First set of exercises: Statistical Mechanics

1) The energy of a system of N localized magnetic ions at temperature T in the presence of fields H and D may be written as $\mathcal{H} = D\sum_{i=1}^{N} S_i^2 - \mu_0 H \sum_{i=1}^{N} S_i$, where D, μ_0 and H are positive and S_i can assume the values $-1, 0$ ou $+1$ for all sites i.
a) Obtain expressions for the inernal energy, entropy and magnetization per site.
b) In zero field $H = 0$, sketch graphs of internal energy, entropy and specifical heat per site versus the temperature. Indicate the behavior of these quantities in the limits of $T \to 0$ and $T \to \infty$.
c) Calculate the "quadrupole moment" $q = \frac{1}{N}\langle S_i^2 \rangle$ versus H, D and T.

2) Consider a system of N particles, in which each one can occupy only two levels with energies 0 e ϵ, respectively. The system is placed in contact with a thermal reservoir of temperature T.
a) Obtain the partition function $Z(T, N)$ as well as the internal energy and specific heat per site $u(T), c(T)$ as a function of T.
b) Obtain an equation of state for the pressure $p = p(T, v)$ by introducing the effect of volume $v = V/N$ according to the following $\epsilon = a/v^\gamma$, with $a > 0$.

4) The energy of a system of N localized magnetic ions at temperature T in the presence of field H is given by the Hamiltonian

$$\mathcal{H} = -J \sum_{i=1,3,\ldots,N-1}^{N} \sigma_i \sigma_{i+1} - H \sum_{i=1}^{N} \sigma_i, \tag{1}$$

where parameters J e H are positive and $\sigma = \pm 1$ for all sites i. Assume that N is old and the first summation is carried out over only odd sites i.
a) Obtain the partition function $Z(T, H)$ and the internal energy $u = u(T, H)$ and entropy $s(T, H)$. Sketch a graph of $u(T, H = 0)$ and $s(T, H = 0)$ versus T.
b) Evaluate the magnetization per particle $m = m(T, H)$ and the magnetic susceptibilitty e para a suscetibilidade magnética $\chi = \chi(T, H) = (\frac{\partial m}{\partial H})_T$. Sketch a graph of $\chi(T, H = 0)$ versus T.

5) Consider a system of N noninteracting and localized particles. The single-particle states have energies $\epsilon_n = n\epsilon$ and are n times degenerate, where $\epsilon > 0$ and $n = 1, 2, 3, \ldots$.
a) Calculate canonical partition function.
b) Obtain expressions for the internal energy and entropy as a function of T. What are their asymptotic expressions in the limit of high temperatures?

6) a) Show that $S/k_B = \beta^2 \frac{\partial F}{\partial \beta}$ and expresses S in terms of Z and its derivatives with respect to β.
b) Show that $c_v = -\beta(\frac{\partial s}{\partial \beta})_v$ and also expresses c_v as a function of Z and its derivatives with respect to β.

7) Consider a system of N ultrarelativistic classical particles constrained in a recipi-

ent of volume V under the temperature T, described by the following Hamiltonian

$$\mathcal{H} = \sum_{i=1}^{N} c|p_i|, \tag{2}$$

where $c > 0$ is a constant. Obtain the classical partition function and the entropy per particle as a function of T and $v = V/N$. Obtain the specific heat at constant volume C_v.

8) Consider a system of N harmonic oscillators given by the following Hamiltonian

$$\mathcal{H} = \sum_{i=1}^{N} [\frac{p_i^2}{2m} + \frac{m\omega^2}{2} x_i^n], \tag{3}$$

where n is an even number and positive. Obtain the specific heat for this system.

9) The equation of state for the nitrogen gas at low densities can be written in the following form

$$\frac{pV}{Nk_B T} = 1 + A(T)\frac{N}{V}. \tag{4}$$

Above are listed some experimental results for the second virial coefficient $A(T)$ as a function of temperature Suppose that the intermolecular potential of gas nitrogen

T(K)	A/k_B (K/atm)
100	-1,8000
200	-0.4260
300	-0,0549
400	+0,1120
500	+0,2050

is given by $V(r) = \infty$ se $0 < r < \sigma$, $-\epsilon$, if $\sigma < r < r_0$ and 0 for $r > r_0$. Use the experimental data of this table to obtain the best values of σ, ϵ e r_0. *Dica: Mostre que a expressão para $A(T)$ pode ser escrita da seguinte forma: $A = k_B[a - b\exp(c/T)]$. Um ajuste não linear fornecerá os valores de a, b e c. Encontre em seguida σ, ϵ e r_0.*

10) Show that the grand-canonical entropy can be written in the following form $S = -k_B \sum_j P_j \ln P_j$, where the probability P_j associate with microscopic state j is given by the expression $\Xi^{-1}\exp(-\beta E_j + \beta\mu N_j)$.

