Janosh Riebesell Lecturer: Carlo Ewerz January 27th, 2010

Statistical Mechanics

Second Exam

General remarks

- Please use a separate sheet for every exercise.
- Write your name and your group on every sheet.
- You are not allowed to use calculators, paper (except blank sheets) or formula cards.

1 Short questions (10 points)

a) What is the mean occupation number $\langle n_\nu \rangle$ for a bosonic and for a fermionic system with energy levels E_ν? (3 points)

b) Consider a system consisting of two identical non-interacting particles. Each particle can have exactly three distinct energies $\epsilon_1 = -\epsilon$, $\epsilon_2 = 0$, and $\epsilon_3 = +\epsilon$. The system is in thermal contact with a heat bath of temperature T. Determine the canonical partition sum of the system for the case where both particles are distinguishable. (2 points)

c) Shortly explain what characterizes Bose-Einstein condensation. (2 points)

d) Specify the thermodynamic quantities to which the energy fluctuations (in the canonical ensemble) and the particle number fluctuations (in the grand canonical ensemble) are related. (3 points)

a) The expected number of bosons/fermions in a state $|\nu\rangle$ with energy E_ν is determined by Bose-Einstein/Fermi-Dirac statistics,

$$\langle n_\nu^\pm \rangle = -\frac{1}{\beta}\frac{\partial}{\partial E_\nu} \ln(Z_g^\pm) = \frac{g_\nu}{e^{\beta\,(E_\nu - \mu)} \mp 1}, \tag{1}$$

where g_ν counts the degeneracy of E_ν and $\beta = \frac{1}{k_B T}$.

b) Since the particles are non-interacting, the partition function factorizes. For a single particle,

$$Z_c^1 = \sum_{i=1}^{3} e^{-\beta\epsilon_1} = e^{\beta\epsilon} + 1 + e^{-\beta\epsilon}. \tag{2}$$

For both,

$$Z_c = (Z_c^1)^2 = e^{2\beta\epsilon} + 2e^{\beta\epsilon} + 3 + 2e^{-\beta\epsilon} + e^{-2\beta\epsilon}. \tag{3}$$

The degeneracies in front of each Boltzmann factor coincide with the number of times an energy level appears in the table below. They sum up to the total number of states $1 + 2 + 3 + 2 + 1 = 9$.

E	-2ϵ	$-\epsilon$	0	$-\epsilon$	0	ϵ	0	ϵ	2ϵ
ϵ			•			•	•	•	••
0		•		•	••	•		•	
$-\epsilon$	••	•	•	•			•		

If instead the particles were indistinguishable, we would have $Z_c = \frac{1}{2!}(Z_c^1)^2$.

c) Bose-Einstein condensation is the phenomenon of macroscopic accumulation of bosons in the ground state wave function below a critical temperature $T < T_c$. T_c is close to absolute zero and determined by the particle density $n(z=1)$ at zero chemical potential ($z = e^{\beta\mu}$).

d) The expected energy in the canonical ensemble is

$$\langle E \rangle = \frac{1}{Z_c}\sum_i E_i e^{-\beta E_i} = -\frac{\partial \ln Z_c}{\partial \beta}. \tag{4}$$

Its derivative w.r.t. temperature gives

$$\begin{aligned} C_V = \frac{\partial \langle E \rangle}{\partial T} &= \frac{1}{Z_c}\sum_i E_i \frac{E_i}{k_\mathrm{B}T^2} e^{-\beta E_i} - \frac{1}{Z_c}\frac{\partial Z_c}{\partial T}\langle E \rangle \\ &= \frac{1}{k_\mathrm{B}T^2}\left(\langle E^2 \rangle - \langle E \rangle^2\right) = \frac{1}{k_\mathrm{B}T^2}\sigma_E^2. \end{aligned} \tag{5}$$

