Statistical physics exam, duration 3h. One handwritten sheet and calculator allowed. **Frame your results**.

1 Melting temperature

In the model of a solid where each atom is identified with an independent classical harmonic oscillator and d is the interatomic distance, Lindemann (1910) suggested that the solid must melt when the average displacement of the atoms x_0 reaches a certain material-independent fraction $r = \frac{x_0}{d}$. We will study this hypothesis.

Let us consider a classical particle of mass m with one degree of freedom, i.e. whose state is characterised by its position $x \in \mathbb{R}$ and its momentum $p \in \mathbb{R}$. Its energy is assumed to be given by

$$E = \frac{1}{2m}p^2 + \frac{1}{2}Kx^2,$$

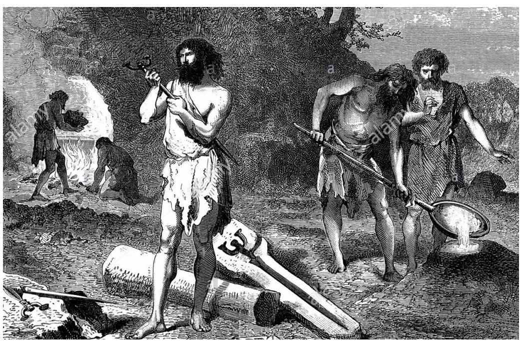
with $K > 0$.

The particle is in an environment at temperature T. We will note N_A the Avogadro number and $R = N_A k = 8.31\, J/K$

1. Express the Boltzmann law that gives the probability measure $P(x,p)\,dxdp$. Deduce the probability $P(x)\,dx$ for $x \in [x, x+dx]$, as a function of kT, K. Help: $\int_{\mathbb{R}} e^{-X^2} dX = \sqrt{\pi}$ and $\int_{\mathbb{R}} X^2 e^{-X^2} dX = \frac{\sqrt{\pi}}{2}$.
2. Deduce the mean values $\langle x \rangle, \langle x^2 \rangle$ as a function of kT, K.
3. Note the atomic mass $M = N_A m$, the Einstein temperature $\Theta = \frac{\hbar\omega}{k}$ with $\omega = \sqrt{\frac{K}{m}}$ and the distance between neighbouring atoms d. Calculate the mean vibration amplitude $x_0 := \langle x^2 \rangle^{1/2}$ as a function of $\Theta, T, M, R, \hbar, N_A$.
4. From the following data for different metals, $\frac{x_0}{d}$ is calculated at the melting temperature:

	Mg	Al	Cu	Zn	Ag	Pb
$M\ \ (g/mole)$	24.3	27.0	63.5	65.4	107.9	207.2
$T_F\ \ (K)$	924	933	1356	692	1234	601
$\Theta\ \ (K)$	340	400	320	230	220	92
$d\ \ (\text{Å})$	3.19	2.86	2.55	2.66	2.88	3.49
x_0/d	0.04	0.036	0.039	0.037	0.037	0.037

Is Lindemann's hypothesis valid? What formula can you propose in general to express Θ from the melting temperature?



2 Ionisation rate of a plasma

Hydrogen is the most abundant element in the universe, present in the atomic form H if the proton p^+ and electron e^- are bound, or in the ionised form, also called **plasma** if p^+ and e^- are separated. It is assumed that the particles p^+, e^- always have the same average density thus guaranteeing electrical neutrality. We will treat H, p^+, e^- as point particles without mutual interaction, i.e. as **perfect gases**. Let us note $\epsilon = 13.6\,\text{eV}$ the internal **binding energy** of each hydrogen atom.

1. The general model of a perfect gas is first studied. We consider N indistinguishable point particles of mass m, each possibly possessing an internal energy $\epsilon \geq 0$, free in a volume V, and of total energy E.

