# Assignments to Condensed Matter Theory I
# Sheet 4


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|---|---|---|
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## **Problem set**: Spin statistics and finite temperatures

In the real world we never encounter zero temperature. Hence we will often need to use statistical physics and thermodynamics. In classical mechanics the state of a system is defined by the position and momentum of all its degrees of freedom. For example the state of N classical particles is defined by the set of 6N coordinates $\mathbf{x}_n, \mathbf{p}_n$ with $n = 1, \dots, N$ in the phase space $\Gamma$. The observables $O(\mathbf{x}_n, \mathbf{p}_n)$ are functions of these coordinates and their thermal averages can be written as:

$$\langle O \rangle_T = \sum_{N=0}^{\infty} \int_\Gamma \mathrm{d}\Gamma \rho(\mathbf{x}_n, \mathbf{p}_n, N) O(\mathbf{x}_n, \mathbf{p}_n)$$

where, according to the Gibbs formula, $\rho(\mathbf{x}_n, \mathbf{p}_n, N) \equiv (1/Z) \exp[-\beta(H(\mathbf{x}_n, \mathbf{p}_n) - \mu N)]$, $\beta = \frac{1}{k_B T}$ and $\mathrm{d}\Gamma \equiv \prod_{n=1}^{N} \mathrm{d}\mathbf{x}_n \mathrm{d}\mathbf{p}_n$. $Z$ is the grancanonical partition function:

$$Z = \sum_{N=0}^{\infty} \int_\Gamma \mathrm{d}\Gamma \exp[-\beta(H(\mathbf{x}_n, \mathbf{p}_n) - \mu N)]$$

The quantum mechanical version of the thermal average is:

$$\langle O \rangle_T = \sum_{N=0}^{\infty} \mathrm{Tr}_N\{\hat{\rho}\hat{O}\}$$

where the operator $\hat{\rho}$ is defined as:

$$\hat{\rho} = (1/Z) \exp[-\beta(\hat{H} - \mu\hat{N})]$$

and the trace $\mathrm{Tr}_N$ is taken only with respect to states with $N$ number of particles. The grancanonical partition function, in the quantum version, reads:

$$Z = \sum_{N=0}^{\infty} \mathrm{Tr}_N\{\exp[-\beta(\hat{H} - \mu\hat{N})]\}$$

### 4.1. Many (non-interacting) bosons

Let us consider the Hamiltonian for non-interacting bosons:

$$H_\mathrm{B} = \sum_\lambda \hbar\omega_\lambda \left( b_\lambda^\dagger b_\lambda + \frac{1}{2} \right) \tag{1}$$

where the quantum number $\lambda$ completely defines the single particle state. For example in the case of a system of phonons $\lambda = (\mathbf{q}, m)$ where $\mathbf{q}$ is the momentum and $m$ the branch index. The chemical potential $\mu$ is taken to be lower than the lowest boson energy and independent from the temperature.

(a) Calculate the grancanonical partition function $Z$ for this system.

(b) What is the average number of bosons in the state defined by the quantum number $\lambda$? This is called Bose-Einstein distribution $n_{\mathrm{BE}}$.

(c) Plot $n_{\mathrm{BE}}(\omega_\lambda, T, \mu)$ vs. $\omega_\lambda$ for different temperatures.

(d) What is the average energy $U$ of the system?
`Hint:` $U = -\frac{\partial}{\partial\beta} \ln Z + \frac{\mu}{\beta}\frac{\partial}{\partial\mu} \ln Z$.

(e) **[Kür]** Calculate the specific heat $c_V = \frac{\partial U}{\partial T}$ using the Einstein model (i.e. only one branch with dispersion $\omega(\mathbf{q}) = \omega_0$).

(f) **[Kür]** Calculate the specific heat $c_V$ at low temperatures for phonons with linear dispersion relation $\omega(\mathbf{q}) = v\|\mathbf{q}\|$ in 1D, 2D, 3D.
`Hint:` It is not (so) difficult to show that:

$$c_V = N k_B \int_0^\infty \mathrm{d}\omega \left(\frac{\hbar\omega}{2k_BT}\right)^2 \frac{DOS(\omega)}{\sinh^2(\hbar\omega/2k_BT)}$$

## 4.2. Many (non-interacting) fermions

Let us now consider the Hamiltonian for non-interacting fermions:

$$H_{\mathrm{F}} = \sum_\lambda \epsilon_\lambda c_\lambda^\dagger c_\lambda \tag{2}$$

where $\lambda$ is a good quantum number for single particle states.

(a) Calculate the grancanonical partition function $Z$ for this system.
`Hint:` Remember that for Fermions the Pauli exclusion principle holds. Formally $\{c^\dagger, c^\dagger\} = 0$ which implies that a single particle state can never be occupied by more than one fermion.

(b) Calculate the average number of fermions in the state defined by the quantum number $\lambda$. You just rediscover the Fermi-Dirac distribution $n_{\mathrm{FD}}$.

(c) Plot $n_{\mathrm{FD}}(\epsilon_\lambda, T, \mu)$ vs. $\epsilon_\lambda$ for different temperatures.

(d) What is the average energy of the system?