Statistical manifestation of quantum correlations via disequilibrium

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That of disequilibrium ($D$) is a statistical notion introduced by López-Ruiz, Mancini, and Calbet (LMC) more than 20 years ago [Phys. Lett. A \textbf{209} (1995) 321]. $D$ 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 simple quantum gaseous systems and 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.

\section{I. INTRODUCTORY MATTERS}

\textbf{A. Historical notes}

Knowledge of the unpredictability and randomness of a system does not automatically translate in an adequate grasping of the extant correlation structures reflected by the current probability distribution (PD). The desideratum is to capture the relations amongst a system’s components in a similar manner as entropy describes disorder. One certainly knows that the antipodal extreme cases of (a) perfect order and (b) maximum randomness are not characterized by strong correlations \cite{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 simple task. Notoriously, Crutchfield has stated in 1994 that \cite{2, 3}:

\begin{quote}
"Physics does have the tools for detecting and measuring complete order equilibria 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 \cite{4, 5, 6, 7, 8, 9, 10}.
\end{quote}

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 \cite{11}. 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. 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 \cite{1, 4}. For $N$–particles one has

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

Here $p_1, p_2, \ldots, p_N$ are the individual normalized probabilities ($\sum_{i=1}^{N} p_i = 1$) \cite{11}. The two ingredients $H$ and $D$ are combined by LMC to yield the complexity $C$ in the fashion $C_{LMC} = DH$ \cite{11, 12, 13}. $C_{LMC}$ vanishes, the two above extreme cases (a) and (b).

\textbf{B. Our present task and its motivation}

In this paper we deal with $D$ properties, within a grand canonical ensemble scenario, for simple gaseous system obeying quantum statistics. We will use $D$ as a structure-indicator so as to compare the classical Maxwell-Boltzmann situation of no quantum correlations vis-a-vis the Bose-Einstein and Fermi-Dirac situations.

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 \cite{14, 15, 16}. 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 the following. In Section II 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 in Section III in which we apply our ideas to quantum gaseous systems, focusing attention on the occupation number. Finally, we present our conclusions en Section IV.

II. Disequilibrium in the Grand Canonical Ensemble

A. López-Ruiz work for the canonical ensemble

We recapitulate first interesting notions of López-Ruiz, for the canonical ensemble \[4, 14\], dealing with a classical ideal gas in thermal equilibrium. One has \(N\) identical particles, confined in a volume \(V\) at the temperature \(T\). The ensuing Boltzmann PD is \[15\]

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

One has \(\beta = 1/k_B T\), \(k_B\) Boltzmann’s constant, while \(\mathcal{H}(x, p)\) is the Hamiltonian, and \(x, p\) the phase space variables. The canonical partition reads

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

with \(\mathrm{d}\Omega = \frac{\mathrm{d}^3N x \mathrm{d}^3N p}{N!h^{3N}}\). The Helmholtz’ free energy \(A\) is \[15\]

\[
A(N, V, T) = -k_B T \ln Q_N(V, T). \tag{4}
\]

R. López-Ruiz (LR) demonstrates in Ref. \[14\] that the disequilibrium \(D(N, V, T)\) displays the following nice 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 now \(T\) by \(T/2\) in Eq. \[1\] and replaces this in Eq. \[5\]. Consequently, he finds

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

B. Our proposal for the grand canonical ensemble

Our goal now is to extend the above LR-formulation to the grand canonical ensemble. As it is well known, the natural quantity associated to this ensemble is the grand potential which is given by \[15\]

\[
\Psi(z, V, T) = -k_B T \ln Z(z, V, T), \tag{7}
\]

where \(Z(z, V, T)\) is the grand partition function of the system and the parameter \(z\) is the fugacity defined by \(z = \exp(-\alpha) = \exp(\mu \beta) \[15\]. One can then extend the ideas presented above for the canonical ensemble, with the help of the relationship between the free energy and the grand potential, that reads

\[
A(z, V, T) = Nk_B T \ln z + \Psi(z, V, T). \tag{8}
\]

Introducing this into Eq. \[5\], one re-express the disequilibrium in the grand canonical ensemble which is now

\[
D(z, V, T) = e^{z^2 \beta [\Psi(z, V, T) - \Psi(z^2, V, T/2)]}. \tag{9}
\]

Note we are adding a dependence on the fugacity \(z\) in \(D\). We observe that, when \(T\) changes to \(T/2\), then \(z\) is replaced by \(z^2\). Thus, using Eq. \[7\], we immediately are led to an original (we believe) disequilibrium expression in terms of the grand partition function

\[
D(z, V, T) = \frac{Z(z^2, V, T/2)}{Z(z, V, T)} \tag{10}
\]

which, depends on the variables \(V, T\), and fugacity \(z\).

