L3 et Magistère de physique fondamentale,
DLMP & ENS-PSay

Mid-term exam of Statistical Physics
Wednesday 10 march 2021

Duration : **2hours**

The use of documents, mobile phones, calculators, . . . , is forbidden.

Recommendations :
Read the text carefully and **write** out your answers as *succinctly* and as *clearly* as possible.
Check your calculations (dimensional analysis, etc.) ; do not forget to **reread yourself**.
Check the **informations at the end of the text**

1 Frenkel defects(∼ 30mn)

Consider a crystalline solid made up of N atoms. In the ground state, atoms occupy the N sites of the crystal lattice, however, an atom can leave a site in the lattice and position itself at an interstitial site, which has an energy cost of $\varepsilon > 0$. We denote by N' the number of available interstitial sites (in general N and N' are of the same order of magnitude). If n atoms occupy interstitial sites (so $N - n$ atoms remain on the N sites of the crystal lattice), the energy of the atoms is $E = n\,\varepsilon$.

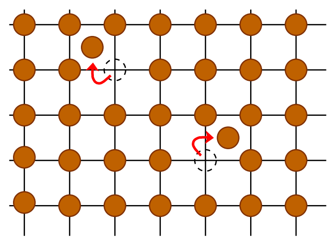

Figure 1 : *Crystal of $N = 35$ atoms with two Frenkel defects.*

1/ State the fundamental postulate of statistical physics.

2/ Recall the definitions of the microcanonical entropy S^* and the microcanonical temperature T^*.

3/ How many ways are there to pick the n atoms leaving the N sites on the lattice ? How many ways are there for these n atoms to occupy the N' interstitial sites ?

4/ Deduce from the previous question the number Ω of microstates corresponding to n atoms on the interstitial sites. Show that for $n \ll N,\ N'$ we have

$$\Omega \simeq \frac{(N'N)^n}{(n!)^2} \tag{1}$$

5/ Deduce the microcanonical entropy S^* atoms of the crystal and give its expression in the limit $N,\ N' \gg n \gg 1$.

6/ Deduce the expression of the temperature $T^*(E)$. Invert this function to determine how the number n of atoms on the interstitial sites depends on the temperature T^*, of N and of N'. Does the hypothesis $n \ll N,\ N'$ of the question **4**/ correspond to high or low temperatures ? Qualitatively plot n as a function of T^* in this regime and comment.

2 Conjugate variables in the microcanonical ensemble (∼ 40mn)

Consider a system whose energy depends on a parameter ϕ, a ≪ force ≫, conjugate to an observable X (for example the magnetic field $\phi \to \mathcal{B}$ and the magnetization $X \to M$). Said differently, the value of the observable in a microstate $|\,\ell\,\rangle$ is related to its energy by

$$X_\ell = -\partial E_\ell / \partial \phi\,. \tag{2}$$

If the system is isolated, we denote by $\overline{X}^*$ the microcanonical average of the observable (i.e. the average over the accessible states $\in [E, E+\delta E]$). Let us note S^* and T^* the microcanonical entropy and temperature. The objective of the exercise is to show the relation

$$\boxed{\overline{X}^* = T^* \frac{\partial S^*}{\partial \phi}} \tag{3}$$

and to discuss a simple application of this very general formula.

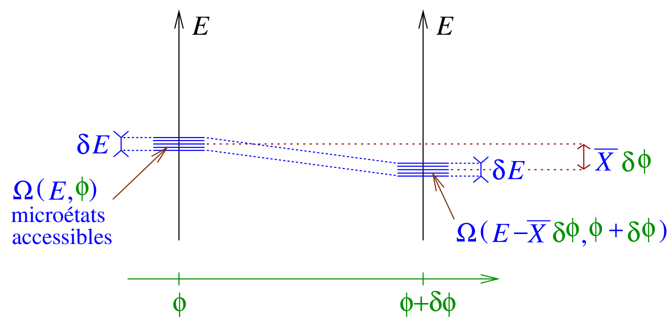

FIGURE 2 : *Evolution of the accessible microstates when changing the parameter $\phi \to \phi + \delta\phi$.*

We note $\Omega(E, \phi)$ the number of accessible microstates.

1/ If we consider an *adiabatic* transformation driven by a "small" variation of the force, $\phi \to \phi + \delta\phi$, the energy of the system changes like $E \to E - \overline{X}^*\,\delta\phi$, according to (2). Under such transformation, the number of accessible microstates is conserved (Fig. 2). Show the relation (3).