   (a) Calculate the expression for the entropy $S(E, V, N)$. Aids: apply Weyl's state counting formula. Divide the number of configurations by $N!$ to account for indistinguishability. The volume of the ball of radius R in $\mathbb{R}^d$ is $V = C_d R^d$ with $\ln(C_d) = \frac{d}{2}\ln\left(\frac{2\pi e}{d}\right) + o(d)$ and $\ln(d!) = d\ln\left(\frac{d}{e}\right) + o(d)$ if $d \gg 1$.

   (b) Recall the definitions of T, P, μ (temperature, pressure, chemical potential) and deduce the three relations

   $$E + N\epsilon = N\frac{3}{2}kT, \quad P = nkT, \quad e^{\frac{\mu+\epsilon}{kT}} = n\lambda^3$$

   with density $n = \frac{N}{V}$ and $\lambda := \left(\frac{2\pi\hbar^2}{mkT}\right)^{1/2}$ called «de Broglie thermal length».

2. The perfect gas model is now applied to each type of co-existing H, p^+, e^- particles. Explain why at equilibrium the temperatures of each gas are equal and the following relationship called **mass action law**

   $$\mu_H = \mu_p + \mu_e$$

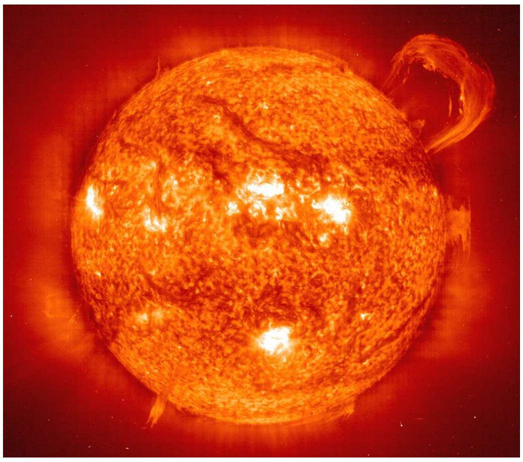
3. Deduce the following relationship for plasma called Saha equation (1920)]

   $$\frac{n_e n_p}{n_H} = \lambda_e^{-3} e^{-\frac{\epsilon}{kT}}$$

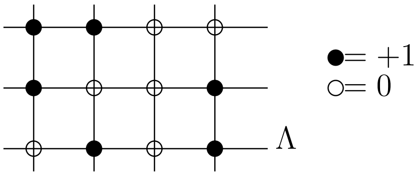
   with $\lambda_e := \left(\frac{2\pi\hbar^2}{m_e kT}\right)^{1/2}$ and electron mass m_e.

4. Let $n := n_H + n_p$. Use plasma neutrality and express the ionisation rate $r := \frac{n_p}{n} \in [0, 1]$ as a function of $\alpha := \frac{1}{n}\lambda_e^{-3} e^{-\frac{\epsilon}{kT}}$. Discuss the limiting cases $\alpha \gg 1$ and $\alpha \ll 1$. Numerical application: calculate r for the photosphere of the sun where $T = 6000K, n = 10^{23} m^{-3}$ giving $\alpha = 4\,10^{-8}$ and calculate r for a nebula where $T = 10^4 K, n = 10^{12} m^{-3}, \alpha = 3\,10^8$.

5. Comment on the physical meaning of α and this observation: in the universe, matter is in a plasma state in most cases, because either (a) the temperature is too high (e.g. star) or (b) the density is too low (e.g. gas in nebulae).



3 Simple gas-liquid transition model



We will study a **very simplified model of condensation of a gas of particles into a liquid** (Lee-Yang model 1952). This model is discrete and uses a finite (but large) size Λ network where each cell is either empty or contains a particle. Each site is denoted x and has a variable $n_x \in \{0, 1\}$ which is the presence or absence of a particle at that site. A **configuration** (or microstate)

$$n : x \in \Lambda \rightarrow n_x \in \{0, 1\}$$

is a choice $n_x \in \{0, 1\}$ for each point $x \in \Lambda$ of the network.

