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Statistical manifestation of quantum correlations via disequilibrium

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ABSTRACT

The statistical notion of disequilibrium (D) was introduced by López-Ruiz, Mancini, and Calbet (LMC) (1995) [1] more than 20 years ago. D measures the amount of "correlational structure" of a system. We wish to use D to analyze one of the simplest types of quantum correlations, those present in gaseous systems due to symmetry considerations. To this end we extend the LMC formalism to the grand canonical environment and show that D displays distinctive behaviors for simple gases, that allow for interesting insights into their structural properties.

1. Introductory matters

1.1. Historical notes

Knowledge about the unpredictability and randomness of a system does not automatically translate into an adequate grasping of the extant correlation structures, reflected by the current probability distribution (PD). The desideratum is to capture the relations amongst the components of a system in a manner similar to that in which entropy captures disorder. One certainly knows that the antipodal extreme cases of (a) perfect order and (b) maximum randomness are not characterized by strong correlations [1]. Amidst (a) and (b) diverse correlation-degrees may be manifested by the features of the probability distribution. The big question is how? Answering the query is not a simple task. Notoriously, Crutchfield has stated in 1994 that [2,3]:

"*Physics does have the tools for detecting and measuring complete order equilibrium and fixed point or periodic behavior and ideal randomness via temperature and thermodynamic entropy or, in dynamical contexts, via the Shannon entropy rate and Kolmogorov complexity. What is still needed, though, is a definition of structure and a way to detect and to measure it [2,3]*".

Famously, Seth Lloyd found as many as 40 ways of introducing a complexity definition, none of which quite satisfactory.

LMC introduced an interesting functional of the PD that does grasp correlations in the way that entropy captures randomness. This may be regarded as a great breakthrough [1]. LMC's statistical complexity did individualize and quantify the bequeath of Boltzmann's entropy (or information H) and that of structure. *The latter contribution came from the notion of disequilibrium D*, which it measures (in probability space) the distance from i) the prevailing probability distribution to ii) the uniform probability. *D reveals the amount of structural details. The larger it is, the more structure exists* [1,4]. For N-particles one has

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

where $p_1, p_2, \ldots, p_N$ are the individual normalized probabilities ($\sum_{i=1}^{N} p_i = 1$) [1]. The two ingredients H and D are combined by LMC to yield the complexity C in the fashion $C_{LMC} = DH$ [1,5–10]. C_{LMC} vanishes in the two above extreme cases (a) and (b).

1.2. Our present task and its motivation

In this paper, we deal with properties of D within of the grand canonical ensemble scenario, for simple gaseous systems obeying quantum statistics. We will use D as a structure-indicator so as to compare the classical Maxwell–Boltzmann situation vis-a-vis the Bose–Einstein and Fermi–Dirac ones.

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Why? Because in this way we have an opportunity of observing the workings of quantum symmetries in the simplest conceivable scenario. We will indeed encounter interesting quantum insights.

The issue of separating quantum (qc) from classical correlations (cc) has revived since the discovery of quantum discord [11–13]. Before, it was a simple matter to distinguish between cc and qc, because the former were associated to separable states and the latter to non-separable ones endowed with entanglement. The discovery that some separable states are also endowed with qc (discord) made the cc-qc distinction a more formidable task, still the subject of much research. This gives our present endeavor some additional contemporary relevance.

The structure of this paper is organized as follows: in Section 2 we recapitulate the relevant background, i.e., the pertinent formalism in the canonical ensemble and we introduce also our proposal referring to extending the disequilibrium notion to the grand canonical ensemble. The main results of the paper are presented in Section 3, in which we apply our ideas to quantum gaseous systems, focusing attention on the mean occupation number. Finally, we present our conclusions en Section 4.

