D-Dimensional Statistical Mechanics in Fractional Classical and Quantum Mechanics

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ABSTRACT: In this work, we focus our study on some systems in statistical mechanics based on the fractional classical and quantum mechanics in any positive spatial dimension D. At the first stage we present the thermodynamical properties of the classical ideal gas and the system of N classical oscillators. In each case, the Hamiltonian exhibits fractional exponents of the phase space (position and momentum). At the second stage, in the context of the fractional quantum mechanics, we have studied the Bose-Einstein statistics with the related problem of the condensation and the Fermi-Dirac.

KEYWORDS: fractional calculus, fractional quantum mechanics, quantum statistics, partition function.

RÉSUMÉ : Dans ce travail, nous nous intéressons à l'étude de certains systèmes en mécanique statistique basée sur la mécanique classique et quantique fractionnaire dans toute dimension D. Au premier lieu, nous présentons les propriétés thermodynamiques du gaz idéal classique et le système de N oscillateurs classiques. Dans chaque cas, l'hamiltonien présente des puissances fractionnaires de l'espace des phases (de position et l'impulsion). En deuxième étape, dans le contexte de la mécanique quantique fractionnaire, nous avons étudié les statistiques de Bose-Einstein et de Fermi-Dirac avec le problème associé de la condensation.

MOTS-CLÉS : calcul fractionnaire, la mécanique quantique fractionnaire, statistiques quantiques, fonction de partition.

1. Introduction

Since some years, research has intensified and diversified in the calculation of the fractional derivatives. These are applied quickly thereafter, to physics and to engineering. This kind of calculation is due to Riemann and Liouville pioneers. This consists to make derivatives with non-integer order of functions. More precisely, instead to make a derivative of the first order (order 1) or a derivative of second order (order 2), we make a derivative of an intermediate order between 1 and 2. We then speak, for example, of the fractional derivative of order 1/2 or 3/4. This concept was developed recently by I. Podlubny (1999) [1]. In physics, we often deal with differential equations or with partial differential equations. What happens if these equations present the fractional derivative? In quantum mechanics, the results arising from this new concept are discussed by several authors [2-5]. The focus of this paper is to see how the fundamental problems of statistical physics, both classical and quantum, will be affected by using the fractional derivatives. Section 2 start with defining fractional classical Hamiltonian for two classical systems: N particles ideal gas and N independent fractional oscillators in D-dimensional space. Using the canonical ensemble, we have developed the thermodynamical properties of the system (N particles ideal gas and N independent fractional oscillators in D-dimensional space). By performing the limit $\alpha = 2$, $\nu = 2$ and D=3, we have recovered the well-known results for the 3-dimensional ideal gas and N independent oscillators. In section 3, we have studied the ideal gases (Bose and Fermi gases) in grand canonical ensemble. We emphasize a subsection to discuss how the critical temperature of the ideal Bose gas is affected by the fraction parameter α. By putting $\alpha = 2$ and D=3, we have recovered the standard results relative to the quantum Bose gas. We close this work by a conclusion in section 4.

2. Classical statistical mechanics

2. 1. Ideal gas

The canonical partition function of a classical ideal gas composed of N particles occupying a volume V at a temperature T is given by:

$$Z_N = \frac{(Z_1)^N}{N!} \tag{1}$$

where Z_1 is the individual partition function of a free particle in the canonical ensemble:

$$Z_1 = \int \frac{d^D p \, d^D x}{h^D} e^{-\beta H_\alpha(\vec{p},\vec{x})} \tag{2}$$

where:

$$H_\alpha(\vec{p},\vec{x}) = D_\alpha |\vec{p}|^\alpha \tag{3}$$

$\beta = (K_B T)^{-1}$ (K_B is Boltzmann constant and T is the temperature) and D_α is a constant to choose preserving the dimension of the energy for $H_\alpha(\vec{p},\vec{x})$. α is a parameter greater than one and less than or equal to two ($1 \leq \alpha < 2$). For $\alpha = 2$ the equation (3) must represent the free particle Hamiltonian, then $D_2 = (2m)^{-1}$. In quantum mechanics $|\vec{p}|^\alpha$ becomes a fractional derivative. As $H_\alpha(\vec{p},\vec{x})$ given by (3) doesn't depend on the position $\vec{x}$, the integral over $\vec{x}$ in (2) gives the system volume V. The integral over $\vec{p}$ in (2) is performed by using the spherical coordinates, we find that:

$$Z_1 = \frac{2\pi^{D/2} V}{\Gamma\left(\frac{D}{2}\right) h^D \alpha (\beta D_\alpha)^{D/\alpha}} \Gamma\left(\frac{D}{\alpha}\right) \tag{4}$$

where $\Gamma(x)$ is Euler Gamma function. Note here that N. Laskin [6] has calculated Z_1 only in one dimension. The last result (4) can be transformed into $Z_1 = \frac{V}{\lambda_g^3}$ where we have defined a novel generalized thermal wave length [7]:

$$\lambda_g = \left(\frac{\Gamma\left(\frac{D}{2}\right) h^D \alpha (\beta D_\alpha)^{D/\alpha}}{2\pi^{D/2} \Gamma\left(\frac{D}{\alpha}\right)} \right)^{1/D} \tag{5}$$

Finally, we get the classical partition function for the ideal gas whose fractional Hamiltonian presents a non integer power of the momentum p (see formula (3)):

$$Z_N = \frac{1}{N!} \left(\frac{2\pi^{D/2} V}{\Gamma\left(\frac{D}{2}\right) h^D \alpha (\beta D_\alpha)^{D/\alpha}} \Gamma\left(\frac{D}{\alpha}\right) \right)^N = \frac{1}{N!} \left(\frac{V}{\lambda_g^D} \right)^N \tag{6}$$

It is easy to see that when putting $\alpha = 2$ and D=3 in formula (5-6), we retrieve the usual thermal wave-length $\lambda_{th} = h/\sqrt{2\pi n K_B T}$ and the usual partition function $Z_N = \frac{1}{N!} \left(\frac{V}{\lambda_{th}^3} \right)^N$. Using Stirling formula we deduce the free energy or Helmholtz energy of the ideal gas

$$F = -K_B T \log Z_N = N K_B T \log\left(\frac{V}{\lambda_g^D N} + 1 \right) \tag{7}$$

When the partition function Z_N and the Helmholtz's energy F are known it is easy to compute all the remaining thermodynamical quantities of the system.

2. 1. 1. Internal Energy and specific heat
The internal energy for the ideal gas is the mean value of its kinetic energy E_c:

$$U = -\frac{\partial \log Z_N}{\partial \beta} = \frac{D}{\alpha} N K_B T \qquad (8)$$

and the specific heat at constant volume:

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V = \frac{D}{\alpha} N K_B \qquad (9)$$

2. 1. 2. Entropy
The entropy of the system in the canonical ensemble is given by:

$$S = -\left(\frac{\partial F}{\partial T}\right)_V = N K_B \log\left(\frac{V}{\lambda_g^D N} + \frac{D}{\alpha} + 1\right) \qquad (10)$$

2. 1. 3. State equation
The canonical pressure of the system is given by:

$$P = -\left(\frac{\partial F}{\partial V}\right)_T = \frac{N K_B T}{V} \qquad (11)$$

We remark here that the state equation is independent of the parameter α whereas all other thermodynamical quantities depend. This remark holds also when we use the micro-canonical ensemble.

2. 2. Fractional oscillators system
Consider now a system composed of N classical independent three-dimensional fractional oscillators. The hamiltonian of this system is given by [8,9]:

$$H_{\alpha,v} = \sum_{i=1}^{N}\left(D_\alpha |p_i|^\alpha + |r_i|^v\right) \qquad (12)$$

where q is a constant with dimension [q] = erg$^{1/2}$cm$^{-v/2}$, α and v are parameters such as $1 \le \alpha < 2$, $1 \le v < 2$.