11) Considere o gás clássico ultra-relativístico do exercício 1) em contato agora com um reservatório térmico e de partículas. Obtenha a grande função de partição e o potencial grande canônico desse sistema.

12) Show that the average quadratic deviation of particle number may be written as

$$\langle(\Delta N)^2\rangle = \langle N_j^2\rangle - \langle N_j\rangle^2 = z\frac{\partial}{\partial z}[z\frac{\partial}{\partial z}\ln\Xi(\beta, z)]. \tag{5}$$

Obtain an expression for the relative deviation $\sqrt{\langle(\Delta N)^2\rangle}/\langle N_j\rangle$ for an ideal monoatomic classical gas.

13) A uma temperatura T, uma superfície com N_0 centros de adsorção tem $N \leq N_0$ moléculas adsorvidas. Supondo que não haja interação entre as moléculas, mostre que o potencial químico do gás adsorvido pode ser escrito da seguinte forma

$$\mu = k_B T \ln \frac{N}{(N_0 - N)a(T)}. \tag{6}$$

Qual seria a interpretação da função $a(T)$?
14) Mostre que a equação de estado

$$pV = \frac{2}{3}U, \tag{7}$$

vale tanto para bósons e férmions quanto no limite clássico. Mostre que para o gás ideal ultrarelativístico, dado pela relação $e = \hbar ck$ também vale esta equação de estado.
15) Mostre que o potencial químico de um gás clássico de N partículas monoatômicas no volume V, a temperatura T pode ser escrito na forma

$$\mu = k_B T \ln(\frac{\lambda^3}{v}), \tag{8}$$

onde $v = \frac{V}{N}$ e $\lambda = \frac{h}{\sqrt{2\pi m k_B T}}$ é o comprimento de onda térmico. Obtenha agora a primeira correção quântica desse resultado. Isto é, mostre que

$$\mu - k_B T \ln(\frac{\lambda^3}{v}) = A(\frac{\lambda^3}{v}) + ... \tag{9}$$

e obtenha explicitamente o prefator A nos casos de férmions e bósons.

16) Considere um sistema de N elétrons livres, dentro de uma região de volume V, num regime ultrarelativístico. O espectro de energia é dado por

$$e = [p^2c^2 + m^2c^4]^{1/2} \sim pc, \tag{10}$$

onde $\vec{p}$ é o momento linear.
a) Calcule a energia de Fermi desse sistema; b) Qual é a energia do sistema no estado fundamental; c) Obtenha uma forma assintótica para o calor específico a volume constante no limite $T << T_F$.

17) Considere um sistema de férmions num espaço $d-$dimensional, com espectro de energia

$$e_{\vec{k},\sigma} = c|\vec{k}|^a, \tag{11}$$

onde $c > 0$ e $a > 1$.
a) Calcule o prefator A da relação $pV = AU$;
b) Calcule a energia de Fermi em função do volume V e do número de partículas N;

c) Calcule uma forma assintótica, quando $T << T_F$, para o calor específico a volume constante.

18) Obtain expressions for the mean energy, pressure and compressibility of a gas of free fermions at null temperature. By using data for the metalic sodium, obtain a numerical estimation for the compressibility and compare with experimental values at room temperature.

19) Let us consider an ideal gas of bosonic particles (spinless) and mass m. Obtain an expression for the Bose-Einstein condensation temperature in the following cases:
a) A spectrum of energy given by $\epsilon = \hbar c k$,
b) For a system whose density of states $D(\epsilon)$ is given by $D(\epsilon) = \alpha\epsilon^2$ for $\epsilon > 0$ and 0 otherwise, with α being a positive constant.

20) Let us consider an ideal gas of bosonic particles (spinless) and mass m constrained in a volume V.
a) Show that the Bose-Einstein condensation temperature T_0 is given by the following expression

$$S = k_B \frac{V}{\lambda^3}[\frac{5}{2} g_{5/2}(z) - \frac{\mu}{k_B T} g_{3/2}(z)], \tag{12}$$

where $g_\alpha = \sum_{n=1}^{\infty} \frac{z^n}{n^\alpha}$.
b) Given N and V, obtain an expression for the entropy below T_0? What is the entropy associated to the condensed?
c) From the expression for the entropy, show that the specific heat c_V at constant volume above T_0 is given by the expression

$$c_V = \frac{3}{4} k_B [5 \frac{g_{5/2}(z)}{g_{3/2}(z)} - 3 \frac{g_{3/2}(z)}{g_{1/2}(z)}], \tag{13}$$

d) Show that c_V is given by the expression

$$c_V = \frac{15}{4} k_B \frac{v}{\lambda^3} g_{5/2}(1) \tag{14}$$

for $T < T_0$.

21) Let us consider a gas of free bosons constrained in a surface of area A. Show that there is no Bose-Einstein condensation in such a case.