

Article

Separable States on Density Matrices and Emergent Systems

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Abstract: In this paper, we propose a quantitative definition of emergence from the density matrix framework as a state of knowledge of the system and its generalized probability formulation, in order to detect emergent properties. We propose the use of a descriptor based on the difference of von Neumann entropy, to calculate if subsystems of systems have inner correlations by defining emergent systems in terms of emergent information.

Keywords: emergence; quantum theory; density matrix; subadditivity

1. Introduction

From quantum mechanics it is well known that any separable state belongs to a composite space which can be factored into individual states from separate subspaces. One state is said to be correlated if it is not separable. As a matter of fact to determine if a state is separable or not is not trivial and the problem is classed as *NP-hard* from the theory of complex systems [1].

A density operator, in quantum mechanics, is used to describe the statistical state of a quantum system. The usual meaning of it is that the eigenvalues are the probabilities to find a system in one state corresponding to the eigenvectors. In a physical sense we can see its elements as relative frequencies corresponding to an appropriate ensemble of N identical copies of the system which are in several possible states, under a certain setup or preparation protocol. Thus we have a superposition of quantum states $|v_i\rangle$ with probabilities p_i (real numbers) satisfying $\sum p_i = 1$ as it was mentioned before. However, it can be shown that the density operator formalism can be recovered in a Bayesian formalism for noncommutative expectations, wherein the system depends on the order of the measurements, this is not restricted just to a quantum mechanical system it can be understood under the framework of what we have called *fragile system* [2]. This operator provides a convenient mean for describing quantum systems whose state is not completely known, being mathematically equivalent to a state vector approach [3] [4].

By applying the entropy to the density matrix we can obtain the degree of desinformation of the state of the system. The systems can be composed of subsystems and by the subadditivity property [5] it is possible to quantify if the entropy of the whole is less than that of its parts. Holzer and De Meer [6], make a comparison between the information at the system level with the information of a lower level. As they state, “this measure gives a high value of emergence for systems with many dependencies (interdependent components) and a low value of emergence for systems with few dependencies (independent components)”, therefore the information of the whole is more than the information of the parts, in that sense the entropy can be a good parameter to measure a type of emergence in systems.

This paper is organized as follows. In Section 2 we talk about emergent systems and its current definitions. In Section 3 we introduce the density matrix formalism. In Section

4 we depict a mathematical formulation of emergent systems within the density matrix formalism. In Section 5 we show a concrete example of a subadditive system. Finally we provide some concluding remarks in Section 6.

2. Emergent Systems

Several definitions of emergence exist, taking into account different aspects of their origin or behavior. For instance, Peter Checkland [7] defines emergence as “the principle that entities exhibit properties which are meaningful only when attributed to the whole, not to its parts.” Emergent systems are structured in such a way that their components interact allowing the structure of global patterns, depicted as a consequence of interrelations/correlations between subsystem elements, being the result of complex and self-organizing processes. This process may be triggered by an external stimulus.

Emergence is, as well, a remarkable representation of life phenomenon and the key aspect of how patterns can emerge from randomness.

There are, basically, three types of emergence: simple, weak and strong ones, described as follows:

Simple emergence is composed by the combination of certain properties and relationships between elements in a non linear behavior. For instance, in order to achieve the flight of an airplane we cannot consider separately the motors, the propulsion system, neither their wings, all these properties must be considered together because they are interconnected and they have interrelations by which flight emerges. This type of emergence can be predicted from the functioning of its parts and it is referred as the concept of synergy, which means interacting or working together [8].

Weak emergence describes the emergence of properties of systems which may be predictable (not completely) and also reducible. It can be reduced to basic rules at an initial time, after a while the behavior can be unpredictable, nevertheless it is possible to make computational simulations about such systems because of the knowledge of the basic rules. Weak emergence is the product of complex system dynamics (i.e. non linear behavior, spontaneous order and adaptation), examples of the latter are cellular automaton known as Conway’s Game of Life [9–11].