The canonical partition function for the classical system is given by:

$$Z_N = \frac{1}{N!}\left(\int_0^\infty d^D p\, d^D r\, e^{-\beta H_{\alpha,v}(p,r)}\right)^N \qquad (13)$$

Then

$$Z_N = \frac{1}{N!}\left(\int_0^\infty d^D p\, d^D r\, e^{-\beta\left(D_\alpha |p|^\alpha + q^2 |r|^\alpha\right)}\right)^N \qquad (14)$$

A simple calculation gives:

$$Z_N = \frac{1}{N!}\left(\frac{4\pi^D \Gamma\left(\dfrac{D}{\alpha}\right)\Gamma\left(\dfrac{D}{v}\right)}{\Gamma^2\left(\dfrac{D}{2}\right) h^D \alpha v \left(\beta D_\alpha\right)^{D/\alpha}\left(\beta q^2\right)^{D/v}}\right)^N \qquad (15)$$

If we express the Helmholtz energy (using the Stirling formula),

$$F = -K_B T \log Z_N = -NK_B T \log\left(1 + \frac{4\pi^D \Gamma\left(\frac{D}{\alpha}\right)\Gamma\left(\frac{D}{v}\right)}{\Gamma^2\left(\frac{D}{2}\right)h^D \alpha v (\beta D_\alpha)^{D/\alpha}\left(\beta q^2\right)^{D/v}}\right) \tag{16}$$

2. 2. 1. Energy and specific heat

The internal energy in the canonical ensemble is given by:

$$U = -\frac{\partial \log Z_N}{\partial \beta} = \left(\frac{D}{\alpha} + \frac{D}{v}\right)NK_B T \tag{17}$$

and the specific heat at constant volume:

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V = \left(\frac{D}{\alpha} + \frac{D}{v}\right)NK_B \tag{18}$$

3. Quantum statistical mechanics

3. 1. Ideal Bose gas

We will now consider N particles with zero spin (bosons) without interaction, enclosed in a volume V. We assume that the system is in thermodynamical equilibrium with a thermostat at temperature T. We will study some properties of the ideal gas of bosons in the fractional case. To address the problem of an ideal gas of bosons, we use the grand canonical partition function D(z, V, T) [10]:

$$D(z,V,T) = \prod_i \frac{1}{1 - ze^{-\beta \varepsilon_i}} \tag{19}$$

where ε_i is the energy of the single-particle. we assume that ε_i is given by:

$$\varepsilon_i = D_\alpha |p|^\alpha \tag{20}$$

and z is the fugacity of the gas which is related to the chemical potential μ through the formula:

$$z = e^{\beta\mu} \tag{21}$$

or equivalently, the grand partition function is:

$$D(z,V,T) = \prod_p \frac{1}{1 - ze^{-\beta D_\alpha p^\alpha}} \tag{22}$$

Using this expression we can derive some thermodynamical properties of the Bose gas system in the case of fractional quantum mechanics.

3. 1. 1. State Equation

In the grand canonical ensemble of equilibrium statistical mechanics, the state equation is given by:

$$\begin{cases} \dfrac{PV}{K_B T} = \log D(z,V,T) = -\sum_1^\infty \log\left(1 - ze^{-\beta D_\alpha p^\alpha}\right) - \log(1 - z) \\[3mm] N = z\dfrac{\partial \log D(z,V,T)}{\partial z} = \sum_1^\infty \dfrac{ze^{-\beta D_\alpha p^\alpha}}{1 - ze^{-\beta D_\alpha p^\alpha}} + \dfrac{z}{1 - z} \end{cases} \tag{23}$$

where P and N are respectively the pressure and the total number average of particles of the system. The last sums can be extended to an integral:

