

Exercise Sheet 13

(1) Grandcanonical ensemble

We consider a quantum many-body system for particles, described by a Hamiltonian \mathbf{H} , which is bounded from below, i.e., the with energy eigenvalues $E \geq 0$. In addition there is a conserved charge Q . The grand-canonical ensemble is defined by a (large) subsystem in (an even larger) closed system of particles, which can exchange energy as well as particles/charges with its environment.

The equilibrium statistical operator \mathbf{R} is determined by giving the average internal energy $U = \langle \mathbf{H} \rangle$ and average charge $q = \langle \mathbf{Q} \rangle$ and fulfilling the normalization condition $\text{Tr} \mathbf{R} = 1$, which is fixed due to the conservation laws and maximizing the entropy

$$S = -\text{Tr}(\mathbf{R} \ln \mathbf{R}) = -\langle \ln \mathbf{R} \rangle. \quad (1)$$

Show that with appropriate Lagrange multipliers to fulfill the above given constraints this statistical operator reads

$$\rho = \exp(-\beta \mathbf{H} - \alpha \mathbf{Q} - \Omega). \quad (2)$$

The normalization condition gives

$$\text{Tr} \rho = 1 \Rightarrow \Omega(\beta, \alpha) = \ln Z(\beta, \alpha), \quad Z = \text{Tr} \exp(-\beta \mathbf{H} - \alpha \mathbf{Q}). \quad (3)$$

Show that the internal energy and mean total charge are given by

$$U = -\partial_\beta \Omega, \quad q = -\partial_\alpha \Omega. \quad (4)$$

Then calculate the entropy, using Eq. (1). Finally show, calculating dS , with help of the thermodynamic relation

$$dU = T dS - P dV + \mu dq \quad (5)$$

the relation of β and α to T and μ .

Hint: to get the pressure, note that Ω also depends implicitly on $L = V^{1/3}$, when introducing a cube of length L as a finite volume with imposing periodic boundary conditions on the (quantum) fields, describing the particles. Then, due to the periodic boundary conditions, the momenta take the discrete values $\vec{p} \in (2\pi/L)\mathbb{Z}^3$.

$$d\Omega = d\beta \partial_\beta \Omega + d\alpha \partial_\alpha \Omega + dV \partial_V \Omega. \quad (6)$$

(2) Thermodynamics of a charged Bose gas

We consider the ideal gas of a charged relativistic Bose gas considering the scalar particles described by a Klein-Gordon field (see Lecture 6 of “Kerne und Teilchen 1”¹), describing charged particles and their antiparticles. We use the “box regularized version”, i.e., take a cube of length L as a finite “quantization volume” with the fields obeying periodic boundary conditions as already assumed in part (1). Then the Hamiltonian and total charge is given by the occupation numbers $\mathbf{N} = \mathbf{a}^\dagger(\vec{p})\mathbf{a}(\vec{p})$ and $\bar{\mathbf{N}} = \mathbf{b}^\dagger(\vec{p})\mathbf{b}(\vec{p})$ with momenta $\vec{p} \in (2\pi/L)\mathbb{Z}^3$ and creation and annihilation operators $\mathbf{a}^\dagger(\vec{p})$ and $\mathbf{a}(\vec{p})$ for a particle with momentum \vec{p} and $\mathbf{b}^\dagger(\vec{p})$ and $\mathbf{b}(\vec{p})$ for an antiparticle, obeying bosonic commutation relations

$$[\mathbf{a}(\vec{p}), \mathbf{a}^\dagger(\vec{q})] = [\mathbf{b}(\vec{p}), \mathbf{b}^\dagger(\vec{p})] = \delta_{\vec{p}, \vec{q}} \quad (7)$$

¹<https://itp.uni-frankfurt.de/~hees/old-teilchen-kerne-1-WS2526/index.html>

and all other commutators of creation and annihilation operators vanishing.
 The Hamiltonian and charge operator are given by

$$\begin{aligned} \mathbf{H} &= \sum_{\vec{p}} E_p [\mathbf{N}(\vec{p}) + \bar{\mathbf{N}}(\vec{p})], \quad E_p = \sqrt{m^2 + \vec{p}^2}, \\ \mathbf{Q} &= \sum_{\vec{p}} [\mathbf{N}(\vec{p}) - \bar{\mathbf{N}}(\vec{p})] \end{aligned} \tag{8}$$

Use the occupation-number basis (Fock basis), i.e., the common eigenvectors $|\{N(\vec{p}), \bar{N}(\vec{p})\}_{\vec{p}}\rangle$ with $N(\vec{p}), \bar{N}(\vec{p}) \in \mathbb{N}_0 = \{0, 1, 2, \dots\}$ of the particle and antiparticle number operators to evaluate the partition sum. Also discuss the physical range of values for temperature, T and chemical potential, μ .

(3) Thermodynamics of a charged Fermi gas

Repeat the steps for an ideal gas of Dirac fermions and antifermions. Here we have anticommutators instead of commutators for the annihilation and creation operators and in addition two spin/ polarization-degrees of freedom $\sigma = \pm 1/2$. Note that the only difference is that one has a sum over momenta and spins and the possible occupation numbers can only take the eigenvalues $N(\vec{p}, \sigma), \bar{N}(\vec{p}, \sigma) \in \{0, 1\}$.
