



# Statistical complexity and classical–quantum frontier

R. Branada <sup>a</sup>, F. Pennini <sup>a,b,\*</sup>, A. Plastino <sup>c,d</sup>

<sup>a</sup> Departamento de Física, Universidad Católica del Norte, Av. Angamos 0610, Antofagasta, Chile

<sup>b</sup> Departamento de Física, Facultad de Ciencias Exactas y Naturales, Universidad Nacional de La Pampa, CONICET, Av. Peru 151, 6300, Santa Rosa, La Pampa, Argentina

<sup>c</sup> Instituto de Física La Plata–CCT-CONICET, Universidad Nacional de La Plata, C.C. 727, 1900, La Plata, Argentina

<sup>d</sup> SThAR - EPFL, Lausanne, Switzerland

## HIGHLIGHTS

- We revisit two very simple systems using the statistical complexity as quantifier.
- We uncover with the help of the statistical complexity, unexplored, interesting features of these simple systems.
- These features are seen to be related to the classical–quantum frontier.

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## ABSTRACT

The classical limit of quantum mechanics (CLQM) is a fascinating subject of perennial interest. Here we deal with it in a novel way for two of the simplest conceivable systems: the classical ideal gas (IG) and the Einstein crystal (EC). Even if at first sight one may not believe that something new could be said about them, it will be seen that some statistical quantifiers do. In particular, the statistical complexity  $C$ , seems to signal the CLQM's zone. The associated two  $C$ –maxima (versus temperature), for, respectively, the IG and the CG, almost coincide.

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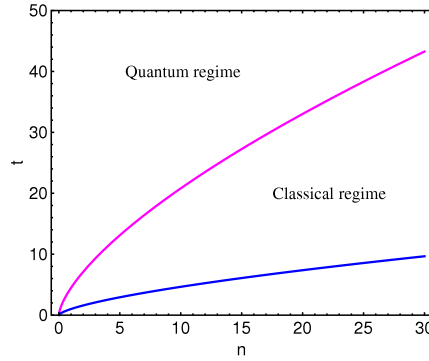
## 1. Introduction

The classical limit of quantum mechanics is an exciting issue of continuous interest, containing beguiling challenges and several open problems (see, for example, Refs. [1–6]). We wish here to address it in conjunction with the notion of statistical complexity (SC) [7,8], discussing novel facets concerning aspects of the classical–quantum frontier (CQF). For an alluring CQF-treatment, we recommend Ref. [1]. We appeal here to the idea that, sometimes, statistical quantifiers can yield different and perhaps deeper insights than purely dynamic quantifiers.

Statistical complexity  $C$  is a quantifier that rivals entropy  $S$  somehow, in the sense that it grasps correlation structures in the manner that  $S$  grasps disorder.

It was introduced, in what many people regard as a great leap forward, in Ref. [7], by appealing to a kind of “distance” to the maximum entropy instance. This distance was called disequilibrium  $D$  [8]. In these last references the distance was determined in probability space: that of a given probability distribution (PD) to the uniform PD. This generates a sort of hierarchy that makes  $D$  non-null only in cases in which some “privileged” states exist amongst the available ones.  $D$  becomes maximal for wholly ordered systems and vanishes for completely random situations. Obviously, for  $S$  matters are exactly

\* Corresponding author at: Departamento de Física, Universidad Católica del Norte, Av. Angamos 0610, Antofagasta, Chile  
E-mail address: [fpennini@ucn.cl](mailto:fpennini@ucn.cl) (F. Pennini).



