

UNIVERSITY OF OSLO

Obligatory assignment 4: FYS2160, Thermodynamics and statistical physics, Fall 2019

Due: November 12. 2019

1 Equilibrium states of macroscopic systems

Learning outcomes: We learn that macroscopic systems at equilibrium have thermodynamic properties (entropy, energy, temperature, etc.) that are independent of how we choose to define the system in relation to its environment. This is a fundamental result in statistical mechanics also known as the ensemble equivalence. A statistical ensemble is a collection of microstates corresponding to a particular way in which the system interacts with the environment. For example, if we consider an isolated system, then we have an ensemble of equally likely microstates at the same energy. Or, if we consider a system in a thermal bath, then we have an ensemble of microstates at the same temperature. The statistical mechanics of these ensembles corresponds to a unique equilibrium state of the system. This is exemplified by showing that, in the thermodynamic limit, the mean entropy of a particle as a function of its mean energy in an isolated system is the same as that for a system in contact with a thermal bath at a corresponding temperature T .

Consider a system of identical, independent and distinguishable particles. Each particle has two energy levels ϵ and $-\epsilon$ that it can occupy. First, we consider an isolated system with a fixed number of particles N and a fixed total energy U . Let us denote the number of particles with energy ϵ by N_+ and the number of particles with energy $-\epsilon$ by N_- . From the constraints of fixed total energy and number of particles, we then have that $U = N_+\epsilon - N_-\epsilon$ and $N = N_+ + N_-$. This implies that $N_{\pm} = N(1 \pm x)/2$, where $x = U/(N\epsilon)$ is the dimensionless mean energy per particle.

1.1 Compute the entropy $S_M(x, N)$ as a function of U (in dimensionless units) and N . Using the Stirling approximation for the thermodynamic limit, determine the entropy per particle as a function of the dimensionless energy per particle, $s_M(x) = \lim_{N \rightarrow \infty} S_M(x, N)/N$.

Now, let us consider that the system with the same fixed N number of particles is in contact with a thermal bath at fixed temperature T .

1.2 Calculate the partition function of one particle $Z_1(T)$.

1.3 Calculate the partition function of N particles $Z_N(T)$.

1.4 Determine the Helmholtz free energy $F(T, N)$ for N particles.

1.5 Calculate the total average energy $U = \langle E \rangle$ for N particles. Invert the equation to express $\beta\epsilon$ as a function of $x = U/(N\epsilon)$. Eliminate the $\beta\epsilon$ -dependence of $F_N(T)$ calculated above and express it as a function of x instead.

1.6 Determine the entropy per particle $s_C(x) = \lim_{N \rightarrow \infty} S_C(x, N)/N$.

1.7 Give a physical interpretation of the identity $s_M \equiv s_C$ for a particle. Why does it not matter for a particle how the system interacts with its environment?

2 Harmonic oscillators

Learning outcomes: We learn how to derive the equilibrium properties of a system at a given temperature and with particles that have infinitely many energy levels. As an example, we consider a system of quantum harmonic oscillators and derive the temperature dependence of the average energy and heat capacity. We can determine the regime where the theorem of equipartition of energy applies.

Consider a system of N independent and distinguishable quantum harmonic oscillators in one dimension, at the same angular frequency ω and in contact with a thermal bath at T . The energy levels for each harmonic oscillator are $\epsilon(n) = (n + 1/2)\hbar\omega$, where $n = 0, 1, \dots$.

2.1 Compute the partition function for one quantum harmonic oscillator $Z_1(T)$.

2.2 Compute the partition function for N particles $Z_N(T)$ and the Helmholtz free energy $F_N(T)$.

2.3 Compute average energy $\langle E_N \rangle$ for N oscillators and discuss its low and high-temperature limit.

2.4 Compute the heat capacity (at constant volume) for N oscillators and discuss its low-temperature limit and its high-temperature limit.

3 Particle in 1D

Learning outcomes: We learn how to derive the equation of state of a quantum ideal gas and compare it with that of the classical ideal gas. For this, we use that the ideal gas is composed of indistinguishable, identical particles and therefore the N -particle partition function is $Z_N = Z_1^N/N!$, where Z_1 is the one-particle partition function. The free energy of N particles is determined by Z_N as $F_N = -kT \ln(Z_N)$.

A quantum in a one-dimensional square of width L has the energy levels

$$E(n) = \frac{n^2 \hbar^2 \pi^2}{2mL^2} = n^2 \theta(L), \quad (1)$$

where the quantum number $n = 1, 2, \dots$ and $\theta(L) = \hbar^2 \pi^2 / (2mL^2)$. We consider a gas of independent quantum particles in contact with a thermal bath at T . **3.1** Find a general expression for one-particle partition function $Z_1(T, L)$ and compute it in the low- T and high- T limits. Give a general expression for N -particle partition function $Z_N(T, L, N)$.

3.2 Derive an expression for the Helmholtz free energy of the particle and evaluate it in the low- T and high- T limit cases.

3.3 Derive an expression for the pressure $P(L, T)$ as function of L , T and N . Plot $(P \cdot L)/\theta$ as a function NkT/θ . Evaluate this expression in the low- T and high- T limit cases and discuss which one of them corresponds to the classical ideal gas.