Strong emergence: it is a case of non expected emergence, as well as weak emergence, the difference lies in its non-reducible behavior which appears just when the system is running. As being systematically determined by low-level attributes it is not possible to deduce it from the components at lower levels. Consciousness phenomenon is one example of this type of emergence which appears as a construction process. There is likely no algorithm from bottom up because it is a dynamical process evolving along time at the highest-level with non-linear relations at the lower ones.

Another way of conceptualizing emergence is the separation of levels of complexity of the system at different spatial or temporal scales [12].

Some main characteristics of strong emergence to consider are the following:

Non reducible phenomenon the global state of the emergent system cannot be explainable neither reducible to its sub-system components.

Downward causation emergent high-level properties appear from a non-obvious consequences of low level properties, but at the same time all processes at the lower level of hierarchy are constrained by and act in coherence to the laws of the higher level [13].

Wholeness is a phenomenon wherein complex, interesting high-level function appears as a result of combining low-level mechanisms in straightforward ways.

Radical novelty emergence is a phenomenon wherein a system is designed according to certain principles. Interesting unexpected properties arise from the behavior of sub-system elements [14].

In general, emergent systems are common in nature and technology, one example of the latter is the speed of a vehicle affected by the center of gravity, the driver skills, weather,

friction, among other attributes (in this case we can predict the emergent property of the speed from the relation between components, being the case of weak emergence). It is possible to find strong emergent properties in the consciousness phenomenon [15], human body and social phenomena, among others. One important example is the “self-awareness” which is a result of the interconnection of neurons in the brain [16].

In the case of biological systems (as well as in the case of social phenomena) emergent models are appropriate to describe those cases. We can observe the characteristic mentioned about strong emergence: non-reducibility, radical novelty, wholeness and downward causation.

The main aspect of biological emergent systems is that they must be observed from inside them by the system [17], This is in concordance with the autopoiesis theory proposed by the Chilean biologists H. Maturana and F. Varela [18] to define the self-maintaining chemistry of any living cell, this is under the perspective of Chemical Organization Theory used to formalize autopoietic structures, “providing a basis to operationalize goals as an emergent process” [19].

3. The density operator

In this section, we are going to formulate the density matrix operator, as a previous concept in order to define emergent systems using the calculation of entropies.

The density operator is a positive semi-definite, Hermitian operator of trace one. If \mathbb{A} is the matrix representation of an arbitrary observable \hat{A} , we can write

$$\mathbb{A} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix} (\bar{a}_1 \bar{a}_2 \cdots \bar{a}_N). \quad (1)$$

Hence, we have

$$\mathbb{A} = \begin{pmatrix} a_1 \bar{a}_1 & \cdots & a_1 \bar{a}_N \\ a_2 \bar{a}_1 & \cdots & a_2 \bar{a}_N \\ \vdots & \ddots & \vdots \\ a_N \bar{a}_1 & \cdots & a_N \bar{a}_N \end{pmatrix}$$

where \bar{a}_i is the conjugate of the element a_i , in the case of real numbers: the same element. We can take the average of different measurements represented by different matrices \mathbb{A} of the same observable, then normalize and diagonalize, finally we obtain the density matrix of a mixture as below,

$$\hat{\rho} = \sum_i^N p_i |v\rangle \langle v| \quad (2)$$

where $p_i = P(\lambda_i|I)$ and λ_i is obtained from the eigen-value problem $\lambda_i |v_i\rangle = \lambda_i \hat{A} |v_i\rangle$ [20].