$$\begin{cases} \dfrac{PV}{K_B T} = -\dfrac{2\pi^{D/2}V}{\Gamma\left(\frac{D}{2}\right)h^D}\int_0^\infty p^{D-1}dp \log\left(1 - ze^{-\beta D_\alpha p^\alpha}\right) - \log(1 - z) \\[4mm] N = \dfrac{2\pi^{D/2}V}{\Gamma\left(\frac{D}{2}\right)h^D}\int_0^\infty p^{D-1}dp \dfrac{ze^{-\beta D_\alpha p^\alpha}}{1 - ze^{-\beta D_\alpha p^\alpha}} + \dfrac{z}{1 - z} \end{cases} \tag{24}$$

Performing the integrals we find:

$$\begin{cases} \dfrac{P}{K_B T} = \dfrac{2\pi^{D/2}\Gamma\left(\dfrac{D}{\alpha}\right)}{\alpha\Gamma\left(\dfrac{D}{2}\right)h^D(\beta D_\alpha)^{D/\alpha}} g_{\left(\frac{D}{\alpha}+1\right)}(z) - \dfrac{1}{V}\log(1-z) \\[4mm] \dfrac{N}{V} = \dfrac{2\pi^{D/2}\Gamma\left(\dfrac{D}{\alpha}\right)}{\alpha\Gamma\left(\dfrac{D}{2}\right)h^D(\beta D_\alpha)^{D/\alpha}} g_{\left(\frac{D}{\alpha}\right)}(z) + \dfrac{z}{V(1-z)} \end{cases} \tag{25}$$

where:

$$g_r(z) = \sum_{l=0}^{\infty} \frac{z^l}{l^r} \tag{26}$$

is Bose function.

The state equation can be obtained by eliminating z from the two following coupled equations:

$$\begin{cases} \dfrac{P}{K_B T} = \dfrac{1}{\lambda_g^D} g_{\left(\frac{D}{\alpha}+1\right)}(z) - \dfrac{1}{V}\log(1-z) \\[4mm] \dfrac{N}{V} = \dfrac{1}{\lambda_g^D} g_{\left(\frac{D}{\alpha}\right)}(z) + \dfrac{z}{V(1-z)} \end{cases} \tag{27}$$

Where λ_g is the generalized thermal wave length. Now look at the equations (27) when we perform the thermodynamical limit (N and V going to infinity keeping the ratio N/V equal to a constant):

a) when z < 1 then (27) becomes:

$$\begin{cases} \dfrac{P}{K_B T} = \dfrac{1}{\lambda_g^D} g_{\left(\frac{D}{\alpha}+1\right)}(z) \\[4mm] \dfrac{N}{V} = \dfrac{1}{\lambda_g^D} g_{\left(\frac{D}{\alpha}\right)}(z) \end{cases} \tag{28}$$

These coupled equations correspond to the state equation for the case z < 1.

b) When z goes to 1 $(z \to 1)$, the term

$$\frac{z}{V(1-z)} = \frac{N_0}{V} \tag{29}$$

becomes a significative fraction of the total particles density, whereas the term

$$\frac{1}{V}\log(1-z) = -\frac{1}{V}\log(N_0+1) \tag{30}$$

is negligible. In this case the coupled state equations become:

$$\begin{cases} \dfrac{P}{K_B T} = \dfrac{1}{\lambda_g^D} g_{\left(\frac{D}{\alpha}+1\right)}(1) \\[4mm] \dfrac{N}{V} = \dfrac{1}{\lambda_g^D} g_{\left(\frac{D}{\alpha}\right)}(1) + \dfrac{N_0}{V} = \dfrac{1}{\lambda_g^D} g_{\left(\frac{D}{\alpha}\right)}(1) + \dfrac{N}{V}\left(1 - \left(\dfrac{T}{T_C}\right)^{D/\alpha}\right) \end{cases} \tag{31}$$

where N_0 is the mean number of bosons occupying the state of zero energy (k=0) and T_C is the Bose temperature that will be defined in the next subsection. We remark here that in the case of z=1, the pressure (31) is independent of the volume V. This case obviously corresponds to situation where the temperature T is less than T_B.

