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Temperature-Dependent Specific Heat of a Monoatomic Gas Based on a Stretched Exponential Partition Function

José Weberszpil [1], Cresus F. L. Godinho[2], Ion V. Vancea [3]
DEFIS/ Universidade Federal do Rio de Janeiro - UFRRJ, Rio de Janeiro, RJ
O. Sotolongo-Costa[4]
Universidad Autónoma del Estado de Morelos: Cuernavaca, Morelos, MX

Abstract. Accurate modeling of complex systems often requires the application of advanced mathematical tools. In this work, we investigate the thermodynamic behavior of monoatomic gases using a stretched exponential probability density function. By constructing the partition function Z within this framework, we derive expressions for the internal energy and temperature-dependent specific heat of the system. The results are shown to be consistent with classical kinetic theory for ideal gases. Furthermore, comparisons with experimental data are presented, highlighting the viability of this approach.

Palavras-chave. Stretched Exponential, Monoatomic Gases, Specific Heat

1 Introduction

Modeling complex systems that exhibit dynamics governed by power laws and non-Gaussian Maxwell–Boltzmann distributions frequently necessitates the use of generalized statistical frameworks. Among these, stretched exponential probability distributions ($SEPD$), also known as the Kohlrausch–Williams–Watts (KWW) functions, are widely recognized for their versatility in describing a broad array of physical phenomena [5]. Experimental studies have shown that these functions effectively characterize relaxation processes across various systems, including biological systems [3, 6, 13]. The presence of nonlinear energy dissipation supports the use of KWW-type relaxation models. As discussed in Ref. [13], there is evidence suggesting that a universal mechanism may underlie KWW dynamics, independent of the microscopic details of individual systems. Moreover, connections have been established between the KWW law and Lévy-type stable probability distributions, which naturally arise from the superposition of numerous independent random events with heavy-tailed distributions. For further insight into this relationship, Ref. [2] provides valuable context, including applications related to system size and scaling effects, as elaborated in Ref. [9]. KWW functions have proven particularly useful in the study of granular gases and particulate systems, where inelastic collisions and dissipative dynamics drive the system far from equilibrium. These systems, known as granular gases (GG), consist of dilute assemblies of particles that deviate from the classical Maxwell–Boltzmann velocity distribution [12]. Instead, they often exhibit stretched exponential velocity distributions [1] and can display collective behaviors such as spontaneous cluster formation. It is also notable that granular media may behave as a hybrid

[1] josewebe@ufrrj.br
[2] crgodinho@ufrrj.br
[3] ionvancea@ufrrj.br
[4] osotolongo@uaem.mx, osotolongo@gmail.com

between fluid and solid phases, effectively forming a multi-particle system with unique thermodynamic properties [4]. In this study, we focus on deriving a temperature-dependent expression for the specific heat of a monoatomic gas, grounded in a stretched exponential probability distribution approach.

Granular gases and monoatomic real gases share fundamental similarities in their kinetic behavior, yet they differ significantly in the nature of their interactions. Both systems consist of particles undergoing random motion and colliding with one another, making kinetic theory a useful tool for their analysis. In monoatomic real gases, collisions are elastic, conserving energy and momentum, and the particles interact through well-defined intermolecular potentials. In contrast, granular gases are composed of macroscopic grains that undergo inelastic collisions, leading to energy dissipation and requiring continuous energy input to maintain a steady state. Despite this key difference, granular gases can often be modeled using adaptations of the Boltzmann equation, drawing formal analogies with molecular gases, especially in dilute regimes. Thus, while granular gases deviate from thermodynamic equilibrium due to energy dissipation, their statistical behavior under certain conditions can closely resemble that of monoatomic real gases.This possible connection justifies the use of non-standard or specialized mathematical tools, such as deformed derivatives, fractional calculus and stretched exponential.

2 Partition Function for Stretched Exponential Probability

To characterize the thermodynamic properties of the system, we adopt the $SEPD$ framework. Following the methodologies of Refs. [10, 11], but modifying for $SEPD$, the partition function Z is given by:

$$Z = \int_v d^\nu q_1 d^\nu q_2 ... d^\nu q_N d^\nu p_1 d^\nu p_2 ... d^\nu p_N e^{-\beta \mathcal{H}^\alpha}, \tag{1}$$

. Here, β is the inverse Boltzmann factor, and the integration spans the generalized coordinates and momenta q_i, p_i. V^N is the volume and the exponent α characterizes the stretched exponential form and will be better determined after some considerations.

