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Classical analogue of the statistical operator

Research Article

Angelo Plastino[1*], Angel R. Plastino[2,3†], Claudia Zander[4‡]

1 *Universidad Nacional de La Plata UNLP-CONICET, C.C. 727, 1900 La Plata, Argentina*

2 *CeBio y Secretaria de Investigacion, Universidad Nacional del Noroeste de la Prov. de Buenos Aires - UNNOBA and CONICET, R. Saenz Peña 456, Junin, Argentina*

3 *Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada, 18071 Granada, Spain*

4 *Physics Department, University of Pretoria, Pretoria 0002, South Africa*

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Abstract: We advance the notion of a classical density matrix, as a classical analogue of the quantum mechanical statistical operator, and investigate its main properties. In the case of composite systems a partial trace-like operation performed upon the global classical density matrix leads to a marginal density matrix describing a subsystem. In the case of dynamically independent subsystems (that is, non-interacting subsystems) this marginal density matrix evolves locally, its behavior being completely determined by the local phase-space flow associated with the subsystem under consideration. However, and in contrast with the case of ordinary marginal probability densities, the marginal classical density matrix contains information concerning the statistical correlations between a subsystem and the rest of the system.

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1. Introduction

The physics of information is a multidisciplinary research field [1–13] that has generated significant advances concerning the limitations imposed by the basic laws of Nature on any real device that processes or transmits information [6, 7, 13–15]. On the other hand, theoretical developments indubitably show that information-related notions are of essence for our understanding of the physical world [1–6]. Information-based methodologies such as the maximum entropy (maxent) principle [16–18] have found application in an immense variety of scenarios, and have paved the way for erecting bridges between physics and other scientific fields, particularly biology. Indeed, biological entities have come to be regarded as being basically information-processing systems [19].

The density matrix constitutes one of the most important

*E-mail: angeloplastino@gmail.com (Corresponding author)
†E-mail: arplastino@ugr.es
‡E-mail: cz@up.ac.za

tools for the study of quantum mechanical aspects of the physics of information, being an essential ingredient both in the analysis of the conceptual foundations of quantum mechanics and in its practical applications. It is the basic tool for describing mixed quantum states. These, in turn, arise when one deals with situations in which one does not possess maximum knowledge (as in the case of pure states) concerning the system's state or when dealing with the state of a quantum system that is entangled with another quantum system. The former scenario corresponds, for instance, to the statistical ensemble of quantum statistical mechanics. The latter is essential in the study of quantum entanglement and quantum information theory.

The density matrix is an essentially quantum-mechanical concept. It is our purpose here to investigate the possibility of concocting a classical analogue of this fundamental concept. Such an inquiry is inscribed within the more general research line that explores classical analogues of diverse aspects of quantum mechanics (see [8] and references therein) in order to better elucidate the basic nature of the quantum state and, in particular, contribute to the underlying ontic *vs.* epistemic debate [20]. In addition to its relevance for the quantum mechanics' foundations, the study of classical analogues of aspects of quantum physics may also lead to new tools for the statistical treatment of classical systems [21].

2. Classical density matrix

Consider a normalized probability density $f(\mathbf{x})$, where $\mathbf{x} \in \mathcal{R}^N$ stands for the relevant N-dimensional phase-space, so that

$$\int f(\mathbf{x})\, d^N x = 1. \tag{1}$$

By analogy with quantum mechanics we now define a "density matrix" $\rho(\mathbf{x}, \mathbf{x}')$ with matrix elements

$$\rho(\mathbf{x}, \mathbf{x}') = \sqrt{[f(\mathbf{x})\, f(\mathbf{x}')]}, \tag{2}$$

where $\sqrt{f(\mathbf{x})}$ is the classical analogue of a probability amplitude in quantum mechanics. In equation (2) $\mathbf{x}$ and $\mathbf{x}'$ represent two arbitrary points in the relevant phase-space. The density matrix (2) clearly exhibits some important properties like normalization and positivity,

$$\rho(\mathbf{x}, \mathbf{x}') \geq 0,$$

$$\int d^N x\, \rho(\mathbf{x}, \mathbf{x}) = 1. \tag{3}$$

From Eq. (2) a basic relation follows, namely

$$P = \int d^N x\, d^N x' \rho^2(\mathbf{x}, \mathbf{x}') = 1, \tag{4}$$

a property that can be regarded as the classical counterpart of the well-known relation $Tr[\hat{\rho}^2] = 1$ characterizing the quantum statistical operator associated with pure quantum states. It is worth mentioning that non-local integrals of the type (4) arise in the analysis of radiative entropy production [22], and also of surface/interfacial tension systems (see, for instance, [23, 24])