**Fig. 1.** Typical inverse square length  $t = 2\pi mk_B T/h^2$  as a function of the particle density  $n = N/V$ . The blue curve is obtained for the condition  $t = n^{2/3}$ , which separates the classical from the quantum domain according to Ref. [18]. The second, magenta curve corresponds to our present study’s proposal, to be discussed below, and given by  $t = t_c = e^{-1}n^{2/3}$ . We purport to show that it constitutes a better delimiter than the first one. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

reversed. In this framework, López-Ruiz, Mancini, and Calvet (LMC) [7] advanced what is today the standard form for a measure of  $C$ , i.e.,

$$C = DS, \tag{1}$$

a functional of the probability distribution [7]. If one deals with a finite number  $N$  particles one has

$$D = \sum_{i=1}^N \left( p_i - \frac{1}{N} \right)^2, \tag{2}$$

where  $p_1, p_2, \dots, p_N$  are the individual normalized probabilities ( $\sum_{i=1}^N p_i = 1$ ) [7], becoming a maximum for a fully ordered state and null for equi-probable states. Above,  $S$  is the Shannon–Boltzmann entropy (or information), which is given by [9]

$$S = - \sum_{i=1}^N p_i \ln p_i. \tag{3}$$

LMC’s proposal generated an immense degree of attention (see Refs. [10–16], as a small sample), having been used in different scientific scenarios for the micro-canonical, canonical, and grand canonical ensembles.

### 1.1. Motivation and goal

Statistical quantifiers often allow for interesting insights into the intricacies of purely dynamical issues [17]. Here we are concerned with the classic–quantum frontier (CQF) and confront, for the ideal gas (IG), the intriguing text-book graph [18] given below, in which we learn that for the IG we confront the scenario of Fig. 1. One depicts there a multiple of the temperature  $T$  against the molar density  $n(T)$ . The book’s author argues that such curve is a separatrix between classical and quantum behavior [18] A second curve is also depicted there, leftwards. We will see below that it provides a better classical–quantum delimiter than the first curve. The classical regime is attained when the mean thermal wavelength of the particles  $\lambda = h/\sqrt{2\pi mk_B T}$  is small compared to  $v^{1/3} = (V/N)^{1/3}$ , the mean molecular separation [19], so that we have a special separation  $d_T = v^{1/3}$

$$h/\sqrt{2\pi mk_B T} = v^{1/3} = d_T. \tag{4}$$

In other words, classicity regions for  $\lambda \ll v^{1/3} = d_T$ . This separatrix is certainly an interesting topic to investigate with our statistical quantities  $D$  and  $C$ , as we do below.

Why? Because we see that even at this elemental level the CQF seems to emerge. The question we want to answer here is: what has the statistical complexity to teach us in this respect? We turn our attention, for an answer, to the fundamentals of the LMC ideas by critically re-examining the two LMC paradigmatic instances: the ideal gas and the perfect crystal, usually considered as opposite examples of disorder versus order. In such contra-position, our disequilibrium–statistical complexity analysis of these two paradigmatic systems will allow for some surprises regarding the classic–quantum frontier.

## 1.2. Paper's structure

The paper is organized as follows. Section 2 describes the SC-formalism while, in Sections 3 and 4 we present concepts related to our two simple systems. Section 5 looks at the quantum–classical frontier. This constitutes a crucial issue. Finally, we draw some conclusions in Section 6.

## 2. Formalism's details

In this preparatory section we present important ideas developed for the canonical ensemble, in Ref. [8], where an ideal gas in thermal equilibrium is described. Let us deal then with a classical system of  $N$  identical particles, confined into a space of volume  $V$ , in thermal equilibrium at temperature  $T$ . The corresponding Boltzmann distribution becomes [19]

$$\rho(x, p) = \frac{e^{-\beta \mathcal{H}(x, p)}}{Q_N(V, T)}, \quad (5)$$

with  $\beta = 1/k_B T$ ,  $k_B$  the Boltzmann constant,  $\mathcal{H}(x, p)$  the Hamiltonian, and  $x, p$  the phase space variables. The canonical partition function reads

$$Q_N(V, T) = \int d\Omega e^{-\beta \mathcal{H}(x, p)}, \quad (6)$$

with  $d\Omega = d^{3N}x d^{3N}p/N!h^{3N}$ , while the Helmholtz' free energy  $A$  is cast as [19]