With system's Hamiltonian $H(q_1, ..., q_n, p_1, ..., p_n, t)$ in a form of stretched exponential, the partition function can be written explicitly as:

$$Z = V^N \int_{-a}^{+a} \exp\left[-\beta \left(\frac{1}{2m}\right)^\alpha \left(p_1^2 + p_2^2 + ... + p_N^2\right)^\alpha\right] dp_1^\nu dp_2^\nu ... dp_N^\nu. \tag{2}$$

Again, as in Ref. [10], transforming to spherical coordinates in νN-dimensional momentum space and calling $p_1^2 + p_2^2 + ... + p_N^2 = p^2$, we obtain for Z,

$$Z = \frac{2\pi^{\nu N/2}}{\Gamma^{\nu N/2}} V^N \int_0^\infty \exp\left(-\frac{\beta}{(2m)^\alpha} p^{2\alpha}\right) p^{\nu N - 1} dp\,. \tag{3}$$

Using the substitution

$$u = \frac{\beta}{(2m)^\alpha} p^{2\alpha} \longrightarrow p = \left[\frac{(2m)^\alpha}{\beta} u\right]^{1/2\alpha}, \tag{4}$$

we derive:

$$du = \frac{\beta}{(2m)^\alpha} 2\alpha p^{2\alpha - 1} dp\,. \tag{5}$$

By this way, we can write dp as

$$dp = \frac{(2m)^\alpha}{2\alpha\beta} p^{1-2\alpha} du = \frac{(2m)^\alpha}{2\alpha\beta} \left[\frac{(2m)^\alpha}{\beta} u\right]^{\frac{1-2\alpha}{2\alpha}} du. \tag{6}$$

The partition function, Z, can now be written as

$$\begin{aligned} Z &= \frac{\pi^{\nu N/2}}{\Gamma^{\nu N/2}} V^N \int_0^\infty e^{-u} \left[\frac{(2m)^\alpha}{\beta} u\right]^{(2\nu-1)/2\alpha} \frac{(2m)^\alpha}{2\alpha\beta} \left[\frac{(2m)^\alpha}{\beta} u\right]^{\frac{1-2\alpha}{2\alpha}} du = \\ &= \frac{\pi^{\nu N/2}}{\Gamma^{\nu N/2}} V^N \left[\frac{(2m)^\alpha}{\beta}\right]^{(2\nu-1)/2\alpha} \frac{(2m)^\alpha}{2\alpha\beta} \left[\frac{(2m)^\alpha}{\beta}\right]^{\frac{1-2\alpha}{2\alpha}} \int_0^\infty e^{-u} u^{(2\nu-1)/2\alpha} u^{1-2\alpha/2\alpha} du = \\ &= C_{1(\nu,N,\alpha,m,\beta)} \int_0^\infty e^{-u} u^{(\nu N-1+1-2\alpha)/2\alpha} du = C_{1(\nu,N,\alpha,m,\beta)} \int_0^\infty e^{-u} u^{(\nu N-2\alpha)/2\alpha} du. \end{aligned} \tag{7}$$

In the eq.(7) we can identified the form of a gamma function Γ as

$$\Gamma(u) = \int_0^\infty e^{-u} u^{(\frac{\nu N}{2\alpha}-1)} du. \tag{8}$$

Following with the calculations, the prefactor in eq.(7) can be written, with some simple algebra as

$$\begin{aligned} C_1 &\equiv C_{1(\nu,N,\alpha,m,\beta)} = \frac{(2m)^{(\nu N-2\alpha)/2}}{\beta^{(\nu N-2\alpha)/2\alpha}} \frac{(2m)^\alpha}{2\beta\alpha} \left(\frac{\pi^{\nu N/2}}{\Gamma(\nu N/2)} V^N\right) = \\ &= \frac{(2m)^{(\nu N)/2}}{2\alpha\beta^{(\nu N)/2\alpha}} \left(\frac{\pi^{\nu N/2}}{\Gamma(\nu N/2)} V^N\right). \end{aligned} \tag{9}$$

Finally, Z can be cast as

$$Z = \frac{(2m)^{(\nu N)/2}}{2\alpha\beta^{(\nu N)/2\alpha}} \left(\pi^{\nu N/2} V^N\right). \tag{10}$$

Note that

$$\frac{\nu N}{2\alpha} > 0 \Longrightarrow \nu N > 0 \Longrightarrow N > 0, \tag{11}$$

ensures physical ensure the validity of the solution, without the restrictions of poles in Plastino's papers [10, 11].