III. Statistical Features of the Quantum Gaseous System Occupation Number

A. Disequilibrium

Following Ref. \[13\], Chapter 6, we focus attention on a gaseous system of \(N\) non-interacting indistinguishable particles contained in a volume \(V\) with energies \(\epsilon_k\) 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 \[13\]

\[
\frac{PV}{k_B T} = \ln Z(z, V, T) = \frac{1}{a} \sum \ln(1 + a z e^{-\epsilon}). \tag{11}
\]

where \(a = +1\) in the Fermi-Dirac (FD) case, \(a = -1\) in the Bose-Einstein (BE) one, and \(a = 0\) for the Maxwell-Boltzmann (MB) instance. The energy \(\epsilon\) runs over every eigenstate. In particular, for the classical case, the grand partitions functions becomes \[13\]

\[
\frac{PV}{k_B T} = \ln Z(z, V, T) = \frac{1}{a} \sum \ln(1 + a z e^{-\epsilon}). \tag{11}
\]
The notion is reinforced in Figs. 3 and 4, by plotting \( Z(z, V, T) = z \sum_\epsilon e^{-\beta \epsilon} \). (12)

Replacing Eqs. (11) and (12) into Eq. (10) we analytically get the disequilibrium whose form is

\[ D(z, V, T) = \prod_\epsilon D_a(z, \epsilon, V, T), \]  

where, for each energy level, we have

\[ D_a(z, \epsilon, V, T) = \begin{cases} 
(1+a z^2 e^{-2z \epsilon})^{1/a} & \text{for } a = \pm 1, \\
2 e^{-\beta \epsilon} & \text{for } a = 0,
\end{cases} \]  

(14)
a disequilibrium expression for the level of energy \( \epsilon \) for the three cases under consideration. From hereafter, in order to simplify the notation, we will drop the variables \( z, V, \) and \( T \). Therefore, only the dependency on \( \epsilon \) will be preserved.

Moreover, since the mean occupation number \( \langle n_\epsilon \rangle \) of the level \( \epsilon \) is given by

\[ \langle n_\epsilon \rangle = \frac{1}{z^{-1}e^{\beta \epsilon} + a}, \]  

(15)
then we immediately have that

\[ z^{-1}e^{\beta \epsilon} = \frac{1}{\langle n_\epsilon \rangle} - a. \]  

(16)

Therefore, replacing Eq. (10) into the couple of Eqs. (14) we obtain \( D_a(\epsilon) \) as a function of the occupation number for the three cases. This reads

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

(17)

The \( D_a(\epsilon) \)–behavior ruled by Eqs. (14) and (17) is displayed in Figs. 1 to 3 by the FD (red), BE (blue), and MB (green) cases. The differences with the classical result are a magnificent illustration of quantum correlations. 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 illustrated 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 minimal 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 in Figs. 5 and 6 by plotting \( D_a(\epsilon) \) versus \( \langle n_\epsilon \rangle \). If we set \( q = (\epsilon - \mu)/k_BT \), we appreciate the fact that \( D_a(\epsilon) \) varies only between \( q = 0 \) and approximately \( q = 10 \), remaining constant equal to 1 for any larger \( q \)–value grater than 10. Remember that the simple gaseous systems’ descriptions converge to the classical one as \( q \) grows.

In the FD instance, instead, 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. At first sight, this behavior near \( \langle n_\epsilon \rangle = 0 \) 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 Matuck in Ref. [10]). 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 \( \langle n_\epsilon \rangle \rightarrow \infty \), 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 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 $\langle n_\epsilon \rangle = 0$, $K_\alpha(\epsilon)$ 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 $\langle n_\epsilon \rangle = 1$.

