^{(j)} : \mathcal{H} \to \mathcal{H}$ are hermitian operators on the Hilbert space $\mathcal{H}$ of the system.

Our final goal is to derive the Fermi-Dirac and Bose-Einstein statistic from the principle of maximal entropy.

The Hilbert space of Bosonic systems are infinite dimensional which leads to technical difficulties that we cannot discuss here. Hence we restrict to the Fermionic case for now and will motivate the Bosonic case later by analogy. Let us furthermore restrict to the case in which the Hamiltonian $\hat{H}$ and the particle number operator $\hat{N}$ commute, i.e., there exists a basis in which both are diagonal.

c) Assume that some density matrix ρ is given in this basis. On which entries of the matrix ρ do the expectation values of $\hat{H}$ and $\hat{N}$ depend on? Which entries of ρ cannot change these expectation values?

An important consequence of Schur's theorem is the following: Among all density matrices with the same diagonal (in some basis), the matrix with all entries outside the diagonal equal to zero has the largest von Neumann entropy.

d) Use the above to show that for finite dimensional systems the density matrix ρ_{gc} which maximizes the von Neumann entropy and at the same time fulfills the two constrains

$$\mathrm{Tr}[\rho_{gc}\,\hat{H}] = E \tag{10}$$

$$\mathrm{Tr}[\rho_{gc}\,\hat{N}] = N, \tag{11}$$

is of the form

$$\rho_{gc} = \frac{\exp(-\beta(\hat{H} - \mu\,\hat{N}))}{\mathrm{Tr}\exp(-\beta(\hat{H} - \mu\,\hat{N}))}. \tag{12}$$

The normalization constant

$$Z := \mathrm{Tr}\exp(-\beta(\hat{H} - \mu\,\hat{N})) \tag{13}$$

is called grand canonical partition sum.

We have derived the expressions for ρ_{gc} and Z only in the finite dimensional case. However, it can be shown that Eqs. (12) and (13) also hold for systems of non-interacting Bosons.

Now consider a quantum mechanical system of identical non-interacting particles (either Fermions or Bosons). The Hamiltonian of the system is given by

$$\hat{H} := \sum_{k=1}^{n} E_k\,\hat{N}_k \tag{14}$$

where $\hat{N}_k$ is the particle number operator that counts how many of the particles are in the k-th of the n modes of the system, which has energy E_k. Obviously the total number of particles is $\hat{N} = \sum_k \hat{N}_k$.

e) Show that $\hat{H}$, $\hat{N}$, and all the $\hat{N}_k$ commute. Y ou can assume that $[\hat{N}_k, \hat{N}_j] = 0$.

f) Show that the expected number of particles $\mathrm{Tr}[\rho_{gc} N_k]$ in the k-th mode in the grand canonical state ρ_{gc} is given by

$$\mathrm{Tr}[\rho_{gc} N_k] = -\beta^{-1}\frac{\partial}{\partial E_k}\ln Z. \tag{15}$$

g) Show that the grand canonical partition sum $Z := \mathrm{Tr}\exp(-\beta(\hat{H} - \mu\,\hat{N}))$ of the system is given by

$$Z = \sum_{N=0}^{\infty}\ \sum_{N_1,\ldots,N_n : \sum_k N_k = N}\ \prod_k \mathrm{e}^{-\beta N_k (E_k - \mu)} \tag{16}$$

and that this can furthermore be written as

$$Z = \prod_k \sum_{N_k} \mathrm{e}^{-\beta N_k (E_k - \mu)}. \tag{17}$$

Hint: Use a clever basis to calculate the trace in Eq. (13) for Hamiltonians of the form (14).

The Fermi exclusion principle states that no two Fermions can share the same quantum state. Thus, if the particles are Fermions $N_k \in \{0, 1\}$. For Bosons no such restriction exists, i.e., N_k can take all non-negative integer values.

h) Show that this implies for

$$\text{Fermions:} \qquad Z_F = \prod_k (1 + \mathrm{e}^{-\beta(E_k - \mu)}) \tag{18}$$

$$\text{Bosons:} \qquad Z_B = \prod_k \frac{1}{1 - \mathrm{e}^{-\beta(E_k - \mu)}} \tag{19}$$

i) Use the previous results to derive $\mathrm{Tr}[\rho_{gc} N_k]$ for Fermions and for Bosons — the famous Fermi-Dirac and Bose-Einstein distribution.