Understanding decoherence as an irreversible process

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Abstract: If decoherence is an irreversible process, its physical meaning might be clarified by comparing quantum and classical irreversibility. In this work we carry out this comparison, from which a unified view of the emergence of irreversibility arises, applicable both to the classical and to the quantum case. According to this unified view, in the two cases the irreversible macro-level arises from the reversible micro-level as a coarse description that can be understood in terms of the concept of projection. This position supplies an understanding of the phenomenon of decoherence different from that implicit in most presentations: the reduced state is not the quantum state of the open system, but a coarse state of the closed composite system; as a consequence, decoherence should be understood not as a phenomenon resulting from the interaction between an open system and its environment, but rather as a coarse evolution that emerges from disregarding certain degrees of freedom of the whole closed system.

Keywords: Decoherence, irreversibility, coarse-graining, partial trace

1. Introduction

The phenomenon of decoherence is usually conceived as the result of the interaction between an open quantum system and its environment. In order to describe it, the open system is endowed with a reduced state, which is obtained from the quantum state of the whole composite system by tracing off the degrees of freedom of the environment. The time-behavior of this reduced state is not confined to unitarity; therefore, the open system may follow an irreversible evolution as that required by decoherence. In fact, as Roland Omnès (2001, 2002) stresses, decoherence is an irreversible process, through which the states of the environment tend to orthogonality and the reduced state of the open system tends to diagonalization in a “preferred basis” of states. If this is the case, the physical meaning of decoherence might be clarified by comparing quantum and classical irreversibility; this is the general framework of the present work.
For this purpose, the present article is organized as follows. After introducing the problem resulting from the orthodox interpretation of decoherence in Section 2, the argument is developed in four stages. In Section 3 and Section 4, the role played by coarse graining to explain irreversibility in classical statistical mechanics and the role played by partial trace in quantum mechanics to explain decoherence are recalled, respectively. Section 5 is devoted to show that both coarse graining and partial trace can be understood from a unified perspective in terms of the concept of projection. On this basis, in Section 6 the parallel between the two cases is completed by considering coarse graining in quantum mechanics and partial trace in classical statistical mechanics. Finally, in Section 7, the consequences of the argumentation for the interpretation of decoherence are presented: the reduced state of the open system is not its quantum state but a coarse description of the closed system; therefore, decoherence should be understood not as a phenomenon resulting from the interaction between an open system and its environment, but rather as a coarse evolution that emerges from disregarding certain degrees of freedom of the whole closed system.

2. Stating the problem

One of the hottest conceptual discussions about quantum mechanics is that referred to the interpretation of the quantum state. Does it represent our knowledge or embody objective propensities? Does it describe a physical field on physical but empirically inaccessible degrees of freedom? This kind of questions has led to a wide spectrum of interpretations about the meaning of the quantum state, which constitute a topic that attracts the interest of researchers up to the present (see, e.g., Ney and Albert 2013). However, despite the seriousness of the interpretive problem, the distinction among the different kinds of states appearing in the quantum discourse is usually not sufficiently emphasized.

On the one hand, the quantum state is represented by an operator \( \hat{\rho} \in \mathcal{H} \otimes \mathcal{H} \), where \( \mathcal{H} \) is a Hilbert space (pure states, represented by vectors \( |\psi\rangle \in \mathcal{H} \), correspond to the particular case \( \hat{\rho} = |\psi\rangle \langle \psi| \)), and its unitary time-evolution is ruled by the von Neumann equation (or, in the particular case of pure states, by the Schrödinger equation).\(^1\) On the other hand, reduced states \( \hat{\rho}_r \) are conceived as quantum states of open systems, even if they do not evolve unitarily according to the dynamical postulate of the theory and they cancel quantum correlations. In spite of these substantial differences, the states of closed and open systems are treated on equal footing. The fact that reduced states do not evolve unitarily is justified by saying that the dynamical postulate of quantum mechanics only applies to closed systems. But this argument disregards that there is no dynamical law for reduced states: the evolution

\(^1\) Here we will not discuss the question of the supposed priority of pure states over mixed states: following certain presentations of the theory (e.g. Ballentine 1998), we will take the generic stance of considering state operators as representing quantum states, and pure states as a particular case.
of open systems always depends, in the final analysis, on the unitary evolution of the whole closed system of which the open system is a part. In turn, the fact that reduced states cancel quantum correlations is viewed as a consequence of the state of the composite system not being uniquely defined by the quantum states of its components. But this view implies that there are quantum states that cannot be used for computations in certain cases.

It might be supposed that assigning or not the name ‘quantum state’ to reduced states is something completely arbitrary. However, this is not the case, since how reduced states are conceptualized has relevant interpretive consequences (see discussion in Fortin and Lombardi 2014). In particular, the meaning of reduced states strongly influences the way in which the phenomenon of decoherence is understood.