We can formulate the density matrix operator by the use of a complex Hilbert space just as in Von Neumann’s formulation of quantum theory [21]. For this we consider an arbitrary orthonormal basis set $|n\rangle$ ($n=1, \dots, N$) with $\langle i|j\rangle = \delta(i, j)$ and define the density operator [22] $\hat{\rho}$ as

$$\hat{\rho} := \sum_{i=1}^N \sum_{j=1}^N \rho_{ij} |i\rangle \langle j|, \quad (3)$$

with ρ_{ij} complex numbers. Imposing that $\hat{\rho}$ is Hermitian, we see that the diagonal elements ρ_{ii} must be real and $\rho_{ij} = \bar{\rho}_{ji}$. It is always possible to make a choice of such complex matrix elements ρ_{ij} so that they are proportional to the elements p_{ij} , these are given by

$$\rho_{ij} = \langle \epsilon_i | \hat{\rho} | \epsilon_j \rangle = \frac{1}{2\eta} \left([p_{ij} + p_{ji}] + i[p_{ij} - p_{ji}] \right), \quad (4)$$

where $\eta = \sum_i p_{ii}$ is a normalization factor that imposes $\text{Tr}(\hat{\rho}) = 1$. 110

3.1. Pure and mixed states 111

Consider an ensemble of measurements $\{|v_i\rangle\}_{i=1}^N$. If all the vectors are in the same state (meaning that the same probability distribution is assigned) the ensemble represents a pure state. Assuming that the system is in the state $|v\rangle$, we can expand it with respect to the eigenvector of an Hermitian operator \hat{A} , as follows: 112
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$$|v\rangle = \sum_n \lambda_n |v_n\rangle, \quad (5)$$

$$\hat{A}|v\rangle = \lambda_n |v\rangle. \quad (6)$$

Finally, we can define a pure state by the following term:

$$\hat{\rho} = |v\rangle\langle v|. \quad (7)$$

Because $\hat{\rho}^2 = (|v\rangle\langle v|)(|v\rangle\langle v|) = |v\rangle(\langle v|v\rangle)\langle v| = \hat{\rho}$, we can distinguish a density operator of a pure state by tracing, we have then

$$\text{Tr}(\hat{\rho}) = \text{Tr}(\hat{\rho}^2) = 1. \quad (8)$$

When we cannot repeat exactly the same initial condition, because of the noise of the system, we represent this situation in a mathematical formulation in terms of an operator called density matrix for mixed states. This is a superposition of pure states

$$\hat{\rho} = \sum_i p_i |v\rangle\langle v|, \quad (9)$$

where the weights of each measurement satisfy the normalization condition $\sum_i p_i = 1$. Each p_i is the probability to find a system in a given pure state. 116
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In contrast to a pure state, when we have a mixed density matrix the trace of the square density matrix is given by the inequality 118
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$$\text{Tr}(\hat{\rho}^2) < 1, \quad (10)$$

hence $\text{Tr}(\hat{\rho}^2)$, known as the *degree of purity* [23], can be used to distinguish between pure and mixed states in a basis-independent manner. 120
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4. Density operator formalism and emergent systems 122

Earlier work by Prokopenko *et al* [12] has set the basis for a discussion of complexity, self-organization and emergence of classical systems in information-theoretical terms, particularly in terms of Shannon entropy and mutual information. 123
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Taking all of this into account, we will rephrase the earlier arguments in terms of the (von Neumann) entropy of density matrices. But first let us review the behavior of the entropy for classical, correlated systems. 126
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Information entropy (or Shannon entropy) is a measure of missing information in a probabilistic model about some aspect of reality. For a state of knowledge I where we ask an arbitrary question with N possible answers, denoted by the proposition A_1, A_2, \dots, A_N , the information entropy is defined as

$$S(I) := - \sum_{i=1}^N p_i \ln p_i \quad (11)$$

where p_i is the probability $P(A_i|I)$ of the answer A_i being true under I . In the case where the question involves the unknown value of one or more variables, the information entropy directly translates in terms of the probability distribution. For instance, for the joint

probability distribution $P(X, Y|I)$ of the variables X and Y under the state of knowledge I we have