2. Disequilibrium in the grand canonical ensemble

2.1. López-Ruiz work for the canonical ensemble

We recapitulate first interesting notions of López-Ruiz for the canonical ensemble [4,14]. These deal with a classical ideal gas in thermal equilibrium. One has N identical particles, confined to a volume V at temperature T. The ensuing Boltzmann PD is [17]

$$\rho(x,p)=\frac{e^{-\beta\mathcal{H}(x,p)}}{Q_N(V,T)}. \tag{2}$$

One has $\beta=1/k_BT$, k_B Boltzmann's constant, while $\mathcal{H}(x,p)$ is the Hamiltonian, and x, p are the phase space variables. The canonical partition reads

$$Q_N(V,T)=\int d\Omega\, e^{-\beta\,\mathcal{H}(x,p)}, \tag{3}$$

with $d\Omega=d^{3N}x\,d^{3N}p/N!h^{3N}$. The Helmholtz free energy A is [17]

$$A(N,V,T)=-k_BT\,\ln Q_N(V,T). \tag{4}$$

López-Ruiz (LR) demonstrates, in Ref. [14], that the disequilibrium D displays the following appearance for continuous probability distributions

$$D(N,V,T)=e^{2\beta\,[A(N,V,T)-A(N,V,T/2)]}. \tag{5}$$

LR changes the variable T by $T/2$ in Eq. (4) and replaces this into Eq. (5). Consequently, he finds

$$D(N,V,T)=\frac{Q_N(V,T/2)}{[Q_N(V,T)]^2}. \tag{6}$$

Employing now definitions (2) and (3), D can also be cast as

$$D(N,V,T)=\frac{\int d\Omega\, e^{-2\beta H(x,p)}}{[Q_N(V,T)]^2}=\int d\Omega\,\rho^2(x,p). \tag{7}$$

This is the orthodox form used by most people (see, for instance, Ref. [15]).

2.2. Our proposal for the grand canonical ensemble

Our goal here is to extend the above ideas of López-Ruiz to the structures of the grand canonical ensemble. In this ensemble, the system has a variable number of particles N, with the average number $\bar{N}$ determined by external conditions. The system can exchange both energy and particles with a reservoir. We assume, as usual, equilibrium with respect to both energy and particle number, i.e., reservoir and system have the same temperature T and the same chemical potential μ [16]. To describe this kind of systems, we appeal to the equilibrium distribution, i.e.,

$$\rho(x,p,N)=\frac{e^{-\beta(\mathcal{H}(x,p)-\mu N)}}{\mathcal{Z}(z,V,T)}, \tag{8}$$

where $\mathcal{Z}(z,V,T)=\sum_N z^N Q_N(V,T)$ is the grand partition function. One usually defines the fugacity $z=\exp(\mu\beta)$ [17]. The disequilibrium is rigorously defined as

$$D(z,V,T)=\sum_N\int d\Omega\,\rho^2(x,p,N), \tag{9}$$

that constitutes an extension of the definition (7) given for the canonical ensemble, except that now we have added a sum over N and incorporated the corresponding equilibrium distribution $\rho(x,p,N)$. In view of Eqs. (3) and (8), D becomes

$$D(z,V,T)=\frac{1}{\mathcal{Z}^2(z,V,T)}\sum_N z^{2N}\int d\Omega\, e^{-2\beta\mathcal{H}(x,p)}. \tag{10}$$

Note that we are adding a dependence on the fugacity z in D. From Eqs. (6) and (7), the above expression can be cast as

$$D(z,V,T)=\frac{1}{\mathcal{Z}^2(z,V,T)}\sum_N z^{2N}Q_N(V,T/2). \tag{11}$$

We see that, when T changes to $T/2$, z is replaced by z^2. In such a situation, we immediately find that $\mathcal{Z}(z^2,V,T/2)=\sum_N z^{2N}Q_N(V,T/2)$, which leads to an original expression for the disequilibrium in terms of $\mathcal{Z}$, namely,

$$D(z,V,T)=\frac{\mathcal{Z}(z^2,V,T/2)}{\mathcal{Z}^2(z,V,T)}, \tag{12}$$

depending on the variables V, T, and z. It is well known that the natural quantity associated to this ensemble is the grand potential, given by [16,17]

$$\Psi(z,V,T)=-k_BT\,\ln\mathcal{Z}(z,V,T). \tag{13}$$

Introducing (13) into Eq. (12), one can re-express D for the grand canonical in terms of the grand potential Ψ

$$D(z,V,T)=e^{2\beta\,[\Psi(z,V,T)-\Psi(z^2,V,T/2)]}. \tag{14}$$

In order to establish another connection with the grand canonical ensemble, we appeal to the relationship between the Helmholtz free energy A given in Eq. (4) and the grand potential Ψ defined in (13) [16]