$$A(N, V, T) = -k_B T \ln Q_N(V, T). \quad (7)$$

It is shown in Ref. [8] that the canonical  $D(N, V, T)$  becomes here

$$D(N, V, T) = e^{2\beta [A(N, V, T) - A(N, V, T/2)]}, \quad (8)$$

where this form is valid only for continuous probability distributions. Set now  $T = T/2$  in (7) and encounter that [8]

$$A(N, V, T/2) = -\frac{k_B T}{2} \ln Q_N(V, T/2). \quad (9)$$

Replacing Eqs. (7) and (9) into Eq. (8) yields

$$D(N, V, T) = \frac{Q_N(V, T/2)}{Q_N^2(V, T)}. \quad (10)$$

The alternative  $D$ -expression is, from definitions (5) and (6),

$$D(N, V, T) = \int d\Omega \rho^2(x, p), \quad (11)$$

which is the orthodox form most people use (see, for example, Ref. [20]).

## 3. The Einstein crystal

The Einstein crystal (EC) is often regarded as a perfect model of order [7], whose statistical complexity should vanish [7]. It is a model in which each crystal-site is a three dimensional quantum harmonic oscillator of frequency  $\omega$  [19]. We deal with an  $N$ -atom's lattice of independent particles. The pertinent, well-known canonical partition function is [19]

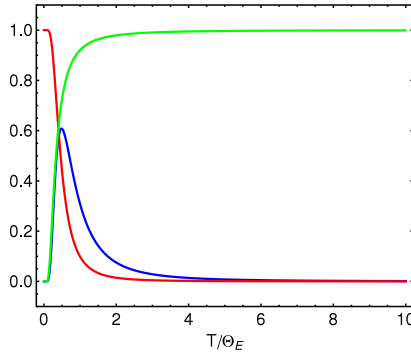
$$Q_N(T) = [2 \sinh(\Theta_E/2T)]^{-3N}, \quad (12)$$

where  $\Theta_E = \hbar\omega/k_B$  is called the Einstein temperature. Accordingly, the disequilibrium becomes

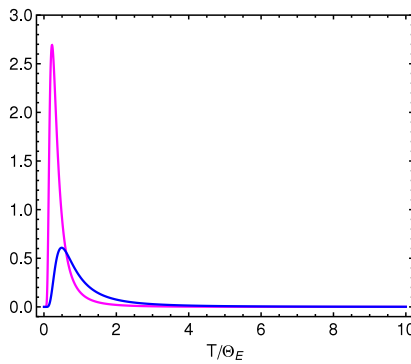
$$D(N, T) = \left[ \frac{2 \sinh^2(\Theta_E/2T)}{\sinh(\Theta_E/T)} \right]^{3N}, \quad (13)$$

while the corresponding entropy is

$$S(N, T) = \frac{3Nk_B(\Theta_E/T)}{e^{\Theta_E/T} - 1} - 3Nk_B \ln(1 - e^{-\Theta_E/T}). \quad (14)$$



**Fig. 2.** Statistical complexity  $c(T)$  (blue curve), disequilibrium  $d(T)$  (red curve), and specific heat  $C_v/3Nk_B$  (green curve) for an Einstein solid, plotted as a function of  $T/\Theta_E$ . The maximum value of  $c$  is 0.608 and occurs at  $T/\Theta_E = 0.488$ . (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



**Fig. 3.** Statistical complexity  $c$  (blue curve) and derivative of the specific heat  $C_v$  respect to  $t = T/\Theta_E$  (magenta curve) for the Einstein solid model. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

For our purposes we need such expressions per particle, which are

$$d(T) = \left[ \frac{2 \sinh^2(\Theta_E/2T)}{\sinh(\Theta_E/T)} \right]^3, \quad (15)$$

while the corresponding entropy is

$$s(T)/k_B = \frac{3(\Theta_E/T)}{e^{\Theta_E/T} - 1} - 3 \ln(1 - e^{-\Theta_E/T}). \quad (16)$$

Therefore, the statistical complexity per particle is

$$c(T) = d(T)s(T)/k_B, \quad (17)$$

where  $d(T)$  and  $s(T)$  are obtained from Eqs. (15) and (16), respectively.