To calculate the mean energy $\langle U \rangle$,we proceed in a similar way, following Refs. [10, 11]: After some tedious algebra explanation of the mean energy, we have the following.

$$\langle U \rangle = \frac{C_{2(\nu,N,\alpha,m,\beta)}}{Z} \Gamma\left(\frac{\nu N + 2}{2\alpha}\right). \tag{12}$$

Note that the argument of the gamma function is positive, that is

$$\frac{\nu N + 2}{2\alpha} > 0. \tag{13}$$

In this way, it follows that $\nu N + 2 > 0 \Longrightarrow N > -2/\nu \Longrightarrow N > 0$, for physical solutions. Again, there are no the restrictions of poles (see Refs. [10, 11]).

After some simple algebra, the term C_2 can be written as

$$C_{2(\nu,N,\alpha,m,\beta)} = \frac{V^N}{2\alpha}\frac{(2m)^{(\nu N)/2}}{\beta^{(\nu N+2)/2\alpha}}\frac{\pi^{\nu N/2}}{\Gamma\left(\frac{\nu N}{2}\right)}. \tag{14}$$

Using a correction factor [7]

$$\frac{1}{N!(2\pi\hbar)^{\nu N}}, \tag{15}$$

we can rewrite the term C_2 as:

$$C_2 \equiv C_{2(\nu,N,\alpha,m,\beta)} = \frac{1}{N!(2\pi\hbar)^{\nu N}}\frac{V^N}{2\alpha}\frac{(2m)^{(\nu N)/2}}{\beta^{(\nu N+2)/2\alpha}}\frac{\pi^{\nu N/2}}{\Gamma\left(\frac{\nu N}{2}\right)}. \tag{16}$$

Finally, the Helmholtz free energy can also be written as:

$$F = -kT\ln Z_\alpha = -KT\left[-lnN! - \ln(2\pi\hbar)^{\nu N} + \ln\left(\pi^{\nu N/2}\right) + \ln\left(\frac{2m^{nuN})}{2\beta^{\nu/2}\alpha}\right) + NlnV\right]. \tag{17}$$

2.1 The Internal Energy and Temperature-Dependent Specific Heat

Let us write explicitly the mean internal energy. With eq. (12) and eq.(10) written as $Z = C_1\Gamma\left(\frac{\nu N}{2\alpha}\right)$,the internal mean energy can be written as

$$\langle U\rangle = \frac{C_2}{C_1}\frac{\Gamma\left(\frac{\nu N+2}{2\alpha}\right)}{\Gamma\left(\frac{\nu N}{2\alpha}\right)}, \tag{18}$$

with $C_1 = \frac{(2m)^{(\nu N)/2}}{2\alpha\beta^{(\nu N)/2\alpha}}\left(\frac{\pi^{\nu N/2}}{\Gamma(\nu N/2)}V^N\right)$. By this way, $\frac{C_2}{C_1}$ is identified as

$$\frac{C_2}{C_1} = \frac{\beta^{\nu N/2}}{\beta^{(\nu N+2)/2}} = \beta^{\frac{\nu N-\nu N-2}{2\alpha}} = \beta^{-1/\alpha}. \tag{19}$$

The internal mean energy of the system is then explained as

$$\langle U\rangle = \beta^{-1/\alpha}\frac{\Gamma\left(\frac{\nu N+2}{2\alpha}\right)}{\Gamma\left(\frac{\nu N}{2\alpha}\right)}. \tag{20}$$

It is possible to give a one parametric equation for the specific heat C_V, that we will show in what follows that depends on the temperature.

Performing a partial derivative on the mean energy, the C_V can now be written as

$$C_V = \frac{\partial\langle U\rangle}{\partial T} = \frac{\partial}{\partial T}\left(\beta^{-1/\alpha}\frac{\Gamma\left(\frac{\nu N+2}{2\alpha}\right)}{\Gamma\left(\frac{\nu N}{2\alpha}\right)}\right), \tag{21}$$

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or

$$C_V = \frac{K^{1/\alpha}}{\alpha} T^{(1-\alpha)/\alpha} \frac{\Gamma\left(\frac{\nu N + 2}{2\alpha}\right)}{\Gamma\left(\frac{\nu N}{2\alpha}\right)}, \tag{22}$$

where K is the Boltzmann constant. The parameter α is an experimental fractal parameter and depends on the composition of the system under study.