$$A(\bar{N},V,T)=k_BT\bar{N}\ln z+\Psi(z,V,T), \tag{15}$$

where A is evaluated for $\bar{N}$ instead of N, due to the fact that N-fluctuations are small, with a peak at $N=\bar{N}$ (we must use the relation $\bar{N}=z\partial\ln\mathcal{Z}(z,V,T)/\partial z$ in order to eliminate z [16]). Accordingly, replacing Eq. (15) into Eq. (14) we arrive at

$$D(\bar{N},V,T)=e^{2\beta\,[A(\bar{N},V,T)-A(\bar{N},V,T/2)]}, \tag{16}$$

where, in this representation, the corresponding variables are $\bar{N}$, V, and T.

Summing up, Eqs. (12), (14), and (16) provide three alternative ways for calculating the disequilibrium in the grand canonical ensemble. One uses, respectively, the grand partition function, the grand potential, or the Helmholtz free energy.

3. Statistical features of quantum gaseous system: mean occupation number

3.1. Disequilibrium

Following Ref. [17], Chapter 6, we focus attention on a gaseous system of N non-interacting undistinguishable particles restricted to a volume V, with energies ϵ_k grouped into cells as described in this classical book. In the grand canonical ensemble, the equation of state for the aforementioned system is given by [17]

$$\frac{PV}{k_B T} = \ln \mathcal{Z}(z, V, T) = \frac{1}{a} \sum_{\epsilon} \ln(1 + aze^{-\beta\epsilon}), \tag{17}$$

where i) $a = +1$ in the Fermi–Dirac (FD) case, ii) $a = -1$ in the Bose–Einstein (BE) one, and iii) $a = 0$ for the Maxwell–Boltzmann (MB) instance. The energy ϵ runs over all eigenstates. In particular, for the classical case, the grand canonical partition function becomes [17]

$$\mathcal{Z}(z, V, T) = z \sum_{\epsilon} e^{-\beta\epsilon}. \tag{18}$$

Replacing Eqs. (17) and (18) into Eq. (12), after a bit of algebra, we analytically find the disequilibrium:

$$D(z, V, T) = \prod_{\epsilon} D_a(z, \epsilon, V, T), \tag{19}$$

where, for each energy level, we have

$$D_a(z, \epsilon, V, T) = \begin{cases} \frac{(1+az^2 e^{-2\beta\epsilon})^{1/a}}{(1+aze^{-\beta\epsilon})^{2/a}} & \text{for } a = \pm 1, \\ ze^{-\beta\epsilon} & \text{for } a = 0. \end{cases} \tag{20}$$

We have here an expression for the disequilibrium (associated to the level of energy ϵ) for each of the three cases under consideration. In what follows, in order to simplify the notation, we will drop the variables z, V, and T. Therefore, only the dependency on ϵ will be indicated. Moreover, since the mean occupation number $\langle n_\epsilon \rangle$ of the level ϵ is given by [17]

$$\langle n_\epsilon \rangle = \frac{1}{z^{-1} e^{\beta\epsilon} + a}, \tag{21}$$

it follows that

$$z^{-1} e^{\beta\epsilon} = \frac{1}{\langle n_\epsilon \rangle} - a. \tag{22}$$

Therefore, replacing Eq. (22) into Eq. (20), we obtain $D_a(\epsilon)$ as a function of $\langle n_\epsilon \rangle$ for our three cases. One has

$$D_a(\epsilon) = \begin{cases} \left[(1 - a\langle n_\epsilon \rangle)^2 + a\langle n_\epsilon \rangle^2\right]^{1/a} & \text{for } a = \pm 1, \\ \langle n_\epsilon \rangle & \text{for } a = 0. \end{cases} \tag{23}$$