When $T > T_B$, we immediately find, the internal energy of the system:

$$U = -\left(\frac{\partial D(z,V,T)}{\partial \beta}\right)_{V,z} = \frac{D}{\alpha}K_B T V \frac{g_{\left(\frac{D}{\alpha}+1\right)}(z)}{\lambda_g^D} \tag{32}$$

and the specific heat at constant volume and mean number N:

$$C_V = \left(\frac{\partial U}{\partial T}\right)_{V,N} \tag{33}$$

Using the properties:

$$z\frac{\partial g_n(z)}{\partial z} = g_{n-1}(z) \tag{34}$$

and

$$\left.\frac{\partial z}{\partial T}\right|_{V,N} = -\frac{Dz}{\alpha T}\frac{g_{D/\alpha}(z)}{g_{D/\alpha-1}(z)} \tag{35}$$

we find:

$$\frac{C_V}{NK_B} = \frac{V(D\alpha+D^2)}{\alpha^2 N}\frac{g_{(D/\alpha+1)}(z)}{\lambda_g^D} - \frac{D^2}{\alpha^2}\frac{g_{D/\alpha}(z)}{g_{(D/\alpha-1)}(z)} \tag{36}$$

and the Helmoltz energy:

$$F = N\mu - PV = NK_B T\left(\log z - V\frac{g_{(D/\alpha+1)}(z)}{\lambda_g^D}\right) \tag{37}$$

and the entropy of the system of bosons:

$$S = \frac{U-F}{T} = \frac{D+\alpha}{\alpha}VK_B\frac{g_{(D/\alpha+1)}(z)}{\lambda_g^D} - NK_B\log z \tag{38}$$

We mention here, that all above results lead to the well known standard results when we put $\alpha = 2$ and D=3.

3. 1. 2. Bose-Einstein Condensation
Following the same procedure to demonstrate the Bose-Einstein condensation (for the case of spin zero), we find for $T < T_B$, that the density of the excited particles (that occupying the energy level $\varepsilon > 0$):

$$N_{\varepsilon>0}^{\max} = \frac{2\pi^{D/2}\Gamma\left(\frac{D}{\alpha}\right)V}{\alpha\Gamma\left(\frac{D}{2}\right)h^D(\beta D_\alpha)^{D/\alpha}}g_{\left(\frac{D}{\alpha}\right)}(1) \tag{39}$$

and the density of particles occupying the fundamental energy level ($\varepsilon = 0$):

$$N_0(\varepsilon = 0) = N\left(1-\left(\frac{T}{T_B}\right)^{D/\alpha}\right) \tag{40}$$

where:

$$T_B = \frac{D_\alpha}{K_B}\left(\frac{\alpha\Gamma\left(\frac{D}{2}\right)h^D N}{2\pi^{D/2}\Gamma\left(\frac{D}{\alpha}\right)Vg_{\left(\frac{D}{\alpha}\right)}(1)}\right)^{\alpha/D} \tag{41}$$

is the Bose temperature.

For D=3, the ground-state fraction can be written as:

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_C}\right)^{3/\alpha} \tag{42}$$

And:

$$\frac{N_e}{N} = \left(\frac{T}{T_C}\right)^{3/\alpha} \tag{43}$$

A plot of $\frac{N_0}{N}$ and $\frac{N_e}{N}$ are shown in curves 1 and 2 in figure 1 for $\alpha = 1, 1.5,$ and $\alpha = 2$
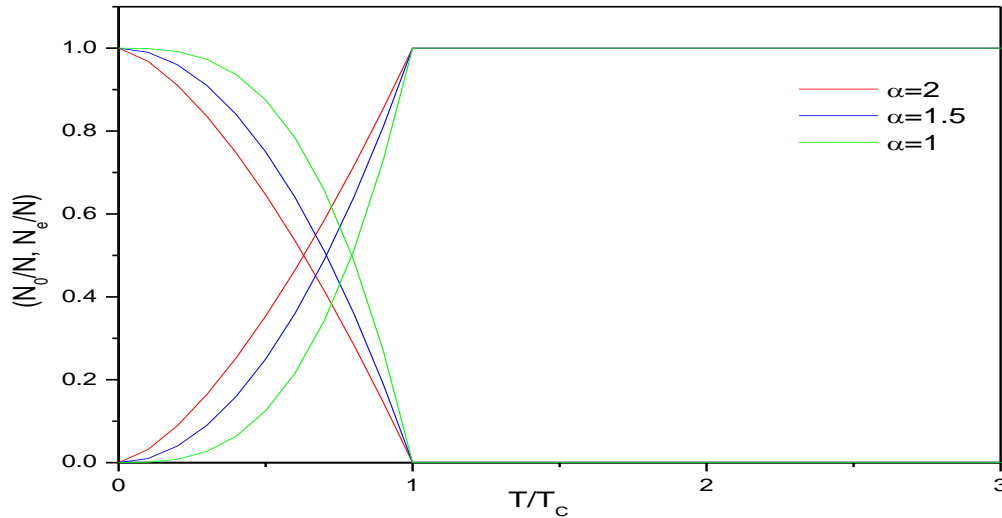

Figure 1: Fractions of the normal phase and the condensed of an ideal Bose gas as a function of the temperature parameter T/T_C

When $T < T_B$ (in the presence of condensation), it is interesting to give some thermodynamical quantities. For example, the internal energy is given by:

$$U = \frac{D}{\alpha} K_B T V \frac{g_{\left(\frac{D}{\alpha}+1\right)}(1)}{\lambda_g^D} \tag{44}$$

and the specific heat at constant volume by:

$$\frac{C_V}{NK_B} = \frac{V(D\alpha + D^2)}{\alpha^2 N} \frac{g_{(D/\alpha+1)}(1)}{\lambda_g^D} \tag{45}$$

For D=3 :

$$\frac{C_V}{NK_B} = \frac{V(3\alpha + 9)}{\alpha^2 N} \frac{g_{(3/\alpha+1)}(z)}{\lambda_g^D} \tag{46}$$

Figure 2 shows the variation of the specific heat of an ideal Bose gas in term of the temperature parameter T/T_C for $\alpha = 1$, $\alpha = 1.5$ and $\alpha = 2$
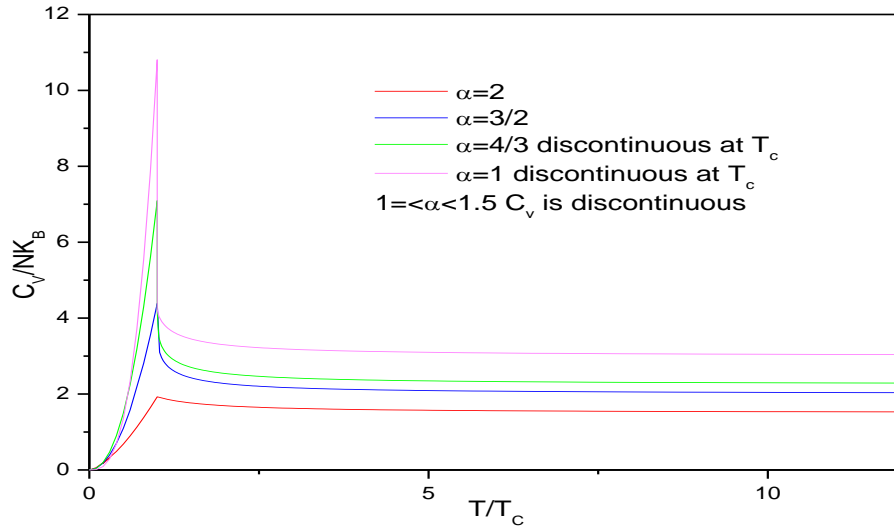
Figure 2: The specific heat of an ideal Bose gas as a function of the temperature parameter T/T_C