To perform the simulation, we will use the Stirling's formula, that allows derivation of the following asymptotic expansion for the ratio of gamma functions:

$$\frac{\Gamma(x+c)}{\Gamma(x)} \approx x^c. \tag{23}$$

With Stirling approximation, the equation (22) can be rewritten as

$$C_V \approx \frac{K^{1/\alpha}}{\alpha} T^{(1-\alpha)/\alpha} \left(\frac{\nu N}{2\alpha}\right)^{1/\alpha} \tag{24}$$

In order to better emulate the nature of a real gas, let us redefine the parameter α as $\alpha = 2-\eta$. The equation (22) can be written now as

$$C_V \approx \frac{K^{1/(2-\eta)}}{2-\eta} T^{(\eta-1)/(2-\eta)} \left(\frac{\nu N}{2-\eta}\right)^{\frac{1}{(2-\eta)}}. \tag{25}$$

As shown in Ref. Ref. [7] (Table 1, column 3), the specific heat at constant volume, C_V, for the noble gas Argon (Ar), exhibits a low degree of fractionality, α, meaning that α is very close to one. This suggests that the appropriate framework for describing the thermodynamics of granular systems such as noble gases is not nonlocal fractional calculus (FC), but rather local and simpler alternatives, such as fractal (or deformed) derivatives.

Here, α and η are purely dimensionless parameters.

Additional values for C_V are provided in Ref. [8].

In Figure (1) we present the experimental data from Ref. [8], along with a fit using eq. (25) for C_V. The results show good agreement with the experimental data, except at low temperatures where quantum effects become significant and the model would require revision.

2.2 Consistence with Classical Approach of Kinetic Theory

Let us now examine the consistence of the relations obtained here with those of the classical kinetic theory approach. For this intention, let us make the parameter α tend to 1, $\alpha \to 1$: In this case

$$C_v \quad \to \quad K\frac{\nu N}{2}, \tag{26}$$

where we have used that, for gamma function, is valid the relation $\Gamma(x+1) = x.\Gamma(x)$.

For $3D$ gas, that is, for $\nu = 3$, the specific heat turns out to be the well known classical one for the ideal gas,

$$C_v = \frac{3}{2} NK, \tag{27}$$

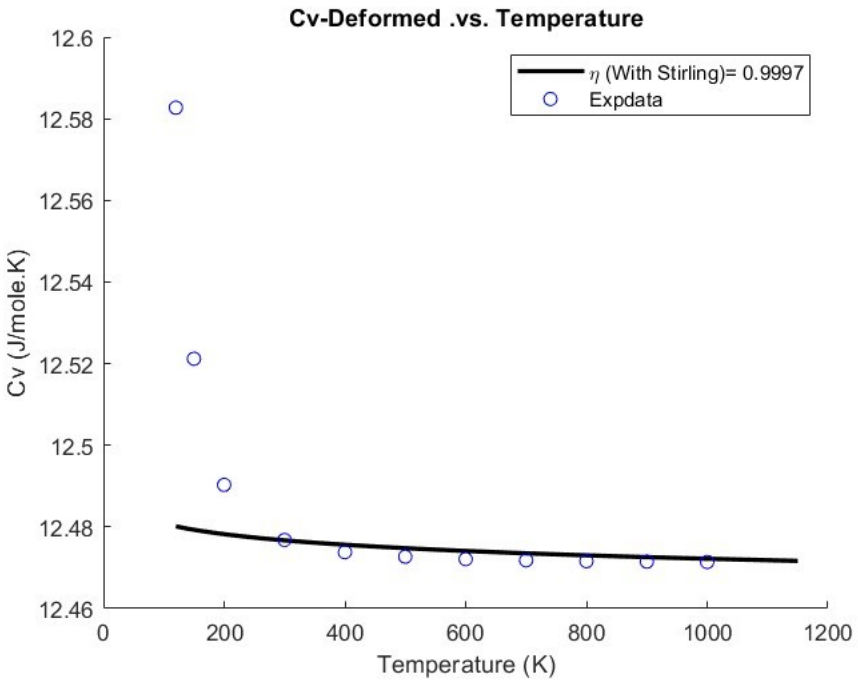

Figure 1: C_V.vs. T for one adjusted η parameter. Experimental data for Argon (Ar) by Ref. [8].

and the internal mean energy is

$$\langle U \rangle = KT\frac{\nu N}{2}. \tag{28}$$

When $\nu = 3$,

$$\langle U \rangle = \frac{3}{2}NKT, \tag{29}$$

that is the well known equipartition principle for classical ideal gases.

3 Conclusions and Final Considerations

In terms of the stretched exponential function, we calculate the partition function Z for a monoatomic gas system by building up the probability density and, from this partition function, we determine the internal energy of the system as well as the specific heat C_V, both dependent on temperature T. Comparisons with experimental data from [8] for Argon have shown good accordance above $250K$. For low temperature experiments, a quantum model is necessary as in Einstein-like model.

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