The $D_a(\epsilon)$-behavior ruled by Eqs. (20) and (23) is displayed in Figs. 1 to 4 for the FD (red), BE (blue), and MB (green) cases. The differences with the classical result are a clear illustration of the effects that quantum correlations generate. The minimum of $D_a(\epsilon)$ occurs when $\langle n_\epsilon \rangle = 1/(1 + a)$, i.e., $\langle n_\epsilon \rangle = 1/2$ for fermions and $\langle n_\epsilon \rangle = \infty$ for bosons, as we illustrate in Figs. 1 and 2. Minimum $D_a(\epsilon)$ entails minimal structure, that in the BE instance is associated to the condensate. Thus, the condensate is endowed with minimum structure, i.e., $D_{-1}(\epsilon)$ clearly identifies the condensate *as having no distinctive* **structural** features, which constitutes a new $D_a(\epsilon)$-result, as far as we know. This notion is reinforced by Figs. 3 and 4, by plotting $D_a(\epsilon)$ versus $\langle n_\epsilon \rangle$. If we set $q = (\epsilon - \mu)/k_B T$, we appreciate the fact that $D_a(\epsilon)$ varies only between $q = 0$ and approximately $q = 10$, remaining constant (and equal to unity) for any q-value greater than 10. Remember that the our system's description converges to the classical one as q grows [17].

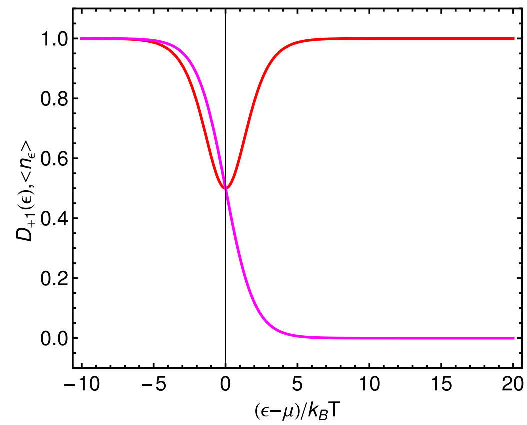

Fig. 1. Disequilibrium $D_{+1}(\epsilon)$ (red curve) and $\langle n_\epsilon \rangle$ (magenta curve) versus $(\epsilon - \mu)/k_B T$ for fermions. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

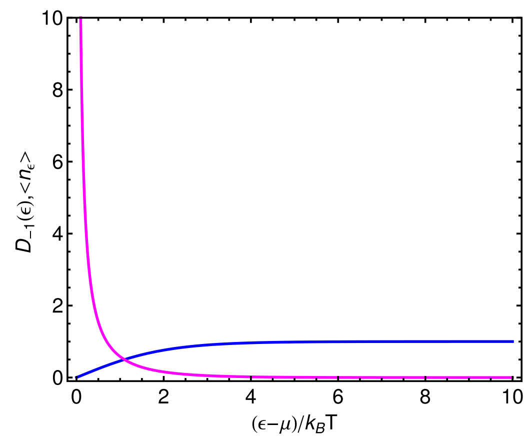

Fig. 2. Disequilibrium $D_{-1}(\epsilon)$ (blue curve) and $\langle n_\epsilon \rangle$ (magenta curve) versus $(\epsilon - \mu)/k_B T$ for bosons. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

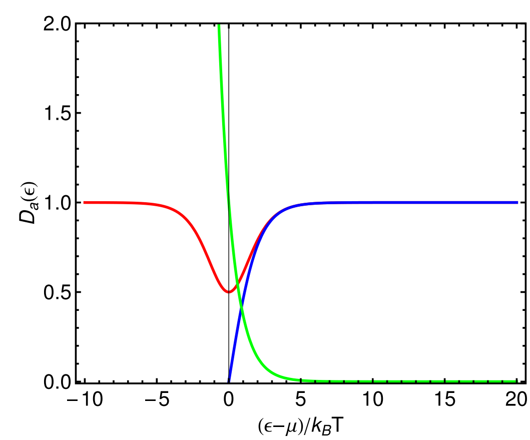

Fig. 3. Disequilibrium $D_a(\epsilon)$ versus $(\epsilon - \mu)/k_B T$. We have a red curve for fermions, a blue line for bosons, and green curve for MB (no quantum correlations). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

In the FD instance, instead, the minimum of $D_{+1}(\epsilon)$ is attained for the situation farthest removed from the trivial instances of zero or maximal occupation. For fermions, complete or zero occupations display maximal structure. At fist sight, this behavior near