It is obvious that for real values of α between 1 and 2 , $\dfrac{C_V}{NK}$ is decreasing function of α.

and the Helmoltz energy:

$$F = -VK_B T g_{(D/\alpha+1)}(1) \tag{47}$$

and the entropy of the system of bosons:

$$S = \frac{D+\alpha}{\alpha} VK_B \frac{g_{(D/\alpha+1)}(1)}{\lambda_g^D} \tag{48}$$

We recover all well known quantities when we put $\alpha = 2$ and D=3.

3. 2. Ideal Fermi gas

For the case of Fermi gas, the same procedure is to be followed except that the energy level cannot be occupied by more than one particle (fermion). Then the Grandpartition function is given by K. Huang [10]:

$$D(z,V,T) = \prod_p \left(1 - ze^{-\beta D_\alpha p^\alpha}\right) \tag{49}$$

This leads us to write:

$$\begin{cases} \dfrac{PV}{K_B T} = \log D(z,V,T) = \sum_1^\infty \log\left(1 + ze^{-\beta D_\alpha p^\alpha}\right) \\ N = z\dfrac{\partial \log D(z,V,T)}{\partial z} = \sum_1^\infty \dfrac{ze^{-\beta D_\alpha p^\alpha}}{1 + ze^{-\beta D_\alpha p^\alpha}} \end{cases} \tag{50}$$

Using the same demarche as the bosons, we find at first the tow coupled state equations:

$$\begin{cases} \dfrac{P}{K_B T} = \dfrac{1}{\lambda_g^D} f_{\left(\frac{D}{\alpha}+1\right)}(z) \\ \dfrac{N}{V} = \dfrac{1}{\lambda_g^D} f_{\left(\frac{D}{\alpha}\right)}(z) \end{cases} \tag{51}$$

where $f_n(z)$ is the Fermi function defined by:

$$f_r(z) = \sum_{l=1}^\infty (-1)^l \frac{z^l}{l^r} \tag{52}$$

All the thermodynamical properties can be found easily, and we list them here:

internal energy

$$U = \frac{D}{\alpha} K_B TN \frac{f_{\left(\frac{D}{\alpha}+1\right)}(z)}{f_{\left(\frac{D}{\alpha}\right)}(z)} \tag{53}$$

the specific heat at constant volume

$$\frac{C_V}{NK_B} = \frac{D\alpha + D^2}{\alpha^2} \frac{f_{(D/\alpha+1)}(z)}{f_{D/\alpha}(z)} - \frac{D^2}{\alpha^2} \frac{f_{D/\alpha}(z)}{f_{(D/\alpha-1)}(z)} \tag{54}$$

the Helmholtz energy and the entropy

$$F = NK_B T \left(\log z - \frac{f_{(D/\alpha+1)}(z)}{f_{D/\alpha}(z)} \right) \tag{55}$$

$$S = \frac{D+\alpha}{\alpha} NK_B \frac{f_{(D/\alpha+1)}(z)}{f_{D/\alpha}} - NK_B \log z \tag{56}$$

4. Conclusion

In this work we have studied some problems of statistical mechanics based on the fractional classical and quantum mechanics. All calculation are made in D dimensional space. We have presented at first the thermodynamical properties relative to the classical ideal gas and to the system of N classical oscillators. In both cases, the Hamiltonian presents fractional exponents of the phase space (position r and momentum p). At the second stage, we have reviewed, in the context of the fractional quantum mechanics, the thermodynamical properties for the cases: the Bose-Einstein condensation and the Fermi-Dirac statistics. When we put D=3 in all the formula, we retrieve all the results obtained earlier by Z. Korichi and M. T. Meftah (2014) [11].

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