Thus in the canonical ensemble, heat capacity and energy fluctuations are directly related. In the grand canonical ensemble, the expected particle number is

$$\langle N \rangle = \frac{1}{Z_g}\sum_{N=0}^{\infty} N z^N Z_c = \frac{1}{Z_g}\frac{1}{\beta}\frac{\partial}{\partial \mu}\sum_{N=0}^{\infty} z^N Z_c = \frac{1}{\beta}\frac{\partial}{\partial \mu}\ln Z_g. \tag{6}$$

The number fluctuations can be written

$$\begin{aligned} \frac{1}{\beta^2}\frac{\partial^2}{\partial^2 \mu}\ln Z_g = \frac{1}{\beta}\frac{\partial}{\partial \mu}\langle N \rangle &= \frac{1}{Z_g}\sum_{N=0}^{\infty} N^2 z^N Z_c - \left(\frac{1}{Z_g}\sum_{N=0}^{\infty} N z^N Z_c\right)^2 \\ &= \langle N^2 \rangle - \langle N \rangle^2 = \sigma_N^2. \end{aligned} \tag{7}$$

Thus

$$\sigma_N^2 = -\frac{1}{\beta}\frac{\partial^2 \Omega}{\partial^2 \mu} = \frac{V}{\beta}\frac{\partial^2 p}{\partial^2 \mu}, \tag{8}$$

where we identified the grand potential $\Omega = -\frac{1}{\beta}\ln Z_g$, inserted $\Omega = -pV$ and used that the grand canonical ensemble keeps the volume fixed. The (isothermal) compressibility is defined

$$\kappa_T = -\frac{1}{V}\frac{\partial p}{\partial V} = \frac{V^2}{N^2}\frac{\partial^2 p}{\partial^2 \mu}, \tag{9}$$

i.t.o. which (8) reads

$$\sigma_N^2 = \frac{N^2}{\beta V}\kappa_T. \tag{10}$$

Thus the grand canonical ensemble relates compressibility and number fluctuations.

2 One-dimensional Ising Model (10 points)

Consider N spins in a chain which can be modeled using the one-dimensional Ising model

$$H = -J\sum_{n=1}^{N-1} s_n s_{n+1}, \tag{11}$$

Where a spin has the values $s_n = \pm 1$.

a) Calculate the partition function. (5 points)

b) Calculate the heat capacity per spin. (5 points)

a) The partition function is the sum over all 2^N possible states $s = \{s_1, \ldots, s_N\} \in \mathcal{S}_N = \{\pm 1\}^N$ weighted by their energy $H(s)$ according to Boltzmann's factor $e^{-\beta H(s)}$,

$$\begin{aligned} Z_c &= \sum_{s\in\mathcal{S}_N} e^{-\beta H(s)} = \sum_{s_1\in\{\pm1\}} \cdots \sum_{s_N\in\{\pm1\}} e^{\beta J \sum_{n=1}^{N-1} s_n s_{n+1}} = \prod_{n=1}^{N-1} \sum_{s_n\in\{\pm1\}} e^{\beta J s_n s_{n+1}} \sum_{s_N\in\{\pm1\}} \\ &= 2 \prod_{j=1}^{N-1} \left(e^{\beta J} + e^{-\beta J}\right) = 2\big[2\cosh(\beta J)\big]^{N-1}, \end{aligned} \tag{12}$$

where we used that $\sum_{s_n\in\{\pm1\}} e^{\beta J s_n s_{n+1}} = 2\cosh(\beta J)$ regardless of the sign of s_{n+1}.

b) The Ising chain's energy is

$$U = -\frac{\partial \ln Z_c}{\partial \beta} = -(N-1)\frac{\sinh(\beta J)}{\cosh(\beta J)} J = -(N-1) J \tanh(\beta J). \tag{13}$$

which results in the per-spin heat capacity

$$c = \frac{C}{N} = \frac{1}{N}\frac{\partial U}{\partial T} = \frac{1}{N}\frac{\partial U}{\partial \beta}\frac{\partial \beta}{\partial T} = \frac{(N-1)J}{N k_\mathrm{B} T^2}\left(J - \frac{\sinh^2(\beta J)}{\cosh^2(\beta J)} J\right) \approx k_\mathrm{B} \frac{\beta^2 J^2}{\cosh^2(\beta J)}, \tag{14}$$

where we used $\sinh^2(x) = \cosh^2(x) - 1$ and $N \gg 1$.