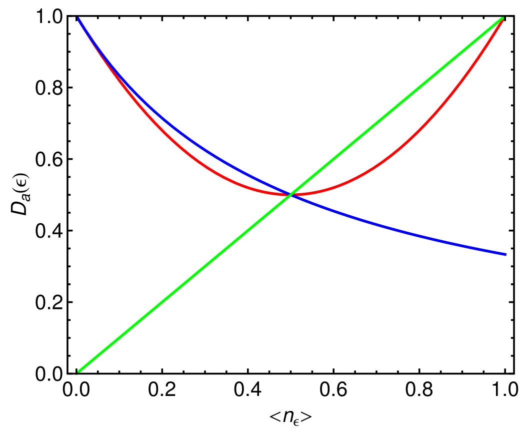

Fig. 4. Disequilibrium $D_a(\epsilon)$ versus $\langle n_\epsilon \rangle$. We have a red curve for fermions, a blue line for bosons, and a green curve for MB (no quantum correlations). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

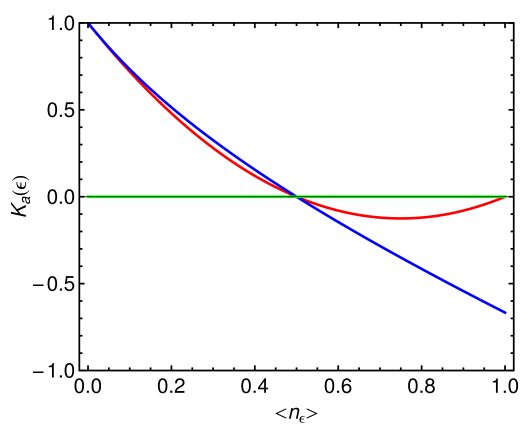

Fig. 5. $K_a(\epsilon) = D_a(\epsilon) - \langle n_\epsilon \rangle$ as a function of $\langle n_\epsilon \rangle$ (red curve for fermions, blue curve for bosons, and green curve for MB), the quantumness indicator. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

$\langle n_\epsilon \rangle = 0$ may seem surprising. The quantum disequilibrium is large while the classical one vanishes. There is no structure, classically. However, it is well known that the quantum vacuum is a very complex, complicated object, as quantum electrodynamics clearly shows. (The quantum–vacuum literature is immense. A suitable introductory treatise is that of Mattuck in Ref. [18].) This is foreshadowed by the quantum disequilibrium at the level of quantum gases! Instead, we note that, for $a = 0$ (the classical case), $D_0(\epsilon)$ coincides with the mean occupation number.

On the other hand, let us reiterate that for $\langle n_\epsilon \rangle \to \infty$, the boson disequilibrium vanishes, on account of dealing with indistinguishable particles. The condensate exhibits no structural details. Instead, the MB $D_0(\epsilon)$ grows with $\langle n_\epsilon \rangle$ because one deals with distinguishable particles, and much more information is needed to label a million particles than to label 10 of them. This fact emphasizes the fact that $D_a(\epsilon)$ tells us about *information* on structural details, either physical or labeling-ones.

Let us define $K_a(\epsilon) = D_a(\epsilon) - \langle n_\epsilon \rangle$, which is a $D_a(\epsilon)$-related "quantumness index", given that it vanishes in the classical case for all mean occupation number. We plot it in Fig. 5. This graph is very instructive. Note that $\langle n_\epsilon \rangle = 1/2$ is a critical value. For it, the curves attain classical values and, for fermions, $D_a(\epsilon)$ is minimum, reflecting on minimal fermion structure. Not surprisingly, in view of previous considerations, $K_a(\epsilon)$ is maximal at the quantum vacuum. From $\langle n_\epsilon \rangle = 0$, $K_a(\epsilon)$ steadily diminishes till we reach the critical point mentioned above. For bosons, it then steadily increases again, in absolute value, towards the condensate. For fermions it grows again, in absolute value, reaches a maximum at $\langle n_\epsilon \rangle = 3/4$, and then tends to zero again at $\langle n_\epsilon \rangle = 1$.

