7. Hausübung, **Statistische Physik**

abzugeben am Donnerstag, 1.12.2011

Aufgabe H12 *Photon gas* (6 Punkte)

a. Consider an ideal gas of relativistic bosons of mass m in a cube of side L at equilibrium at temperature τ and chemical potential μ. Assuming that the momenta are quantized in the same way as for a non-relativistic particle, and knowing that the energy of a relativistic particle of mass m and momentum p is

$$E = \sqrt{p^2c^2 + m^2c^4},$$

where c is the speed of light, write down the expected number $\langle s \rangle_{\vec{n}}$ of particles with a given discrete momentum state $\vec{p}(\vec{n})$ as a function of τ and μ.

b. Consider the quantum electromagnetic field in a cube of side L at thermal equilibrium at temperature τ. Suppose that instead of treating the electromagnetic field as a collection of harmonic oscillators, we want to view it as an ideal gas of relativistic particles called photons, as above. Find a consistent choice for the mass m of the photon and the chemical potential μ so as to make this interpretation hold.

c. Suppose that μ has the value found above, but that the particles are massive and non-relativistic, i.e. $p \ll mc$. Compute the heat capacity as a function of temperature (ignoring any constant proportionality factor). Observe that it is smooth, hence indicating the absence of a phase transition. In particular, there is no Bose-Einstein condensation. Explain what we have done differently that prevents the Bose-Einstein condensation. Note that for the same reason there is no Bose-Einstein condensation either for a photon gas (i.e. with $m = 0$).

Aufgabe H13 *Metropolis-Hastings algorithm* (6 Punkte)

The Metropolis-Hastings algorithm is an efficient way of sampling from a given probability distribution with a computer.
Suppose that the possible energy eigenstates of the system that we want to model are labelled by an integer i, and that ϵ_i is the energy of state i. We want to generate state i with a probability proportional to the Boltzmann factor $e^{-\beta\epsilon_i}$, where $\beta := 1/\tau$. The main problem in doing so is that we cannot in general compute the actual probabilities, because that would entail computing the partition function

$$Z = \sum_i e^{-\beta\epsilon_i}.$$

But this is rarely possible, and in doing so we would have solved the problem anyway.
The Metropolis-Hastings algorithm starts from an arbitrary state of the system, and successively modify it stochastically until, after a sufficient number of step, the probability of reaching any given state of the system is effectively given by Boltzmann's distribution.

a. Suppose that we take a certain state i and transition to state j with probability π_{ij}. The matrix π with elements π_{ij} is called a transition matrix. It must satisfy $\pi_{ij} > 0$ and $\sum_j \pi_{ij} = 1$.

   We say that π together with a probability distribution $p = \{p_1, p_2, \dots\}$ satisfy the *detailed balance* equation if

   $$p_i \pi_{ij} = p_j \pi_{ji} \quad \text{for all } i, j.$$

   Show that this conditions implies that, if the system is initially described by the probability distribution p then, after performing a random transition according to the matrix π, the state is still given by the same distribution p. We say that p is a fixed point of π.

b. In general, if a transition matrix has a fixed point p, then a recursive application of the transition matrix will make the probability distribution ultimately converge to that fixed point independently of the state we started from, provided certain conditions of ergodicity hold. This is how the Metropolis-Hastings algorithm works.

   The detailed balance condition provides an easy way to build a transition matrix whose fixed point is the Boltzmann distribution, without having to compute Z. Indeed, we just need to ensure that, for all pairs of states i, j, either $p_i \pi_{ij} = 0 = p_j \pi_{ji}$ or

   $$\frac{\pi_{ij}}{\pi_{ji}} = \frac{p_j}{p_i} = e^{-\beta(\epsilon_j - \epsilon_i)}.$$

   Use this to prove that one step of the algorithm you applied in the computer exercise C2 implements a transition matrix π which has the correct Boltzmann distribution as a fixed point.