Our interest is piqued by inspecting a plot of the specific heat  $C_v$  given in Fig. 2, that reflect the effects of an internal structure for the system. At low temperatures  $C_v$  tends to vanish, according to thermodynamics' third law, while at high enough  $T$  it becomes constant, according to the Dulong–Petit classical law. We are thus clearly in the presence of the classic–quantum frontier. Fig. 2 depicts the variation of the statistical complexity, of the disequilibrium and of the specific heat with  $T/\Theta_E$ .

Fig. 3 displays  $dC_v/dt$  ( $t = T/\Theta_E$ ), which exhibits a clear maximum near the  $t$ -value  $t = t^*$  at which  $c$  becomes maximal. It makes sense then to conclude that in the vicinity of  $t^*$  we find the CQF, where the system reaches its maximum complexity, as also illustrated by the behavior of  $dC_v/dt$ . The CQF is the relatively small temperature-range in which  $C_v$  changes from its quantum value towards the classic (Dulong–Petit) one. In this small range,  $dC_v/dt$  rapidly varies. At the speediest rate, the system becomes the most structurally complex, a rather convincing picture.

#### 4. The ideal gas

As it is well known, the model consists of  $N$  mono-atomic identical particles confined to a space of volume  $V$  and in thermal equilibrium at temperature  $T$ , whose Hamiltonian is  $\mathcal{H} = \sum_{i=1}^N p_i^2/2m$ , with  $m$  the mass of the particles and  $p_i$  the related momenta,  $i = 1, \dots, N$ . We will emphasize here questions related to the classical–quantum transition zone.

The corresponding canonical partition function is [19]

$$Q_N^{(0)}(V, T) = \frac{1}{N!} \left( \frac{V}{\lambda^3} \right)^N, \quad (18)$$

with  $\lambda$  the particles' mean thermal wavelength [19]. The Helmholtz free energy, after using Stirling's approximation ( $\ln N! \approx N \ln N - N$ ) becomes

$$A(N, V, T) = Nk_B T [\ln(n\lambda^3) - 1], \quad (19)$$

where  $n = N/V$  is the molar density [19].

The classical entropy, provided by the Sackur-Tetrode equation, is [19]

$$S/k_B = -\ln(n\lambda^3)^N + \frac{5N}{2} = \ln\left(e^{5N/2} (n\lambda^3)^{-N}\right), \quad (20)$$

which is positive definite if we fulfill the requirement  $n\lambda^3 \ll e^{5/2}$ . This is an important feature, to which we refer below.

##### 4.1. Remarks on disequilibrium and statistical complexity

We observe that, inserting Eq. (20) into the definitions (1) and (8), we obtain the disequilibrium and the LMC-statistical complexity, given by [21]

$$D(N, V, T) = (n\lambda^3)^N e^{-N} 2^{-3N/2}, \quad (21)$$

and

$$C(N, V, T) = (n\lambda^3)^N e^{-N} 2^{-3N/2} \ln\left(e^{5N/2} (n\lambda^3)^{-N}\right). \quad (22)$$

We note that for  $N \rightarrow \infty$  and/or  $T \rightarrow \infty$  the quantities  $D$  and  $C$  vanish, as they should [7]. This is not the whole story, though. Some kind of “structural” details will emerge if the above mentioned restrictions are lifted. These “structural” details however cannot be of physical origin, because the ideal gas does not exhibit any structure. We may speak of fake-structure, meaning that the inadequacy of the formalism at low temperatures or high densities generates complexity or disequilibrium.