3.2. Probability distributions as a function of $D_a(\epsilon)$

It is well-known the probability to encounter exactly n particles in a state of energy ϵ is $p_\epsilon(n)$ [17], which for the Fermi–Dirac instance reads

$$p_\epsilon(n)|_{FD} = \begin{cases} 1 - \langle n_\epsilon \rangle & \text{for } n = 0, \\ \langle n_\epsilon \rangle & \text{for } n = 1. \end{cases} \tag{24}$$

Thus, considering Eqs. (23) and (24), the disequilibrium becomes

$$D_{+1}(\epsilon) = \sum_{n=0}^{1} p_\epsilon^2(n) = p_\epsilon^2(0) + p_\epsilon^2(1). \tag{25}$$

Since $p_\epsilon(0) + p_\epsilon(1) = 1$, replacing this into above equation, we also have

$$D_{+1}(\epsilon) = (1 - p_\epsilon(1))^2 + p_\epsilon^2(1), \tag{26}$$

the disequilibrium as a function of the occupation probability $p_\epsilon(1)$. Solving Eq. (26) we find

$$p_\epsilon(1)|_{FD} = \frac{1}{2}(1 \pm \sqrt{2D_{+1}(\epsilon) - 1}), \tag{27}$$

which leads to bi-valuation in expressing probabilities as a function of D_{+1}, a novel situation uncovered here.

In the Bose–Einstein case, the probability is given by the distribution [17]

$$p_\epsilon(n)|_{BE} = \frac{\langle n_\epsilon \rangle^n}{(1 + \langle n_\epsilon \rangle)^{n+1}}, \tag{28}$$

and, accordingly, the disequilibrium is now of the form

$$D_{-1}(\epsilon) = \frac{1 - p_\epsilon(n)}{1 + p_\epsilon(n)}. \tag{29}$$

From the above equation then we obtain the probability distribution as a function of the disequilibrium. It reads as follows

$$p_\epsilon(n)_{BE} = \frac{1 - D_{-1}(\epsilon)}{1 + D_{-1}(\epsilon)}. \tag{30}$$

For the MB-instance, p_ϵ is a Poisson distribution given by [17]

$$p_\epsilon(n)|_{MB} = \frac{(\langle n_\epsilon \rangle)^n}{n!} e^{-\langle n_\epsilon \rangle}, \tag{31}$$

that, for Eq. (23) becomes

$$p_\epsilon(n)|_{MB} = \frac{D_0(\epsilon)^n}{n!} e^{-D_0(\epsilon)}. \tag{32}$$

We represent Eqs. (27), (30), and (32) in Fig. 6, where we plot the probability as a function of the disequilibrium $D_a(\epsilon)$ for the three cases, here discussed, with $a = 0, \pm 1$. All of them are different. The classical one is a Poisson distribution. The boson-one decreases steadily as $D_{-1}(\epsilon)$ augments. The FD distribution is bi-valuated save at the $D_{+1}(\epsilon) = 1/2$ instance. Note that for $D_{+1}(\epsilon) = 1$ the probability can be either zero or one, a kind of "cat"-effect.

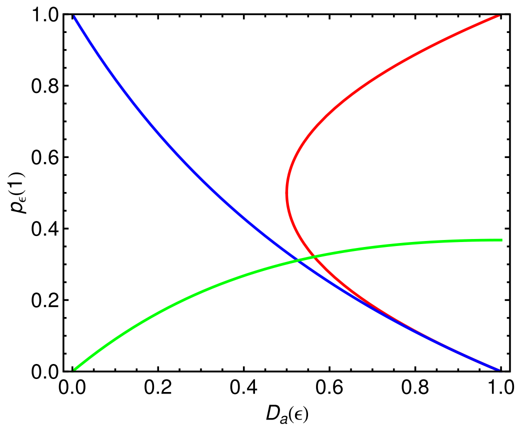

Fig. 6. Probability $p_\epsilon(1)$ versus $D_a(\epsilon)$ for our three cases. We have a red curve for fermions, a blue curve for bosons, and a green curve for MB (no quantum correlations). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

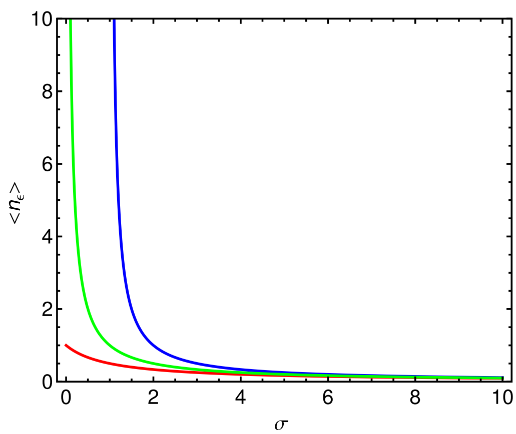

Fig. 7. The mean occupation number $\langle n_\epsilon \rangle$ versus σ.