The environment-induced decoherence program was born in the seventies, when the measurement problem began to be addressed from an open-system perspective: according to that view, macroscopic systems such as measurement devices are never closed, but interact significantly with their environments (see Zeh 1970, 1973). On the basis of those previous contributions, the theory of decoherence was systematized and developed by Wojciech Zurek and his collaborators in a great number of works. According to Zurek (1982, 1991, 1993, 1994), decoherence is a process resulting from the interaction between a quantum system and its environment. Therefore, the first step is to split the universe into the degrees of freedom which are of direct interest to the observer, “the system of interest”, and the remaining degrees of freedom usually referred to as “the environment”, which can be external, such as particles of air or photons scattered off the system, or internal, such as collections of phonons or other internal excitations.

In many models, in which the number of degrees of freedom of the environment is huge, it can be proved that, after an extremely short “decoherence time”, the reduced state of the open system becomes diagonal in a “pointer basis” representing the classically behaving observable. Zurek conceives this decoherence process as the dynamical description of the phenomenon of collapse (Zurek 1981) and, as a consequence, as the explanation of the emergence of classicality: “the environment distills the classical essence of a quantum system.” (Zurek 2003: 3). This explanation is based on conceiving the reduced state as the quantum state of the open system and supposing that such an open system becomes classical.

As some point out (Leggett 1987, Bub 1997), the theory of environment-induced decoherence became the “new orthodoxy” in the quantum physicists community: many authors considered that decoherence finally supplies the right answer to the measurement problem (see, e.g., Auletta 2000, Anderson 2001). However, in the philosophy of physics community, many voices were raised up against the account of measurement given by the decoherence approach (see, e.g., Healey 1995, Bacciagaluppi 2016). For instance, Stephen Adler (2003) explicitly stressed that the diagonalized reduced state does not allow us to say
that the open system is in one of the eigenstates of the “pointer” observable. Jeffrey Bub (1997), in turn, took a step further by claiming that, if the eigenstate-eigenvalue link is accepted, the problem is even worst: the reduced state is not only unable to explain the occurrence of only one of the eigenvalues of the pointer observable, but it is also inconsistent with that occurrence, since the state of the closed system to which the open system belongs is still in a superposition of the eigenstates of that observable. In spite of these severe criticisms, the idea that decoherence solves the quantum measurement problem is still in the air, not only in the physicists community, but also in some conceptual discussions. For instance, decoherence has been appealed to in the context of the many-worlds interpretation (see Wallace 2012), and with the purpose of solving the problem of optical isomerism (see Scerri 2011, 2013; for a criticism, see Fortin, Lombardi and Martínez González 2016).

The persistence of the “orthodox” interpretation of the phenomenon of decoherence justifies the need of insisting on the issue. Here we will show that decoherence can be better understood as an irreversible process, by analogy to classical irreversibility: this strategy will lead us to conclude that the reduced state of the decohering system $S$ must not be conceived as its quantum state.

3. Coarse graining in classical statistical mechanics

In Gibbsian statistical mechanics, the system under study is represented by an ensemble of abstract systems in different microstates, which are compatible with the macrostate of that system. The statistical state of the system under study is represented by a density function $\rho(r,t)$ –normalized to unity–, defined on a phase space $\Gamma$, where $r \in \Gamma$ represents a possible microstate (position and momentum) of the system. In turn, the physical magnitudes depending on the microstates $r$ are represented by observables $O(r)$, such that $O: \Gamma \rightarrow \mathbb{R}$. The density function $\rho(r,t)$ allows computing the phase average (average on all the members of the ensemble) of any observable $O(r)$ as

$$\langle O(r) \rangle_{\rho(r,t)} = \int_{\Gamma} \rho(r,t)O(r)\, dr.$$  \hspace{1cm} (1)

In this Gibbsian approach, statistical equilibrium is defined as the situation in which the phase averages are independent of time; this situation is represented by the microcanonical ensemble, whose density distribution is uniform over all the accessible region of the phase space. As a consequence, in statistical equilibrium the phase average of any observable is time independent.

During the last decades, many discussions focused on the use of ensembles in the definition of the density function, the connection of the density function with the different interpretations of probability, etc. (see, e.g., Frigg 2007, Uffink 2007). One of the central problems in this theoretical context is how to explain the approach to equilibrium by means
of the reversible time-evolution of the density function. In fact, the evolution of $\rho(r,t)$ is ruled by the Liouville equation and, as a consequence, has no limit for $t \to \infty$: the volume of the support of $\rho(r,t)$ in $\Gamma$ is time-invariant as a consequence of the Liouville theorem. Therefore, the problem of irreversibility in classical statistical mechanics turns out to be how to account for an irreversible approach to equilibrium in systems ruled by a time-invariant evolution law (see Lombardi 2003, Frigg 2007).