The set of classical density matrices satisfying (3) is convex. Given two density matrices (from here on we omit the adjective "classical") ρ_1 and ρ_2 verifying (3), it is clear that any convex linear combination

$$\rho(\mathbf{x}, \mathbf{x}') = \lambda_1 \rho_1(\mathbf{x}, \mathbf{x}') + \lambda_2 \rho_2(\mathbf{x}, \mathbf{x}'), \tag{5}$$

with $\lambda_1 + \lambda_2 = 1$ and λ_1, λ_2 non-negative real numbers, also verifies (3). In contrast, property (4) is not preserved by convex linear combinations. In fact, as we shall see when considering composite systems, marginal classical density matrices describing subsystems may not comply with (4), having instead $0 < P < 1$. Consequently, it is convenient to regard as legitimate density matrices all those $\rho(\mathbf{x}, \mathbf{x}')$ belonging to the convex set defined by the conditions (3).

Assume now that the original probability density f is time-dependent and describes the evolution of a statistical ensemble of realizations of a classical dynamical system governed by the equations of motion

$$\dot{\mathbf{x}} = \mathbf{V}(\mathbf{x}), \qquad \mathbf{x}, \mathbf{V} \in \mathcal{R}^N. \tag{6}$$

Accordingly, the ensemble probability density $f(\mathbf{x}, t)$ evolves following the Liouville equation

$$\frac{\partial f}{\partial t} + \nabla_{\mathbf{x}} \cdot (f\, \mathbf{V}) = 0, \tag{7}$$

where

$$\nabla_{\mathbf{x}} = \left(\frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_N} \right) \tag{8}$$

is the N-dimensional nabla operator. The density matrix $\rho(\mathbf{x}, \mathbf{x}')$ satisfies then the (non-linear) evolution equation

$$2\rho \frac{\partial \rho}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho^2\, \mathbf{V}(\mathbf{x})) + \nabla_{\mathbf{x}'} \cdot (\rho^2\, \mathbf{V}(\mathbf{x}')) = 0. \tag{9}$$

We are specially interested in dynamical systems with divergenceless phase-space flows, which encompass Hamiltonian systems amongst their members and are characterized by the fact that their dynamics is information-conserving [25]. Indeed, divergenceless dynamical systems constitute the classical version of dynamical systems

where information is preserved during the time evolution of the system. This conservation of information is given by the conservation of appropriate entropic functionals evaluated upon time dependent probability densities that are solutions of the associated Liouville equation. This kind of dynamics constitutes (at the classical level) the most fundamental one. According to our present understanding of Nature, the basic laws of physics satisfy this information-preserving property [26, 27]. Indeed, the conservation of information has been hailed by some leading theoreticians as the most fundamental law of physics [28]. Dynamics where information is not preserved arise from the approximate treatment of open systems, or from reduced descriptions of the evolution of dynamical systems based on coarse-graining or on related approximation methods. Divergenceless dynamical systems abound both in physics and theoretical biology (among several other areas of knowledge). Besides the celebrated Hamiltonian systems, there are other important divergenceless systems that are not Hamiltonian, or do not admit their more natural representation in terms of canonical variables. Special mention can be made of the Lotka-Volterra predator-prey systems [29, 30] and those of Nambu [31]. Both receive considerable attention [29–37]. In the particular case of a Hamiltonian system with n degrees of freedom the phase space dimension is $N = 2n$, and the location $\mathbf{x}$ in phase space is given by the complete set of n generalized coordinates and the corresponding n conjugate momenta, $\mathbf{x} = (q_1, \ldots, q_n, p_1, \ldots, p_n)$. The flow $\mathbf{v}$ in phase space is determined by the Hamiltonian function H and, expressing $\mathbf{v}$ explicitly in terms of its components, one has, $\mathbf{v} = (\partial H/\partial p_1, \ldots, \partial H/\partial p_n, -\partial H/\partial q_1, \ldots, -\partial H/\partial q_n)$. In the case of a divergenceless dynamical system one has

$$\nabla_{\mathbf{x}} \cdot \mathbf{V}(\mathbf{x}) = 0, \tag{10}$$

and the density matrix obeys the linear, Liouville-like equation

$$\frac{\partial \rho}{\partial t} + (\nabla_{\mathbf{x}}\rho) \cdot \mathbf{V}(\mathbf{x}) + (\nabla_{\mathbf{x}'}\rho) \cdot \mathbf{V}(\mathbf{x}') = 0. \tag{11}$$