2/ Application : crystal of 1/2 spins

We apply these considerations in a very simple case : we consider an (isolated) crystal of N spins 1/2, under a magnetic field $\mathcal{B}$. We note $n_\pm$ the number of spins in the state $|\pm\rangle$ of energy $\varepsilon_\pm = \mp\varepsilon_{\mathcal{B}}$ with $\varepsilon_{\mathcal{B}} = m_0\,\mathcal{B}$ where m_0 is the magnetization of one spin.

a) Give the expression of the number of accessible microstates Ω as a function of N, n_+ and n_-.

b) Deduce the microcanonical entropy S^* (assuming N, $n_\pm \gg 1$). Justify that it can be written in the form $S^*(E, N, \mathcal{B}) = N\,k_B\,s(E/N\varepsilon_{\mathcal{B}})$ and give the expression of the dimensionless function $s(x)$.

c) Apply the formula (3) for the magnetization (i.e. $X \to M$ and $\phi \to \mathcal{B}$) and interpret the result.

d) *High temperature limit.*– Show that $s(x) \simeq \ln 2 - x^2/2$ for $x \ll 1$. Deduce an approximate expression of the magnetic temperature T^*. Give $\overline{M}^*$ as a function of N, m_0, $\mathcal{B}$ and T^*. Interpret the result.

e) Bonus (optional) : In the more general case of spins $s > 1/2$, which part of the analysis would change and which results would be unchanged ?

3 Anharmonic oscillator (∼ 45mn)

We consider a system in contact with a thermostat at temperature T.

1/ Give the definition of the canonical partition function Z (we note $|\,\ell\,\rangle$ the microstates and E_ℓ the energies).

2/ How do we deduce the average energy $\overline{E}^{\mathrm{c}}$ of the partition function (recall the demonstration).

3/ We consider a one-dimensional system described by its Hamiltonian $H(x,p)=\frac{p^2}{2m}+V(x)$. The system is treated classically.

a) Show that the partition function factorizes in the form $Z=Z_{\mathrm{cin}}Z_{\mathrm{pot}}$ where Z_{cin} and Z_{pot} are respectively associated with the kinetic and potential parts of the energy.

b) Calculate Z_{cin} and deduce the average kinetic energy $\overline{E}^{\mathrm{c}}_{\mathrm{cin}}$.

c) We will analyse Z_{pot} using an approximate potential $V(x)=\frac{1}{2}\kappa\,x^2+\lambda\,x^4$. In that respect, we write $\mathrm{e}^{-\beta V(x)}=\mathrm{e}^{-\frac{1}{2}(x/a_2)^2}\,\mathrm{e}^{-(x/a_4)^4}$. Give the expressions of the two length scales a_2 and a_4 as a function of T.

d) By plotting the shapes of $\mathrm{e}^{-\frac{1}{2}(x/a_2)^2}$ and $\mathrm{e}^{-(x/a_4)^4}$, justify that the quartic term is negligible within the limit of low temperatures. Deduce Z_{pot} and the contribution of the potential energy $\overline{E}^{\mathrm{c}}_{\mathrm{pot}}$ to the total average energy.

e) In the high temperature limit, the quadratic term of $V(x)$ is negligible. Show that $Z_{\mathrm{pot}}\propto\beta^{-\theta}$ and specify the value of the exponent θ. Infer $\overline{E}^{\mathrm{c}}_{\mathrm{pot}}$.

f) Calculate the specific heat $C_V=\partial\overline{E}^{\mathrm{c}}/\partial T$ in the two limits (with $\overline{E}^{\mathrm{c}}=\overline{E}^{\mathrm{c}}_{\mathrm{cin}}+\overline{E}^{\mathrm{c}}_{\mathrm{pot}}$). Identify the temperature scale $T_{\mathrm{crossover}}$ separating the two regimes, that you will express in terms of κ and λ. Qualitatively plot C_V and provide a physical interpretation.

Reread yourself (∼ 5mn)

Annex

- Stirling formula : $\ln N!\approx N\ln N-N$ for $N\gg 1$.
- $N!/(N-m)!\simeq N^m$ for $N\gg m$.
- $\int_{\mathbb{R}}\mathrm{d}x\,\mathrm{e}^{-a\,x^2}=\sqrt{\pi/a}$

Solutions sur la page du cours `http://lptms.u-psud.fr/christophe_texier/`