$$S_{XY}(I) := - \sum_x \sum_y P(x, y|I) \ln P(x, y|I). \quad (12)$$

Using the product rule of probability,

$$P(x, y|I) = P(y|x, I)P(x|I), \quad (13)$$

this entropy can always be separated into two terms [24],

$$S_{XY}(I) = S_X(I) + \left\langle S_{Y|X} \right\rangle_I, \quad (14)$$

where the first term is the entropy of the variable X , and the second term,

$$\left\langle S_{Y|X} \right\rangle_I := - \sum_x P(x|I) \sum_y P(y|x, I) \ln P(y|x, I) \quad (15)$$

is the expected value of the conditional entropy of Y given X . This conditional entropy cannot be negative, being the expected value of a non-negative quantity. 129
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It is possible to extend the Bayesian idea of probabilities as degrees of belief constrained on the available information to quantum systems [25,26]. Let be $\rho_{12} = \rho_1 \times \rho_2$. We can obtain the eigenvalues of ρ_1 $a_i = \{\rho_1\}_{ii}$ and ρ_2 $b_j = \{\rho_2\}_{jj}$. Hence the diagonal elements of ρ_{12} are given by all products of the form $a_i b_j$, where $i = 1, \dots, n_1$ and $j = 1, \dots, n_2$. Here n_1 and n_2 are the dimensions of ρ_1 and ρ_2 , respectively, then: 131
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$$\begin{aligned} S(\rho_{12}) &= - \text{Tr}(\rho_{12} \ln \rho_{12}) \\ &= - \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} (a_i b_j) \ln(a_i b_j). \end{aligned} \quad (16)$$

On the other hand, the sum of the entropy of each system is given by

$$S(\rho_1) + S(\rho_2) = - \sum_{i=1}^{n_1} a_i \ln(a_i) - \sum_{j=1}^{n_2} b_j \ln(b_j). \quad (17)$$

Thus, the entropy for an ensemble (ρ_{12}) for which the subsystems are uncorrelated is just equal to the sum of the entropies of the reduced ensembles for the subsystems. When there are correlations, we should expect an inequality instead (called subadditivity property of entropy [5,27,28]), since in this case ρ_{12} contains additional information concerning the correlations, which is not present in ρ_1 neither in ρ_2 (those are the partial traces of ρ_{12} , respectively), as in

$$S(\rho_{12}) \leq S(\rho_1) + S(\rho_2). \quad (18)$$

Given this inequality, we can use a dimensionless and normalized measure of the deviation from additivity, namely

$$\mathcal{E} := \frac{S(\rho_1) + S(\rho_2) - S(\rho_{12})}{S(\rho_{12})}, \quad (19)$$

such that $\mathcal{E} > 0$ whenever there is subadditive behavior and $\mathcal{E} = 0$ for additivity. 136

From equation (19) we obtain a descriptor of weak emergency in systems which are correlated. In this type of systems new information emerges from the relation of its parts in terms of correlations. 137
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5. An example of a subadditive system

As it is depicted in equation (4) we can write the density matrix as follows,

$$\rho_{ij} = \langle \epsilon_i | \hat{\rho} | \epsilon_j \rangle = \frac{1}{2\eta} \left([p_{ij} + p_{ji}] + i[p_{ij} - p_{ji}] \right). \quad (20)$$

but where we now interpret p_{ij} as

$$p_{ij} = P(\epsilon_i, \epsilon'_j | I), \quad (21)$$

$$\eta = \sum_i p_{ii} \quad (22)$$

where primed states are states after a measurement, and where

$$E(s) \in \{\epsilon_1, \dots, \epsilon_N\}.$$

Because of the marginalization rule, it must hold that

$$\sum_i p_{ij} = P(\epsilon'_j | I) \quad \text{for all } j = 1, \dots, N, \quad (23)$$

