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

université PARIS-SACLAY

MID-TERM EXAM OF STATISTICAL PHYSICS

Wednesday 9th march 2022

Duration : **2h.**

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**.
Note that there is an **appendix**

1 Questions related to the lectures (∼ 15mn)

Consider a system in contact with a thermostat at temperature T. We denote by ℓ a microstate of the system and by E_ℓ the corresponding energy.

1/ Give the expression of the canonical distribution P^{c}_ℓ and recall the definition of the canonical partition function Z.

2/ How can one deduce the average energy $\overline{E}^{\mathrm{c}}$ from the canonical partition function ? (demonstrate the formula).

3/ Recall the definition of the free energy F. Let us introduce an observable X and its conjugated force ϕ (i.e. the mean value of the observable in the microstate ℓ is $X_\ell = -\partial E_\ell/\partial\phi$). Show that $\overline{X}^{\mathrm{c}} = -\partial F/\partial\phi$.

2 Einstein theory of specific heat (∼ 40mn)

Consider N identical quantum harmonic oscillators

$$H = \sum_{i=1}^{N} \left(\frac{p_i^2}{2m} + \frac{1}{2} m\omega^2\, q_i^2 \right) \tag{1}$$

We recall that the energy level $E_M = \hbar\omega\,(M + N/2)$, with $M \in \mathbb{N}$, has degeneracy $g_M = \frac{(M+N-1)!}{M!(N-1)!}$ (cf. tutorials).

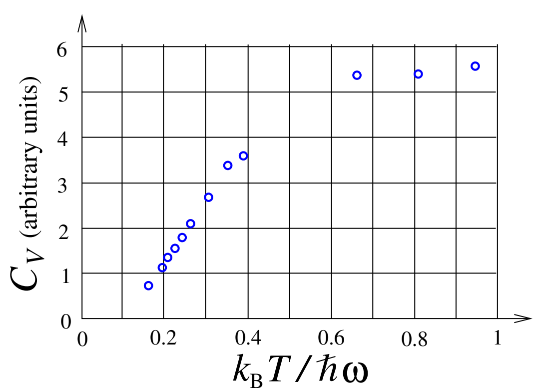

Figure 1: C_V (for one mole) as a function of $k_{\mathrm{B}}T^*/\hbar\omega$ for different solids. Data from the article : A. Einstein, "*Die Plancksche Theorie der Strahlung und die Theorie der spezifischen Wärme*" Annalen der Physik, **22**, p. 180 (1907).

1/ Question related to the lectures : Denote by Ω the number of accessible microstates. Recall the expression of the microcanonical entropy S^* and the definition of the microcanonical temperature T^*.

2/ If the energy of the system is $E = \hbar\omega\,(M + N/2)$, fixed, give the corresponding entropy $S^*(E)$ as a function of M and N (assume $M \gg 1$ and $N \gg 1$).

3/ Compute the microcanonical temperature T^*. Deduce an expression of E as a function of T^*.

4/ Compute the heat capacity $C_V = \partial E/\partial T^*$. Show that the result can be written under the form $C_V(T^*) = N k_\mathrm{B}\,\psi(\hbar\omega/k_\mathrm{B}T^*)$ where $\psi(x)$ is a dimensionless function. Give $\psi(x)$. Analyze the limiting behaviours in the low and high temperature regimes (define these two regimes). Plot *very neatly* C_V as a function of T^*.

5/ In his 1907 article on solid specific heat, Einstein has reported some experimental data for the heat capacity of various solid bodies (figure 1). Compare with your results and discuss physically.

3 Directed polymer (∼ 60mn)

Consider an **isolated** polymer made of N monomers of length a. The monomers are free to **choose one among three orientations** in the xOy plane : towards the left, the right or the top (but not towards the bottom, hence the terminology "directed polymer"). One end of the polymer is attached at the origin $(0,0)$ and the other end is at position (x,y). Different choices of orientations of the monomers correspond to different "microstates" of the polymer.

