Condensed Matter Theory — problem set 1

Dr. Tilman Enss & Valentin Kasper
Institut für Theoretische Physik, Universität Heidelberg
20 April 2016
due date: 27 April 2016
Course homepage: `http://www.thphys.uni-heidelberg.de/~enss/teaching.html`

Problem 1: Ideal quantum gas

Consider a system of free bosonic or fermionic particles with Hamiltonian

$$\hat{\mathcal{H}} = \sum_\alpha \varepsilon_\alpha \hat{a}_\alpha^\dagger \hat{a}_\alpha \,. \tag{1}$$

Compute the partition function $Z = \operatorname{Tr}\exp[-\beta(\hat{\mathcal{H}} - \mu\hat{\mathcal{N}})]$ with $\beta = 1/k_B T$ and $\hat{\mathcal{N}} = \sum_\alpha \hat{n}_\alpha = \sum_\alpha \hat{a}_\alpha^\dagger \hat{a}_\alpha$, as well as the grand potential $\Omega = -(1/\beta)\ln Z$. What are the thermal expectation values of the occupation numbers in equilibrium, $n_\alpha = \langle \hat{a}_\alpha^\dagger \hat{a}_\alpha \rangle$ and $N = \langle \hat{\mathcal{N}} \rangle = -\partial\Omega/\partial\mu$?

Problem 2: Correlation functions [written homework problem: 10P]

Please hand in your written solution to this problem on Wednesday, April 27, before the start of the lecture; it will be discussed in the following tutorial session on Friday, April 29. You may work in teams (two names per solution).

Even a noninteracting quantum gas has nontrivial correlations due to Bose or Fermi statistics. In this case all correlations are determined by the one-particle density matrix

$$G_1(\boldsymbol{x},\boldsymbol{x}') = \langle \hat{\psi}^\dagger(\boldsymbol{x})\hat{\psi}(\boldsymbol{x}')\rangle = \sqrt{n(\boldsymbol{x})n(\boldsymbol{x}')}\, g_1(\boldsymbol{x},\boldsymbol{x}'). \tag{2}$$

In the homogeneous case these functions depend only on $|\boldsymbol{x}-\boldsymbol{x}'|$, *i.e.*, one can set $\boldsymbol{x}' = 0$ and $r = |\boldsymbol{x}|$. Consider an ideal Bose or Fermi gas (without spin) in a box of volume $V \to \infty$ with single-particle energies $\varepsilon_{\boldsymbol{k}} = \hbar^2\boldsymbol{k}^2/2m$ and a mean particle density $n = N/V$.

(a) [3 P]
Using the representation of the field operators $\hat{\psi}(\boldsymbol{x}) = V^{-1/2}\sum_{\boldsymbol{k}} \hat{a}_{\boldsymbol{k}} \exp(i\boldsymbol{k}\boldsymbol{x})$ in terms of the annihilation operators $\hat{a}_{\boldsymbol{k}}$ for particles with momentum $\boldsymbol{k}$ and $\langle \hat{a}_{\boldsymbol{k}}^\dagger \hat{a}_{\boldsymbol{q}}\rangle = \delta_{\boldsymbol{k}\boldsymbol{q}} n_{\boldsymbol{k}}$, show that the one-particle density matrix for free particles is given by the Fourier transform of the momentum distribution of an ideal Bose or Fermi gas,

$$G_1(\boldsymbol{x}-\boldsymbol{x}') = \int \frac{d^3k}{(2\pi)^3} \frac{e^{-i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}')}}{e^{\beta(\epsilon_{\boldsymbol{k}}-\mu)} \mp 1}\,. \tag{3}$$

(b) [2 P]
Compute $g_1(r)$ explicitly in the classical limit $\exp(\beta\mu) \ll 1$, expressed in terms of the thermal wavelength $\lambda_T = h/\sqrt{2\pi m k_B T}$.

(c) **3 P**

The pair correlation function g_2 is defined via the density correlation function

$$\langle \hat{n}(\boldsymbol{x})\hat{n}(\boldsymbol{x}')\rangle = \langle \hat{n}(\boldsymbol{x})\rangle \langle \hat{n}(\boldsymbol{x}')\rangle g_2(\boldsymbol{x},\boldsymbol{x}') + \langle \hat{n}(\boldsymbol{x})\rangle \delta(\boldsymbol{x}-\boldsymbol{x}') . \tag{4}$$

Show that for free particles the pair correlation function is given by $g_2(\boldsymbol{x},\boldsymbol{x}') = 1 \pm |g_1(\boldsymbol{x},\boldsymbol{x}')|^2$. Bosons thus have a tendency to *bunch* ($g_2(0) = 2$) while fermions *anti-bunch* ($g_2(0) = 0$) due to the Pauli principle.

[*Hint*: Use the identity $\langle a_1^\dagger a_2 a_3^\dagger a_4\rangle = \delta_{12}\delta_{34} n_1 n_3 + \delta_{14}\delta_{23} n_1(1 \pm n_2)$.]

(d) **2 P**

Compute $g_2(r)$ explicitly for an ideal Fermi gas at temperature $T = 0$ and discuss the characteristic spatial extent of the resulting "exchange hole" in comparison to the mean particle spacing.

Problem 3: Algebra with Creation and Annhilation Operators

We use the $N \times N$ matrices A and B to define the operators

$$\hat{A} = \sum_{m,n} a_m^\dagger A_{mn} a_n \quad \text{and} \quad \hat{B} = \sum_{m,n} a_m^\dagger B_{mn} a_n \tag{5}$$

with $m, n = 1, \ldots, N$ and the bosonic creation (annihilation) operators $a_m^\dagger (a_m)$. Furthermore, we introduce the vector $\mathbf{v}$ with length N and the components v_m

$$\hat{\mathbf{v}}^\dagger = \sum_m v_m a_m^\dagger . \tag{6}$$

(a) Show that $[\hat{A}, \hat{B}] = \sum_{m,n} a_m^\dagger ([A, B])_{mn} a_n$ and $[\hat{A}, \hat{\mathbf{v}}^\dagger] = \sum_m (A \cdot \mathbf{v})_m a_m^\dagger$.

(b) We define the spin operator

$$\hat{S}^\alpha = \frac{1}{2} \sum_{m,n=1}^{2} a_m^\dagger \sigma_{mn}^\alpha a_n$$

with $\alpha \in \{x, y, z\}$ and the Pauli matrices

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Show that $[\hat{S}^\alpha, \hat{S}^\beta] = i \sum_\gamma \varepsilon^{\alpha\beta\gamma} \hat{S}^\gamma$. Find the eigenstates (in Fock space) and eigenvalues of $\hat{S}^z$.

(c) Prove the identity $e^{\hat{A}}\, \hat{\mathbf{v}}^\dagger\, e^{-\hat{A}} = \sum_m (e^A \cdot \mathbf{v})_m a_m^\dagger$.

(d) Reconsider (a), (b) and (c) with a_m and $a_m^\dagger$ being fermionic operators.