while simultaneously,

$$\sum_j p_{ij} = P(\epsilon_i | I) \quad \text{for all } i = 1, \dots, N \quad (24)$$

must be true. As an example, consider a system with only four possible states, namely

$$s_1 = (0, 0), \quad (25)$$

$$s_2 = (0, 1), \quad (26)$$

$$s_3 = (1, 0), \quad (27)$$

$$s_4 = (1, 1), \quad (28)$$

such that $E(s_i) = i$ for $i=1,2,3,4$. Tables 1 and 2 show a particular set of values for the marginal and joint probabilities, respectively, of these states. Notice that the system is fragile, because $P(\epsilon_i, \epsilon'_j | I)$ is not diagonal. The reduced density matrices are

$$\rho_A = \begin{pmatrix} 0.66845 & 0.20701 + 0.0069579i \\ 0.20701 - 0.0069579i & 0.33155 \end{pmatrix},$$

$$\rho_B = \begin{pmatrix} 0.61953 & 0.15116 + 0.0073659i \\ 0.15116 - 0.0073659i & 0.38047 \end{pmatrix},$$

hence the matrix ρ_{AB} is not separable. The values of the von Neumann entropy are $S_A=0.54291$, $S_B=0.61680$ and $S_{AB} = 0.93465$, therefore our emergence index is $\mathcal{E}=0.24081$, and the system is subadditive. With this example we have found a density operator that is not only correlated but could describe an emergent system, since $\mathcal{E} > 0$, i.e., the entropy of the whole is less than that of its parts.

6. Concluding remarks

In this work we review the idea of emergence in the context of quantum mechanics, in order to test weak emergence in systems under the framework of the density matrix theory. We propose a descriptor in terms of the difference of the entropy between the systems and subsystems to contrast the amount of information present in the whole regarding to its parts. When the parameter $\mathcal{E} > 0$ there is more information in the whole than its parts, therefore new information emerges as a result of the interaction of the subsystems as

i	$P(\epsilon_i I)$	$P(\epsilon'_i I)$
1	0.25	0.3
2	0.32	0.25
3	0.28	0.25
4	0.15	0.20

Table 1. An example set of probabilities for a system having 4 distinct microstates, before (second column) and after (third column) an observation.

i	j	$P(\epsilon_i, \epsilon'_j I)$	ρ_{ij}
1	1	0.18	0.39
1	2	0.00	$0.06-0.05i$
1	3	0.04	0.09
1	4	0.03	0.07
2	1	0.05	$0.06+0.05i$
2	2	0.12	0.28
2	3	0.09	$0.18+0.02i$
2	4	0.06	0.12
3	1	0.38	0.09
3	2	0.07	$0.18-0.02i$
3	3	0.10	0.23
3	4	0.07	$0.09+0.06i$
4	1	0.03	0.07
4	2	0.05	0.12
4	3	0.02	$0.09-0.06i$
4	4	0.05	0.10

Table 2. An example set of joint probabilities $P(\epsilon_i, \epsilon'_j|I)$ for a fragile system (third column), consistent with the values of Table 1. The fourth column shows the values of the elements of the corresponding density matrix.

correlations. We have presented a concrete example of an operator that could describe a subadditive system. 153

Under the knowledge of this framework we can consider for a future work an adaptive, self-sustainable and interconnected model to describe how the observer participates in the proposition, being part of the system as the side effect which produces the act of measurement. 154
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Author Contributions: Conceptualization, Y.N.; methodology, Y.N. and S.D.; software, S.D.; validation, Y.N. and S.D.; formal analysis, Y.N. and S.D.; writing—original draft preparation, Y.N. and S.D.; writing—review and editing, Y.N. and S.D. All authors have read and agreed to the published version of the manuscript. 159
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Funding: This research was funded by ANID FONDECYT 1220651 grant. 163

Data Availability Statement: Not applicable. 164

Conflicts of Interest: The authors declare no conflict of interest. 165

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