The standard answer in the context of the Gibbsian approach consists in relying on coarse graining: the phase space $\Gamma$ is partitioned into cells $C_i$ of the same volume $\mu(C_i)$ in $\Gamma$, and a coarse-grained distribution $\rho_{cg}(r)$ is defined such that

$$
\rho_{cg}(r) = \begin{cases} 
\frac{1}{\mu(C_1)} \int_{C_1} \rho(r) \, dr & \text{if } r \in C_1 \\
\frac{1}{\mu(C_2)} \int_{C_2} \rho(r) \, dr & \text{if } r \in C_2 . 
\end{cases}
$$

It is quite clear that, since the coarse-grained state $\rho_{cg}$ is not the original statistical state, it is not ruled by the dynamical law of classical statistical mechanics and, as a consequence, its evolution is not constrained by the Liouville theorem: $\rho_{cg}(r,t)$ may approach a definite limit for $t \to \infty$. This is what effectively happens when the system has a sufficiently high degree of instability: if the system is mixing, it can be proved that the coarse-grained state approaches a time-independent equilibrium state, $\rho_{cg}(r,t) \to \rho_{cg(eq)}(r)$ (see, e.g., Berkovitz, Frigg, and Kronz 2006).

The expectation values of the observables of the system can be computed in the coarse-grained state $\rho_{cg}(r)$ analogously to eq. (1):

$$
\langle O(r) \rangle_{\rho_{cg}(r)} = \int_{\Gamma} \rho_{cg}(r) O(r) \, dr .
$$

It is quite clear that the same result could be obtained if certain “gross observables” were defined as follows:

$$
O_{cg}(r) = \begin{cases} 
\frac{1}{\mu(C_1)} \int_{C_1} O(r) \, dr & \text{if } r \in C_1 \\
\frac{1}{\mu(C_2)} \int_{C_2} O(r) \, dr & \text{if } r \in C_2 . 
\end{cases}
$$

In fact,

$$
\langle O(r) \rangle_{\rho_{cg}(r)} = \langle O_{cg}(r) \rangle_{\rho(r)} = \langle O_{cg}(r) \rangle_{\rho_{cg}(r)} .
$$

In spite of the precise formalism, conceptual discussions also focus on the meaning of the coarse-grained state: Does it supply the objective description of an emergent process? Or
does it only describe our ignorance about the real underlying evolution? These questions express the different interpretations of irreversibility, in the context of a debate that is still as alive as in the birth of statistical mechanics (see, e.g., Nicolis and Prigogine 1989, Lebowitz 1993, 1994a, 1994b, Driebe 1994, Bricmont 1995, Earman and Rédei 1996, Callender 1999, Frigg 2007). Nevertheless, despite the heated discussions and the deep disagreements about interpretation, nobody ignores the difference between the statistical state, which evolves unitarily according to the dynamical postulate of the theory, and the coarse-grained state, which may tend to a final stable state. Even those authors who take a heterodox position by claiming the priority of the coarse-grained state regarding objectivity, are clear that such a move requires a reformulation of the dynamical law of the theory (see, e.g., Misra, Prigogine, and Courbage 1979, Nicolis and Prigogine 1989). In other words, independently of the particular disagreements, nobody attempts to endow the statistical state and the coarse-grained state with the same interpretation.

4. Partial trace in quantum mechanics

The key idea of the decoherence program is that macroscopic systems are never isolated, but always interact with their environments. Let us consider a quantum system $S$ in the state $\sum_i c_i |\phi_i\rangle$. When the environment $E$ is taken into account, the initial state of the whole system $SE$ becomes

$$|\psi(0)\rangle = \sum_i c_i |\phi_i\rangle \otimes |\epsilon_0\rangle.$$  

(6)

where $|\epsilon_0\rangle$ is the state of the environment before its interaction with the open system $S$. It can be proved that, when the interaction Hamiltonian satisfies certain conditions, $|\psi(0)\rangle$ evolves into $|\psi(t)\rangle$, such that the density operator $\hat{\rho}(t) = |\psi(t)\rangle \langle \psi(t)|$ results

$$\hat{\rho}(t) = \sum_{ij} c_i c_j^* |\phi_i\rangle \langle \epsilon_i(t)| |\phi_j\rangle \langle \epsilon_j(t)|.$$  

(7)

where the $|\epsilon_i(t)\rangle$ are the states of the environment associated with the different states $|\phi_i\rangle$, and the $c_i c_j^* \neq 0$, with $i \neq j$, represent the quantum correlations that preclude classicality.