It can be verified after some algebra that the conditions (3) characterizing a classical density matrix are preserved under the Liouville-like dynamics given by (11). Another important property of the evolution equation (11) is that the quantity P given by (4) is conserved,

$$\frac{dP}{dt} = 0. \tag{12}$$

The time independence of P also holds in the case of non-divergenceless dynamical systems, whose classical density matrix obeys the non-linear evolution equation (9). Consider now a bipartite system with a phase-space of $N = N_1 + N_2$ dimensions. A point in this phase-space can be represented as $(\mathbf{x}, \mathbf{y})$ with $\mathbf{x} \in \mathcal{R}^{N_1}$ (subsystem A) and $\mathbf{y} \in \mathcal{R}^{N_2}$ (subsystem B). If the composite system is described by a normalized joint probability density $f(\mathbf{x}, \mathbf{y})$, we have a joint density matrix

$$\rho(\mathbf{x}, \mathbf{y}; \mathbf{x}', \mathbf{y}') = \sqrt{[f(\mathbf{x}, \mathbf{y})\ f(\mathbf{x}', \mathbf{y}')]}. \tag{13}$$

A crucial stage is that of introducing a *reduced* density matrix $\rho(\mathbf{x}, \mathbf{x}')$ associated with subsystem A, obtained by recourse to a partial trace-like operation,

$$\rho_A(\mathbf{x}, \mathbf{x}') = \int d^{N_2}y\, \rho(\mathbf{x}, \mathbf{y}; \mathbf{x}', \mathbf{y}). \tag{14}$$

It is clear that $\rho_A(\mathbf{x}, \mathbf{x}')$ verifies the requisites of positivity and normalization (3). However, ρ_A will not comply, in general, with condition (4). In fact,

$$P_A = \int d^{N_1}x d^{N_1}x'\, \rho_A^2(\mathbf{x}, \mathbf{x}') = \int d^{N_1}x d^{N_1}x' d^{N_2}y d^{N_2}y' \, [f(\mathbf{x}, \mathbf{y}) f(\mathbf{x}, \mathbf{y}') f(\mathbf{x}', \mathbf{y}) f(\mathbf{x}', \mathbf{y}')]^{1/2} \leq 1. \tag{15}$$

If subsystems A and B are statistically independent in the sense that

$$f(\mathbf{x}, \mathbf{y}) = f_A(\mathbf{x}) f_B(\mathbf{y}), \tag{16}$$

where $f_A(\mathbf{x}) = \int d^{N_2}y f(\mathbf{x}, \mathbf{y})$ and $f_B(\mathbf{y}) = \int d^{N_1}x f(\mathbf{x}, \mathbf{y})$ are the marginal probability densities respectively associated with the subsystems A and B, we find

$$P_A = \int d^{N_1}x d^{N_1}x'\, \rho_A^2(\mathbf{x}, \mathbf{x}') = 1. \tag{17}$$

On the other hand, assuming that $P_A = 1$, leads to the factorizability of $f(\mathbf{x}, \mathbf{y})$. Indeed, appealing to the Schwartz inequality we have

$$\rho_A^2(\mathbf{x}, \mathbf{x}') = \left[\int d^{N_2}y \sqrt{f(\mathbf{x}, \mathbf{y}) f(\mathbf{x}', \mathbf{y})}\right]^2 \leq \left[\int d^{N_2}y\, f(\mathbf{x}, \mathbf{y})\right]\left[\int d^{N_2}y\, f(\mathbf{x}', \mathbf{y})\right] = f_A(\mathbf{x})\, f_A(\mathbf{x}'). \tag{18}$$

Consequently,

$$P_A = \int \rho_A^2(\mathbf{x},\mathbf{x}')\, d^{N_1}x d^{N_1}x' \leq \left[\int d^{N_1}x\, f_A(\mathbf{x})\right]\left[\int d^{N_1}x'\, f_A(\mathbf{x}')\right] = 1. \tag{19}$$

The equality in (18) is verified iff $f(\mathbf{x},\mathbf{y})$ and $f(\mathbf{x}',\mathbf{y})$ are proportional to each other. In other words, iff for each pair $\mathbf{x}$, $\mathbf{x}'$ there exists a number $\delta(\mathbf{x},\mathbf{x}')$ such that

$$f(\mathbf{x},\mathbf{y}) = \delta(\mathbf{x},\mathbf{x}')\, f(\mathbf{x}',\mathbf{y}) \tag{20}$$

holds for all $\mathbf{y}$. Now, (20) clearly implies that $f(\mathbf{x},\mathbf{y})$ is factorizable. Indeed, defining

$$f_B(\mathbf{y}) = \left[\int d^{N_1}x'\, f(\mathbf{x}',\mathbf{y})\right]^{-1} f(\mathbf{x}',\mathbf{y})$$