B. Probability distributions as a function of $D_\alpha(\epsilon)$

It is well-known the the probability to encounter exactly $n$ particles in a state of energy $\epsilon$ is $p_\epsilon(n)\text{[13]}$, which for the Fermi-Dirac instance reads

$$p_\epsilon(n|FD) = \begin{cases} 1 - \langle n_\epsilon \rangle & \text{for } n = 0, \\ \langle n_\epsilon \rangle & \text{for } n = 1. \end{cases} \quad (18)$$

Thus, considering Eqs. [17] and [18], the disequilibrium becomes

$$D_{+1}(\epsilon) = \sum_{n=0}^{1} p_\epsilon^2(n) = p_\epsilon^2(0) + p_\epsilon^2(1). \quad (19)$$

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

$$D_{+1}(\epsilon) = (1 - p_\epsilon(1))^2 + p_\epsilon(1)^2, \quad (20)$$

the disequilibrium as a function of the probability of the occupation of the level of energy $\epsilon$ with one fermion.

Solving Eq. (20) we get

$$p_\epsilon(1|FD) = \frac{1}{2}(1 \pm \sqrt{2D_{+1}(\epsilon) - 1}), \quad (21)$$
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 the geometrical distribution \[ p_\epsilon(n)_{BE} = \frac{\langle n_\epsilon \rangle^n}{(1 + \langle n_\epsilon \rangle)^{n+1}}, \] (22) and, accordingly, the disequilibrium is now of the form \[ D_{-1}(\epsilon) = \frac{1 - p_\epsilon(n)}{1 + p_\epsilon(n)}. \] (23) From the above equation then we get the probability distribution as a function of the disequilibrium that it reads as follows \[ p_\epsilon(n)_{BE} = 1 - \frac{D_{-1}(\epsilon)}{1 + D_{-1}(\epsilon)}. \] (24)

For the MB-instance, $p_\epsilon$ is a Poisson distribution given by \[ p_\epsilon(n)_{MB} = \frac{(\langle n_\epsilon \rangle)^n}{n!} e^{-\langle n_\epsilon \rangle}, \] (25) that, for Eq. (17) becomes \[ p_\epsilon(n)_{MB} = \frac{D_0(\epsilon)^n}{n!} e^{-D_0(\epsilon)}. \] (26)

We represent Eqs. (21), (24) and (26) in Fig. 6, where we plot the probability as a function of the disequilibrium that it reads as follows

\[ p_\epsilon(1) \text{ versus } D_a(\epsilon) \text{ for three cases mentioned. We label red curve for fermions, blue curve for bosons and green curve for MB (no quantum correlations).} \]

\[ \text{FIG. 6: Probability } p_\epsilon(1) \text{ versus } D_a(\epsilon) \text{ for three cases mentioned. We label red curve for fermions, blue curve for bosons and green curve for MB (no quantum correlations).} \]

\[ \text{FIG. 7: The mean occupation number } \langle n_\epsilon \rangle \text{ versus } \sigma. \]

\[ \text{FIG. 7: The mean occupation number } \langle n_\epsilon \rangle \text{ versus } \sigma. \]

\[ \text{statistical correlation} \]

\[ \text{We observe all this in Figs. 4 and 8.} \]

\[ \text{Therefore, in terms of the fluctuations we get} \]

\[ D_a(\sigma) = \begin{cases} \left( \frac{a+\sigma^2}{a+\sigma} \right)^{1/a} & \text{for } a = \pm 1, \\ 1/\sigma & \text{for } a = 0. \end{cases} \] (28)

We see that, in quantum terms, $D_a(\sigma)$ strongly depends also upon the symmetry parameter $a$. We plot the couple of Eqs. (28) in Fig. 7. As $\sigma$ grows, fermion’s and boson’s $D_a(\sigma)$s tend to coincide. Once again, for fermions the normal situation is that of minimum $D_a(\sigma)$.

\[ \text{IV. CONCLUSIONS} \]

We have shown in this note that quantum effects are clearly reflected by the disequilibrium’s $D_a(\epsilon)$ behavior.
• 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 in Fig. 8 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 10 of them.

• We then gather that $D_\epsilon(\epsilon)$ tells us about information on structural details, either physical or labeling-ones.

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