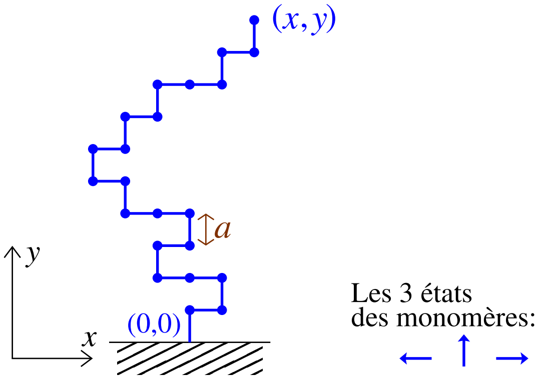

Figure 2: *A polymer attached on a substrate at the origin. Each monomer can have three orientations.*

In a first time, we assume that (x,y) are **fixed**. Denote by n_+ and n_- the number of monomers oriented to the right and to the left, respectively, and m the numbers of monomers oriented to the top (for exemple, on the figure one has $N = 22$, $n_+ = 7$, $n_- = 5$ and $m = 10$).

1/ One wishes to relate $n_\pm$ and m to x, y and $L = Na$. Express m and show that $n_\pm = (L - y \pm x)/2a$.

2/ Give the expression of the number of accessible microstates $\Omega(x,y)$, as a function of N, m, n_+ and n_-. Check you result by computing $\Omega_\mathrm{tot} = \sum_{x,y}\Omega(x,y)$ (in practice $\sum_{x,y} \to \sum_{n_+,\,n_-,\,m}$ with the constraint $n_+ + n_- + m = N$).

3/ Show that the microcanonical entropy of the polymer (for N, m, $n_\pm \gg 1$) is given by

$$S(x,y) \simeq -k_\mathrm{B}\left(n_+ \ln\frac{n_+}{N} + n_- \ln\frac{n_-}{N} + m\ln\frac{m}{N}\right) \tag{2}$$

4/ Compute $\frac{\partial S}{\partial x}$ and $\frac{\partial S}{\partial y}$ (as a function of m, n_+ and n_-). Deduce the values of m, n_+ and n_- (as a function of N) which maximize this entropy. We denote these values m^*, n_+^* and n_-^*. Give the corresponding values of x^* et y^* (as a function of L).

5/ We introduce $\phi_y(x,y) \overset{\text{def}}{=} T\,\frac{\partial S(x,y)}{\partial y}$ where T is the (microcanonical) temperature. What represents physically this quantity ? Express it as a function of x and y. Give the value of y for which $\phi_y(0,y) = 0$ and plot *neatly* $\phi_y(0,y)$ for $y \in [0,L]$. Interpret physically (in particular the behaviour $y \sim y^*$).

6/ For values of (x,y) close to (x^*,y^*), show that the entropy presents the limiting behaviour of the form

$$S(x,y) \simeq \text{cste} - \frac{k_\mathrm{B}}{2}\left[\frac{(x-x^*)^2}{\sigma_x^2} + \frac{(y-y^*)^2}{\sigma_y^2}\right] \qquad \text{pour } x\sim x^* \text{ et } y\sim y^* \tag{3}$$

and express σ_x^2 and σ_y^2.

7/ We now assume that **the constraint on** x **et** y **is removed** (i.e. x and y are now considered as *internal* variables). Express the distribution $p(x,y)$ of the end of the polymer as a function of $\Omega(x,y)$ and Ω_tot, and then as a function of $S(x,y)$. Discuss the result (where is the end of the polymer on average and the typical extensions in the two directions).

Reread yourself (~ 5mn)

Appendix :

- Multinomial Newton formula :

$$(x_1+\cdots+x_d)^N = \sum_{\substack{n_1,\cdots,n_d=0\\ \text{with } n_1+\cdots+n_d=N}}^{N} \frac{N!}{n_1!\cdots n_d!}\, x_1^{n_1}\cdots x_d^{n_d}$$

- Stirling formula : $\ln N! \simeq N\ln N - N + \mathcal{O}(\ln N)$ for $N\gg 1$.
- Fundamental identity of the *thermodynamic* : $\mathrm{d}E = T\,\mathrm{d}S - p\,\mathrm{d}V + \mu\,\mathrm{d}N + \cdots$

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