In order to capture these “fake” structural details, it is useful to consider the values of both  $D$  and  $C$  per particle (involving the particle-density  $n$ ). First, we introduce for convenience the typical inverse square length (a function of  $T$ )

$$t = \frac{2\pi mk_B T}{h^2} = \lambda^{-2}. \quad (23)$$

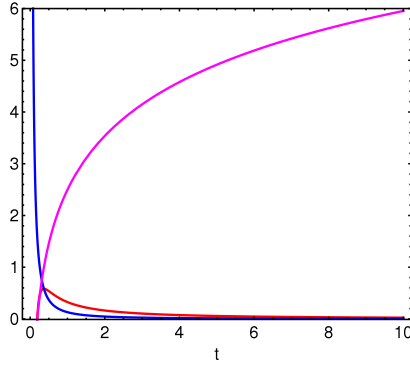
As mentioned in the Introduction,  $\lambda$  is the thermal de Broglie wavelength, that is, roughly, the mean de Broglie wavelength of the gas molecules at the temperature  $T$ . The mean interparticle spacing  $d_T$  is, approximately,  $(V/N)^{1/3}$ . Whenever  $\lambda$  is much smaller than this  $d_T$ , the gas can be regarded as classical. Contrarily, when  $\lambda$  is of the order of or larger than  $d_T$ , quantum effects should dominate and the gas ought to be treated as quantal. The critical temperature is the transition point between these two regimes, and at this critical temperature, the thermal wavelength will be approximately equal to  $d_T$  [19]. Returning to our quantifiers per particle, we have

$$d(n, t) = \left(\frac{n}{e}\right) \left(\frac{1}{2t}\right)^{3/2}, \quad (24)$$

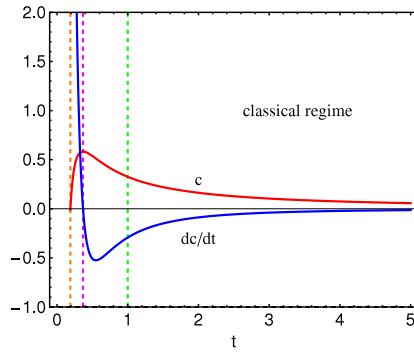
and

$$c(n, t) = \left(\frac{n}{e}\right) \left(\frac{1}{2t}\right)^{3/2} \ln\left(e^{5/2} n^{-1} t^{3/2}\right). \quad (25)$$

From Eq. (25) we see that  $c \geq 0$  whenever  $nt^{-3/2} \leq e^{5/2}$ . Typical behaviors of Eqs. (20), (24) and (25) are displayed in Fig. 4.



**Fig. 4.** Statistical complexity  $c(n, t)$  (red), disequilibrium  $d(n, t)$  (blue), and entropy  $s(n, t)$  (magenta) versus  $t$  for  $n = 1$ . (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



**Fig. 5.** Statistical complexity  $c(n, t)$  (red curve) and  $dc(n, t)/dt$  (blue curve) versus  $t$  for  $n = 1$ . The maximum of  $c$  is  $c_{max} = \sqrt{e/8} = 0.58$  for  $t_c = e^{-1} = 0.36$  (magenta line). The other two vertical dashed lines are located, respectively, at  $t = 1$  (green line) which is usually regarded as signaling the classical limit, and  $e^{-5/3}$  (orange line), that corresponds to a null Boltzmann’s entropy (that becomes negative for smaller  $t$ ’s, violating the requirements imposed by Eq. (20)). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

On the other hand, we note the maximum of  $c(n, t)$  is, for  $n$  fixed,  $c_{max} = \sqrt{e/8}$  that occurs for a  $t = t_c$  that satisfies, as promised in the Introduction,

$$n t_c^{-3/2} = e^{3/2} \Rightarrow t_c = n^{2/3} e^{-1}, \tag{26}$$

as announced in the caption of Fig. 1. This maximum is attained for all isotherms of the effective quasi-temperature  $t$ . In Fig. 5 we show the statistical complexity  $c(n, t)$ . We can interpret things this way. When the two above classicality criteria start being violated, the statistical complexity “notes” it and begins to grow, because it now detects fake structural features beginning to take place. These fake structural details arise from a regime-change, from classic to quantal. We are again in the presence of the classic-to-quantum transition.