3 Ideal quantum gases (10 points)

Note: a) and b) can besolved independently.

a) A system of N non-interacting, spin-$\frac{1}{2}$ fermions are confined to move in two dimensions. They are confined within a rectangular area with dimensions L_x and L_y. The wave vectors allowed by periodic boundary conditions are $\boldsymbol{k} = \frac{2\pi}{L_x} n_x \boldsymbol{e}_x + \frac{2\pi}{L_y} n_y \boldsymbol{e}_y$, where n_x and n_y can take on all positive and negative integer values. The energy for a single fermion is given by $\epsilon = \frac{\hbar^2 \boldsymbol{k}^2}{2m}$.

   i) Determine $N(k)$, the number of single-particle states with wavevector magnitude smaller than k. (1 point)

   ii) Determine $D(\epsilon)$, the density of single-particle states as a function of their energy ϵ. (2 points)

   iii) Find an expression for the total energy E of the system of fermions at $T = 0$. (2 points)

b) Now, we consider a system of N non-interacting bosons that have no spin degrees of freedom. They are distributed among 3 single-particle states: Υ_1 and Υ_2 with energy $\epsilon = 0$ and Υ_3 with energy $\epsilon = \Delta$.

   i) Write down a closed form expression for the partition function $Z(T)$ for the system of bosons. The following formulae may be useful: $\sum_{n=0}^{N} x^n = \frac{1-x^{N+1}}{1-x}$ and $\sum_{n=0}^{N} (N - n + 1)\, x^n = \frac{(N+1)-(N+2)x+x^{N+2}}{(1-x)^2}$. (1 point)

   ii) Determine the internal energy E in the limit of large N at low temperatures $k_\mathrm{B}T \ll N\Delta$. (3 points)

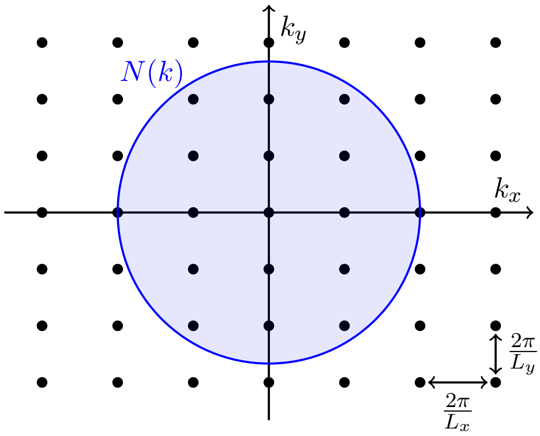
   iii) Shortly explain why E is not an extensive variable in this model at low temperature. (1 point)

   Note: iii) can be solved independently from ii).

a) Ideal Fermi gas

i) The k-space region of wavevectors up to a given magnitude is a disk of area πk^2. The k-space area occupied by a single particle state is $\frac{1}{2}\frac{2\pi}{L_x}\frac{2\pi}{L_y} = \frac{2\pi^2}{A}$, where the factor of $\frac{1}{2}$ is due to the spin degeneracy $g_s = 2s + 1 = 2$. The number of states with wavevector magnitude smaller than k is thus

$$N(k) = \frac{\pi k^2}{2\pi^2/A} = \frac{Ak^2}{2\pi}. \tag{15}$$



ii) The (single-particle) density of states is

$$D(\epsilon) = \frac{\partial}{\partial \epsilon} N(k) = \frac{\partial}{\partial \epsilon} \frac{A}{2\pi} \frac{2m}{\hbar^2} \epsilon = \frac{Am}{\pi \hbar^2}, \tag{16}$$

independent of ϵ.