and

$$f_A(\mathbf{x}) = \left[\int d^{N_2}y\, f(\mathbf{x}',\mathbf{y})\right]^{-1} \delta(\mathbf{x},\mathbf{x}'),$$

we have $f(\mathbf{x},\mathbf{y}) = f_A(\mathbf{x})f_B(\mathbf{y})$. Note that in the above equations we consider a given, fixed $\mathbf{x}'$-value and focus on the dependence of the involved quantities upon $\mathbf{x}$ and $\mathbf{y}$. In other words, $\mathbf{x}'$ is just an auxiliary quantity used to construct the densities $f_A(\mathbf{x})$, $f_B(\mathbf{y})$, which in turn constitute the "final" result of the preceding argument and do not depend on $\mathbf{x}'$. They are in fact marginal probability densities

$$f_A(\mathbf{x}) = \int d^{N_2}y\, f(\mathbf{x},\mathbf{y})$$

$$f_B(\mathbf{y}) = \int d^{N_1}x\, f(\mathbf{x},\mathbf{y}). \tag{21}$$

Summing up, the condition $P_A = 1$ is both necessary and sufficient for the statistical independence of A and B. This fact makes the difference

$$D_A = 1 - P_A, \tag{22}$$

a *measure of the correlations between A and B*. The form of the functional $D_A[\rho_A]$ resembles that of the linear entropy of quantum mechanical density matrices. Notice that P_A is expressed only in terms of A-quantities, but nevertheless contains some B-information. Usually, statistical correlations are measured by recourse to quantities that explicitly refer to both subsystems A and B. For instance, we have the mutual information I_{AB}, given by

$$I_{AB} = S_A + S_B - S_{AB}, \tag{23}$$

where $S[f] = -\int f \ln f\, d^N x$ is the Shannon entropy of the probability density f.

As a simple illustration of the above ideas let us consider a correlated Gaussian probability density,

$$f(x,y) = \frac{\sqrt{4\sigma_1\sigma_2 - \sigma_{12}^2}}{2\pi}\, \exp\left[-(\sigma_1 x^2 + \sigma_2 y^2 + \sigma_{12} xy)\right], \tag{24}$$

describing a composite system consisting of two one-dimensional subsystems with coordinates x and y, respectively. In this case the quantity D_A is equal to

$$D_A = 1 - \sqrt{1 - \frac{\sigma_{12}^2}{4\sigma_1\sigma_2}}, \tag{25}$$

while the mutual information is

$$I_{AB} = -\frac{1}{2}\ln\left(1 - \frac{\sigma_{12}^2}{4\sigma_1\sigma_2}\right). \tag{26}$$

Therefore, we have

$$D_A = 1 - e^{-I_{AB}}, \tag{27}$$

which illustrates the fact that D_A constitutes a measure of statistical correlations between subsystems A and B. Indeed, one can see in this example that D_A is a monotonically increasing function of the mutual information I_{AB} (see Figure 1).

It is important to mention that the classical partial trace-like operation does not commute with the operation of constructing the density matrix ρ from a probability density f. That is, if one starts from the joint probability density $f(\mathbf{x},\mathbf{y})$, computes the marginal probability density for subsystem A, $f_A(\mathbf{x}) = \int d^{N_2}y f(\mathbf{x},\mathbf{y})$, and then constructs its associated density matrix $\tilde{\rho}_A^2(\mathbf{x},\mathbf{x}') = f_A(\mathbf{x})f_A(\mathbf{x}')$, this $\tilde{\rho}_A$ is not, in general, going to coincide with the marginal density matrix ρ_A given by (14). In fact, the marginal probability density $f_A(\mathbf{x})$ does not contain any information concerning the correlations between subsystems A and B, while the marginal density matrix ρ_A (obtained via a partial trace operation conducted upon the joint density matrix ρ) does. In other words, the operation of partial trace performed at the level of probability densities "removes" information concerning correlations, while partial-tracing over density

Figure 1. Measured D_A against mutual information I_{AB} for the correlated Gaussian density (24). All depicted quantities are dimensionless.

matrices does not. Therefore, the appropriate strategy for applying the present density matrix formalism to composite classical systems is the following. Start with the probability density describing the full composite system under consideration and construct the associated classical density matrix. Then, in order to describe the subsystems, determine the concomitant marginal density matrices, obtained via the partial trace operation performed over the global density matrix.