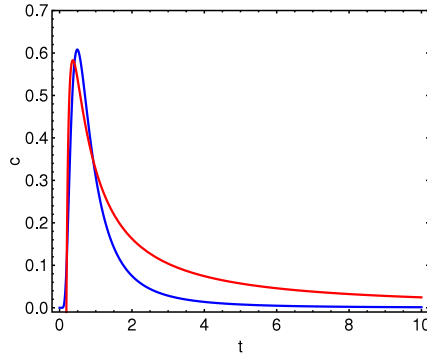
#### 4.2. Details regarding the classical regime

Let us delve in deeper fashion on the validity’s region of the classical regime (CR). To illustrate this, we will consider the occupation numbers,  $n_\epsilon$ , of the single-particle state with energy  $\epsilon$ , in the canonical ensemble [19,22]. The canonical probability distribution is

$$P \equiv \frac{\langle n_\epsilon \rangle}{N} = \frac{e^{-\beta\epsilon}}{Q_1(V, T)}, \tag{27}$$

where  $\langle n_\epsilon \rangle$  is the Maxwell–Boltzmann mean occupation number of a single-particle state with energy  $\epsilon$  [19]. Thus, using Eq. (18) for the canonical partition function of one particle, we find

$$\langle n_\epsilon \rangle = n \lambda^3 e^{-\beta\epsilon}. \tag{28}$$



**Fig. 6.** Statistical complexity  $c(n, t)$  versus  $t$  for  $n = 1$ . The blue curve corresponds to the Einstein solid model and the red refers to the ideal gas instance. In this plot we take the molar density of the gas  $n = 1$  and  $\Theta_\epsilon = h^2/(2\pi mk_B)$ . (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

In the CR the occupancy of any single-particle state is  $\ll 1$  [19,22]. Accordingly

$$\langle n_\epsilon \rangle \ll 1, \text{ for all } \epsilon, \quad (29)$$

and from (29) we immediately obtain

$$n \lambda^3 \ll e^{\beta \epsilon}. \quad (30)$$

Since the mean kinetic energy of a gas molecule in the classical gas is  $\epsilon = 3k_B T/2$  we finally reach

$$n \lambda^3 \ll e^{3/2}, \quad (31)$$

which constitutes the ‘‘Maxwell–Boltzmann limit’’ [22]. Now, after the change of variables (23) we have

$$n t^{-3/2} \ll e^{3/2}. \quad (32)$$

Comparing the limit (31) with our Eq. (26) we obtain

$$n t^{-3/2} \ll n t_c^{-3/2}, \quad (33)$$

telling us that in the CR region

$$t \gg t_c, \quad (34)$$

where  $t_c$  is obtained from the maximum of the statistical quantifier  $C$ .

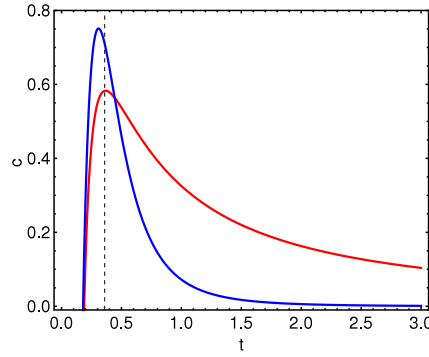
#### 4.3. Illustration regarding the classical–quantum transition

An instructive picturing of our results can be visualized in Fig. 6, where we depict the statistical complexity for the two models described in previous subsections as a function of the typical inverse square length  $t$ . It is seen that for these two models the associated complexities reach their peaks at approximately the same  $t$ , that we can call  $t^*$ . This common inverse square length  $t^*$  is too high for the Einstein crystal to remain being a quantum object and simultaneously too low for the ideal gas to remain in the classical regime. One could then convincingly assert that the statistical complexity notion is indeed a good signal post for the classical–quantum frontier.  $C$  becomes maximal at the same temperature for two totally different systems when they are about to change regimes, from classical to quantum and vice versa.