Let $\mu \in \mathbb{R}$ be given which is the chemical potential (imposed by an external environment). Denote $x \sim y$ if the x, y sites are close neighbours. The energy of configuration n is

$$E_{\text{gaz}}(n) := \sum_{x \sim y} (-n_x n_y) \tag{3.1}$$

where the sum relates to all pairs of neighbouring sites. For a given configuration n, we denote $N(n)$ the total number of particles,

$$E_{GC}(n) := E_{\text{gaz}}(n) - \mu N(n)$$

the canonical grand energy and

$$\rho(n) := \frac{1}{|\Lambda|} N(n)$$

the density of particles, where $|\Lambda|$ the number of sites on the lattice. According to Boltzmann's law, the probability that a configuration n appears is

$$p_T(n) = \frac{1}{Z} \exp\left(-\frac{1}{kT} E_{GC}(n)\right),$$

where T is the temperature and k the Boltzmann constant. The objective of the problem is to study the mean density

$$\langle \rho \rangle := \sum_n p_T(n) \rho(n)$$

as a function of the temperature T and the chemical potential μ (i.e. phase diagram). For that we will use the known results of the Ising model.

We recall that in the **Ising model**, on the same lattice Λ, we note $f_x \in \{-1, +1\}$ the magnetization at the site x and

$$x \in \Lambda \rightarrow f_x \in \{-1, 1\}$$

a configuration. The energy is

$$E_{\text{Ising}}(f) := \sum_{x \sim y} (-f_x f_y) - B \sum_{x \in \Lambda} f_x$$

where $B \in \mathbb{R}$ is the external magnetic field. The magnetisation is

$$M(f) := \frac{1}{|\Lambda|} \sum_{x \in \Lambda} f_x.$$

1. For a given configuration n, express the total number of particles $N(n)$.

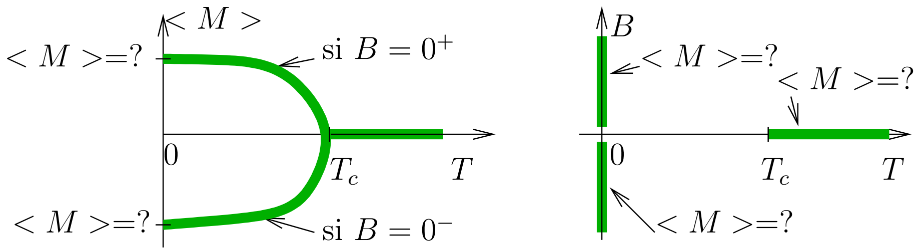
It will be shown that the Lee-Yang gas model can be matched to the Ising model.

2. A configuration $n : x : x \in \Lambda \to n_x \in \{0,1\}$ corresponds to a configuration $f : x : x \in \Lambda \to f_x \in \{-1,1\}$. For each $x \in \Lambda$, express $f_x \in \{-1,1\}$ from $n_x \in \{0,1\}$ by a simple formula?

3. With this correspondence, we write $\frac{1}{kT_{\text{gaz}}} E_{GC}(n) = \frac{1}{kT_{\text{Ising}}} E_{\text{Ising}}(f) + C$ where C is a constant. Express T_{gaz} from T_{Ising} and express μ from B.

4. Express the density $\rho(n)$ from the magnetisation $M(f)$ and similarly for the mean density $\langle \rho \rangle$ from the mean magnetisation $\langle M \rangle$.

We recall some known results for the Ising model in a square two-dimensional lattice: There is a phase transition temperature $kT_c = \left(\frac{1}{2} \ln\left(1+\sqrt{2}\right)\right)^{-1}$ and a phase diagram of the following form (where $B = 0^{\pm}$ means $0 < \pm B \ll 1$)



5. Complete this phase diagram by replacing the "?" signs with precise values for the Ising model.

6. Derive the analogous phase diagram for the gas model by replacing the axes, quantities and values with the appropriate ones. Comment.