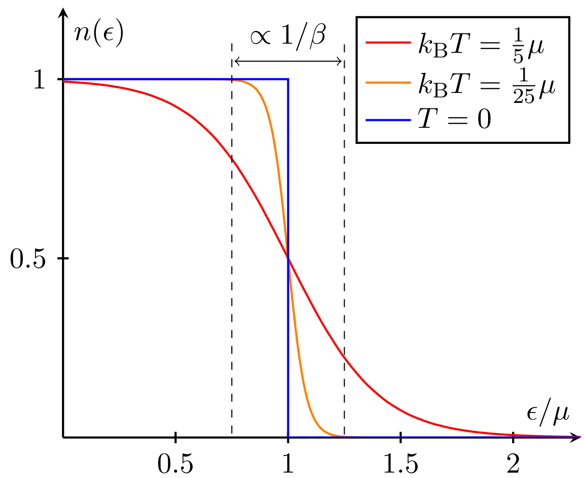
iii) We can calculate the system's total Energy E by integrating ϵ times the density of states $D(\epsilon)$ times the number $n(\epsilon)$ of particles with energy ϵ over all energies,

$$E = \int_0^\infty \epsilon D(\epsilon) n(\epsilon) \, \mathrm{d}\epsilon, \tag{17}$$

where $n(\epsilon)$ is given by the Fermi-Dirac distribution[1]

$$n(\epsilon) = \frac{1}{e^{\beta(\epsilon - \mu) + 1}}, \tag{18}$$

plotted below for different temperatures.



[1]Note that we already took care of the spin degeneracy $g_s = 2$ in the density of states $D(\epsilon)$, so we don't need to include another factor of g_s in $n(\epsilon)$.

At $T = 0$, $n(\epsilon)$ becomes a step function dropping from g_s to zero at the chemical potential μ. Thus the integral (17) simplifies to

$$E = \int_0^\mu \epsilon D(\epsilon)\,\mathrm{d}\epsilon = \frac{1}{2}\frac{Am}{\pi\hbar^2}\,\mu^2 = \frac{N\mu}{2} = \frac{2\pi\hbar^2}{Am}N^2, \tag{19}$$

where we inserted the Fermi energy ϵ_F for $\mu(T = 0)$ obtained from (15) rewritten as

$$N(\epsilon) = \frac{Am}{\pi\hbar^2}\,\epsilon_\mathrm{F} \quad \Rightarrow \quad \epsilon_\mathrm{F} = \frac{\pi\hbar^2 N}{Am}, \tag{20}$$

At $T = 0$ all energy levels from $\epsilon = 0$ up to the chemical potential μ are fully occupied. Thus the second-to-last expression in (19) reflects that the total energy is just the average single-particle energy $\frac{\mu}{2}$ times the number of particles.

b) Ideal Bose gas

i) The canonical partition function of a single boson in this three-state system is

$$Z_c^1 = \sum_{i=1}^{3} e^{-\beta\epsilon_i} = 2 + e^{-\beta\Delta}. \tag{21}$$

Since the N bosons are non-interacting, the total partition function is just

$$Z_c = \frac{1}{N!}(Z_c^1)^N = \frac{1}{N!}\big(2 + e^{-\beta\Delta}\big)^N, \tag{22}$$

where $\frac{1}{N!}$ ensures correct counting of states for indistinguishable particles.

ii) The internal energy is

$$E = -\frac{\partial \ln Z_c}{\partial\beta} = \frac{\Delta N}{1 + 2e^{\beta\Delta}}. \tag{23}$$

At very high temperatures, we expect thermal fluctuations to be so strong that all single-particle states are equally occupied. Indeed, (23) suggests that $E \to \frac{N\Delta}{3}$ for $T \to \infty$, i.e. $\beta \to 0$. For low temperatures on the other hand, the denominator of (23) diverges (assuming $\Delta > 0$) and we get $E = 0$. This is consistent with the interpretation that near absolute zero, all bosons coalesce into either of the two zero-energy ground states.

iii) If all particles occupy states of zero energy, E is not extensive at low temperatures because it remains zero no matter the size of the system.