### 5. Internal degrees of freedom for diatomic molecules

We now consider in this section a diatomic ideal gas. Thus, in addition to the translational part of the molecular motion, we have to add also the internal atomic motion. In particular, we assume that the only internal motion is due to the vibrational states. The canonical partition function of this model reads [19]

$$Q_N(V, T) = \frac{1}{N!} [Q_1^{(0)}(V, T) \zeta_{int}(T)]^N, \quad (35)$$



**Fig. 7.** Qualitative behavior of the statistical complexity  $c(n, t)$ , that incorporates quantum information regarding internal motion, versus  $t$  for  $n = 1$ . The red curve represents  $c$  for translational degrees of freedom, and the blue color corresponds to the case of the system with internal degrees of freedom. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

where  $Q_1^{(0)}(V, T)$  corresponds to the translational degrees of freedom of the individual (identical) diatomic molecules and  $\zeta_{int}(T) = \zeta_{vib}(T)$  is the contribution to the partition function due to internal (quantum) degrees of freedom, in particular, associated with vibrations.

Thus, in this case, the total disequilibrium (10) is due to the contribution of the internal motion together with the translational motion which is given by Eq. (35) and it is expressed as

$$D(N, V, T) = D_0(N, V, T)D_{vib}(N, V, T), \quad (36)$$

where  $D_0$  obviously corresponds to the translational disequilibrium, given by Eq. (21), and the disequilibrium due to the vibrational states is  $D_{vib}$ , given by Eq. (13).

Therefore, after a bit of algebra, the disequilibrium finally adopts the appearance

$$D(N, V, T) = (n\lambda^3)^N e^{-N} 2^{-3N/2} \left[ \frac{2 \sinh^2(\Theta_E/2T)}{\sinh(\Theta_E/T)} \right]^{3N}, \quad (37)$$

where we have added quantum information to  $D$ .

To calculate the statistical complexity we need first to find the total entropy of the system. Thus, from the additivity property of the entropy by using Eqs. (14) and (20), i.e.,  $S = S_0 + S_{vib}$ , we immediately get [19]

$$S = Nk_B \ln \left[ e^{5/2} n^{-1} \lambda^{-3} (1 - e^{-\Theta_E/T})^{-3} e^{3\Theta_E/(T(e^{\Theta_E/T} - 1))} \right]. \quad (38)$$

Finally, the statistical complexity per particle  $c(n, T) = D^{1/N} S / Nk_B$  is constructed by joining Eqs. (37) and (38), obtaining a complexity-measure that incorporates information regarding internal quantum motion. This new  $c$  is depicted in Fig. 7. We appreciate in this figure as the maximum of the system, when we incorporate the quantum vibrational internal degrees, moves towards the left of the classical–quantum frontier, as one should expect. The quantum information added forces the  $c$ –maximum to move further into the quantum region.

## 6. Conclusions

We have studied in this effort the classical–quantum frontier from the view point of two very simple models: (1) the Einstein crystal and (2) the ideal gas. These models are paradigms for, respectively, perfect order and total randomness. This fact makes them relevant for our complexity-exploration, as one would expect their statistical complexities to vanish [7]. *The fact that it does not is due to the presence of the quantum–classical transition zone.* This fact is indeed the focus of our interest here and the motivation for our present research. Now, the specific heat  $C_v$  in the case of model (1) clearly shows that, according to the temperature  $T$ , there is a classical region (Dulong–Petit validity) and a quantum one (third law compliance). For model (2), one has to appeal to Fig. 1 for a somewhat similar situation.

Accordingly, structural details emerge that make  $c$  non-null in the quantum–classical transition zone. These details are physical ones for the Einstein crystal. For the ideal gas they reflect on *the inadequacy of the model at low enough temperatures.* In both cases, the CQF plays a protagonist role. Remarkably enough, critical temperatures that are too high for the EC coincide with those that are too low for the IG. These critical temperatures are thus CQF signatures.

Summing up:

- We have revisited two very simple systems using the statistical complexity as quantifier.



- We have uncovered with the help of the statistical complexity, unexplored, interesting features of these simple systems.
- These features are seen to be related to the classical–quantum frontier.

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