Problem Sheet 4

for the lecture "Statistical Physics", Master course "Computational Science", year 2007/08

due date: Tuesday, November 27, 2007

Problem 1 2.5 points

Prove that in the canonic ensemble

$$\langle (\Delta E)^3 \rangle = -\frac{\partial^3 [ln(Z)]}{\partial \beta^3} \tag{1}$$

where Z is the partition function, and $\beta = 1/(k_B\, T)$. Using the previous result, show that in the canonic ensemble, it is possible to write

$$\langle (\Delta E)^3 \rangle = \langle (E - \langle \Delta E \rangle)^3 \rangle = k_B^2 \left\{ T^4 \left(\frac{\partial C_V}{\partial T} \right)_V + 2T^3 C_V \right\} \tag{2}$$

[**hint:** Take into account that $\langle (\Delta E)^2 \rangle = k_B\, T^2\, C_V$].

Problem 2 2.5 points

Consider a system which has only two states, one at energy 0, the other one at energy ϵ,

1. Calculate the canonical partition function $Z(\tau)$ and thereafter show that the internal energy U is given by
$$U(\tau) \;=\; \frac{\epsilon}{e^{\epsilon/\tau} + 1}\;.$$
2. The specific heat at constant volume (and constant number of particles) is defined as $C_V := \frac{\partial U}{\partial \tau}\big|_{V,N}$. Calculate C_V by using the result you just derived above.
3. Sketch both observables, the internal energy $U(\tau)$ and the specific heat $C_V(\tau)$, as a function of temperature. Pay special attention to their limiting behaviour at $\tau \to 0$ and $\tau \to \infty$. Did you expect such a behaviour?

Problem 3 2.5 points

Consider a one-dimensional harmonic oscillator. From Quantum Mechanics we know that the harmonic oscillator levels are discrete, labelled with their quantum number $n = 0, 1, 2, 3, \ldots$, and that their energy is given by $H(n) = \hbar\omega(n + \frac{1}{2})$, where $\hbar$ is Planck's constant (divided by 2π) and ω is the frequency of the oscillator. We will now be interested in the thermodynamic properties of such an oscillator.

1. Show that the canonical partition function of the harmonic oscillator is given by

$$Z(\tau) = \frac{e^{-\frac{\hbar\omega}{2\tau}}}{1 - e^{-\frac{\hbar\omega}{\tau}}} .$$

Hint: you will need the geometric series $\sum_{n=0}^{\infty} q^n = \frac{1}{1-q}$, valid for $|q| < 1$.

2. Calculate the internal energy $U(\tau) = \langle H \rangle$ and the specific heat at constant volume, which is defined as $C_V = \frac{\partial U}{\partial \tau}\big|_{V,N}$.

3. Either plot the internal energy $U(\tau)$ and the specific heat $C_V(\tau)$ numerically (any tool is fine) or sketch them roughly. In the latter case, first find the asymptotic behaviour of $U(\tau)$ and $C_V(\tau)$ for $\tau \to 0$ and for $\tau \gg \hbar\omega$.

Problem 4 2.5 points

Consider a particle of mass m in a constant gravitational field (i.e., a constant acceleration g downwards). Let the state of the particle be characterised by its height h above ground (see the little figure above). If we forget about the kinetic energy of the particle, the Hamiltonian is given by $H(h) = mgh$.

1. Calculate the partition function $Z(\tau)$. Notice that the height is a *continuous* variable; $0 \le h < \infty$. Therefore the sum occurring in the partition function must be replaced by an integral.

2. Calculate the probability $P(h)$ of finding the particle at height h and sketch your result.

3. Assume that the particle is an oxygen molecule ($m = 5.3 \times 10^{-26}\,\mathrm{kg}$) and that the temperature is $280\,\mathrm{K}$, *independent of height.* At which height $h_{1/2}$ has the probability of finding the particle dropped to half its value at sea level ($h = 0$)? This experiment is done on earth, hence $g \approx 10\,\mathrm{m/s^2}$.

4. What do you think: Would we have obtained a different result if we had not forgotten about the kinetic energy of the particle? (No points for this one, so you may freely speculate (or calculate)!)