Another conceptually interesting feature of D_A that we shall discuss now is that the marginal classical density matrix ρ_A evolves autonomously when the subsystems A and B are non-interacting. That is, its evolution is determined entirely by the structure of the dynamical system A. When the two subsystems A and B are dynamically independent (that is, they do not interact) the concomitant equations of motion are of the form,

$$\dot{\mathbf{x}} \;=\; \mathbf{V}(\mathbf{x}), \qquad \mathbf{x}, \mathbf{V} \in \mathcal{R}^{N_1}$$

$$\dot{\mathbf{y}} \;=\; \mathbf{W}(\mathbf{y}), \qquad \mathbf{y}, \mathbf{W} \in \mathcal{R}^{N_2}. \tag{28}$$

As done before, we shall assume a divergenceless phase-space flow,

$$\nabla_{\mathbf{x}} \cdot \mathbf{V} = \nabla_{\mathbf{y}} \cdot \mathbf{W} = 0. \tag{29}$$

The joint density matrix ρ then evolves according to,

$$\begin{aligned} \frac{\partial \rho}{\partial t} \;&+\; (\nabla_{\mathbf{x}}\rho)\cdot\mathbf{V}(\mathbf{x}) + (\nabla_{\mathbf{y}}\rho)\cdot\mathbf{W}(\mathbf{y}) \\ &+\; (\nabla_{\mathbf{x}'}\rho)\cdot\mathbf{V}(\mathbf{x}') + (\nabla_{\mathbf{y}'}\rho)\cdot\mathbf{W}(\mathbf{y}') \\ &=\; 0. \end{aligned} \tag{30}$$

Note that the subsystems A and B are assumed to be dynamically independent, but not necessarily statistically independent. That is, the joint density matrix ρ may arise from a non-factorizable joint probability density $f(\mathbf{x}, \mathbf{y})$. Setting now in the evolution equation (30) $\mathbf{y} = \mathbf{y}'$, and integrating over the N_2-dimensional phase-space of subsystem B, one obtains the equation of motion for the marginal density matrix ρ_A,

$$\frac{\partial \rho_A}{\partial t} \;+\; (\nabla_{\mathbf{x}}\rho_A)\cdot\mathbf{V}(\mathbf{x}) + (\nabla_{\mathbf{x}'}\rho_A)\cdot\mathbf{V}(\mathbf{x}') \;=\; 0. \tag{31}$$

This equation has the form (11), and describes an autonomous evolution of ρ_A completely determined by the phase-space flow $\mathbf{V}(\mathbf{x})$ characterizing the dynamics of subsystem A. To derive equation (31) one has to use the divergenceless condition (29) and also assume that $f \to 0$ fast enough as $|\mathbf{y}| \to \infty$, so that the surface terms arising after integration by parts vanish. These assumptions imply, for instance, that

$$\int d^{N_2}y (\nabla_{\mathbf{y}}\rho(\mathbf{x},\mathbf{y};\mathbf{x}',\mathbf{y}))\cdot\mathbf{W}(\mathbf{y}) = -\int d^{N_2}y \rho(\mathbf{x},\mathbf{y};\mathbf{x}',\mathbf{y})(\nabla_{\mathbf{y}}\cdot\mathbf{W}(\mathbf{y})) = 0. \tag{32}$$

A consequence of the evolution equation (31) is that P_A is constant in time,

$$\frac{dP_A}{dt} \;=\; 0. \tag{33}$$

This corresponds to the fact that the amount of statistical correlation between the subsystem A and the rest of the system does not change in time if subsystem A is not interacting with the other subsystems.

It is important to emphasize that the linear, Liouville-like evolution equation for the global classical density matrix, and its locally autonomous version corresponding to the marginal density matrices describing independent subsystems, only hold for dynamical systems exhibiting a divergenceless phase-space flow. These facts highlight the fun-

damental nature of these information-preserving systems.

3. Conclusions

We have introduced the concept of a classical density matrix as a classical counterpart of the statistical operator in quantum mechanics. We explored the main properties of this classical density matrix, paying special attention to the case of composite systems. When dealing with these systems, a partial trace-like operation conducted on the global classical density matrix describing the multipartite system yields a marginal density matrix for a subsystem. When the subsystems are dynamically independent (that is, they do not interact) marginal density matrices evolve locally, their behavior being governed solely by the local phase-space flows of the concomitant subsystems. Remarkably enough, and contrary to what happens with standard marginal probability densities, the marginal classical density matrices incorporate information concerning the statistical correlations between the different subsystem constituting the composite system under consideration. When discussing the time-depending aspects of the classical density matrix we have focused upon divergenceless dynamical systems, which constitute the most fundamental ones. However, the case of systems characterized by phase-space flows with finite divergence is also relevant, both from the conceptual and the practical points of view. We plan to address these systems in a forthcoming contribution.

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