3.3. *Disequilibrium in term of fluctuations*

The relative mean-square fluctuation is [17]

$$\sigma = \frac{\langle n_\epsilon^2 \rangle - \langle n_\epsilon \rangle^2}{\langle n_\epsilon \rangle^2} = \frac{1}{\langle n_\epsilon \rangle} - a. \tag{33}$$

In the classical case ($a = 0$) the relative fluctuation is "normal", in the sense that it is proportional to the inverse occupation number and exhibits the statistical behavior of uncorrelated events. In the Fermi–Dirac case σ becomes subnormal and fermions exhibit a negative statistical correlation. Since $0 \le \langle n_\epsilon \rangle \le 1$, then $\sigma \ge 0$. On the other hand, in the Bose–Einstein case, the fluctuation is super-normal [17] ($\sigma \ge 1$), and thus bosons exhibit positive statistical correlation [17]. We illustrate these considerations in Figs. 7 and 8.

Accordingly, in terms of fluctuations one has

$$D_a(\sigma) = \begin{cases} \left(\frac{a+\sigma^2}{(a+\sigma)^2}\right)^{1/a} & \text{for } a = \pm 1, \\ 1/\sigma & \text{for } a = 0. \end{cases} \tag{34}$$

We see that, in quantum terms, $D_a(\sigma)$ strongly depends also upon the symmetry parameter a. We plot the couple of Eqs. (34) in Fig. 7. As σ grows, curves of $D_a(\sigma)$ for fermions and bosons tend to coincide. Once again, for fermions the "normal" situation is that of minimum $D_a(\sigma)$.

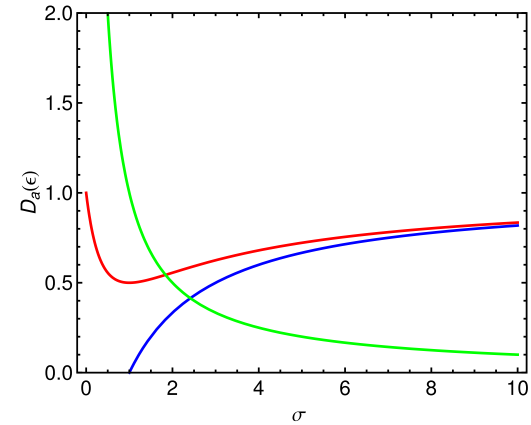

Fig. 8. Disequilibrium $D_a(\epsilon)$ versus σ. We have a red curve for fermions, a blue curve for bosons, and a green curve for MB (no quantum correlations). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

4. Conclusions

We have shown in this note that quantum effects are clearly reflected by the disequilibrium's $D_a(\epsilon)$ behavior. In particular, we observe that:

- For instance, minimum $D_{-1}(\epsilon)$ entails minimal structural correlations, that in the BE instance are associated to the condensate. Thus, the condensate is endowed with minimum structure, i.e., $D_{-1}(\epsilon)$ clearly identifies the condensate as having no distinctive structural features. This is reinforced by Fig. 4, by plotting $D_{-1}(\epsilon)$ versus $\langle n_\epsilon \rangle$.
- On the other hand, in the FD instance, the minimum of $D_{+1}(\epsilon)$ obtains for the situation farthest removed from the trivial instances of zero or maximal occupation. For fermions, complete or zero occupations display maximal structure.
- The behavior near $\langle n_\epsilon \rangle = 0$ is remarkable. The quantum disequilibrium is large while the classical one vanishes. There is no structure, classically. However, the quantum vacuum is a very complicated object, as quantum electrodynamics clearly shows. This is foreshadowed by the quantum disequilibrium at the level of simple gaseous systems.
- For $\langle n_\epsilon \rangle \to \infty$, the boson disequilibrium vanishes, on account of dealing with indistinguishable particles. The condensate exhibits no structural details. On the contrary, the MB $D_0(\epsilon)$ grows with $\langle n_\epsilon \rangle$ because one deals with distinguishable particles, and much more information is needed to label a million particles than to do so with 10 of them.
- We gather that $D_a(\epsilon)$ tells us about *information* on structural details, either physical or labeling-ones.

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