The clue of the decoherence approach is to consider that the state of the open system $S$ is represented by the reduced density operator $\hat{\rho}_S^\gamma (t)$ resulting from tracing over the environmental degrees of freedom:

$$\hat{\rho}_S^\gamma (t) = Tr_E \hat{\rho}(t) = \sum_{ij} c_i c_j^* |\phi_i\rangle \langle \epsilon_i(t)| |\phi_j\rangle \langle \epsilon_j(t)|.$$  

(8)

where the factor $\langle \epsilon_i(t)| \epsilon_j(t)\rangle$, with $i \neq j$, determines the size of the off-diagonal terms at each time. Many standard models for the interaction Hamiltonian show that, when the environment is composed of a very large number of degrees of freedom, the states $|\epsilon_i\rangle$ of the
environment rapidly approach orthogonality: \( \langle e_i(t) \mid e_j(t) \rangle \rightarrow \delta_{ij} \). This means that the reduced density operator rapidly becomes approximately diagonal in the basis \( \{|\phi_i\rangle\} \):

\[
\hat{\rho}_r^S(t) \rightarrow \hat{\rho}_r^S = \sum_i |c_i|^2 |\phi_i\rangle\langle \phi_i|
\]  

(9)

According to the orthodox interpretation of decoherence, the decohered state \( \hat{\rho}_r^S \) denotes a quantum mixture that contains only the terms corresponding to classical correlations. It is precisely for this reason that decoherence would offer the essential ingredient for solving the quantum measurement problem and for explaining the quantum-to-classical transition of the open system \( S \). In a certain sense, decoherence would explain collapse since “quantum entanglement will be converted into an effectively classical correlation as a result of the interaction” between the open system and its environment (Paz and Zurek 2002: 90).

It is quite clear that much of the appealing of decoherence as the explanation of the emergence of classicality relies on the interpretation of the reduced state as the quantum state of the open system. Nevertheless, several authors have warned against this interpretation; the best known among them is Bernard d’Espagnat (1976), who introduced the already classical distinction between proper and improper mixtures: whereas a proper mixture is the quantum state of a closed system, an improper mixture is a density operator obtained by disregarding some degrees of freedom of the closed system. In the case of the open system \( S \), if we could only make measurements on \( S \) and could not make any on the environment \( E \), then we would not be able to differentiate the improper mixture denoted by the reduced density operator \( \hat{\rho}_r^S \) from the analog proper mixture denoted by the density operator \( \hat{\rho}_S^S \). But, as d’Espagnat stresses (1995), there is no theoretical reason that prevents us from having access to, at least, some of the traced over degrees of freedom, and this access would permit us to show that the proper mixture and the improper mixture are, in principle, testably different. In the context of decoherence, the difference is also pointed out by Heinz-Dieter Zeh, one of the founding fathers of the theory: “The conceptually important difference between true and apparent ensembles was clearly pointed out by Bernard d’Espagnat (1976) when he distinguished between proper and improper mixtures. In the case of virtual (reversible) decoherence, this difference can even be observed as recoherence (a relocalization of the superposition, that would be impossible for a proper mixture)” (Zeh 2005: 2).

It is interesting to notice that the discussion about the difference between proper and improper mixtures relies on the fact that both are represented by the same kind of mathematical object—a density operator--; perhaps this fact is what leads many authors to suppose that the improper mixture of the open system is its quantum state in the same sense as the proper mixture is the quantum state of a closed system. However, that mathematical fact essentially depends on the Hilbert space formalism used to articulate the theory, but the situation is different in other cases. For instance, it can be proved (Masillo, Scolarici, and
Sozzo 2009) that proper and improper mixtures are represented by different kinds of density operators in the quaternionic formulation of quantum mechanics (see Adler 1995); therefore, in this formalism they can be distinguished not only physically but also mathematically.

The insistence on interpreting the reduced state of an open system as its quantum state seems to forget the very definition of the concept of reduced state. The reduced state \( \hat{\rho}_r \) of the open system \( S_1 \) is defined as the density operator by means of which the expectation values of all the observables of \( S_1 \) can be computed. Precisely, if \( \mathcal{H}_1 \) and \( \mathcal{H}_2 \) are the Hilbert spaces of the open systems \( S_1 \) and \( S_2 \) respectively, \( \mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \) is the Hilbert space of the closed system \( S \), \( \hat{O}_1 \in \mathcal{H}_1 \otimes \mathcal{H}_4 \) is an observable of \( S_1 \), \( \hat{I}_2 \) is the identity in \( \mathcal{H}_2 \otimes \mathcal{H}_5 \), and \( \hat{\rho} \in \mathcal{H} \otimes \mathcal{H} \) is the state of \( S \), then the reduced state of \( S_1 \) is defined as the density operator \( \hat{\rho}_r \) such that

\[
\forall \hat{O}_1^{12} = \hat{O}_1 \otimes \hat{I}_2 \in \mathcal{H} \otimes \mathcal{H}, \quad \langle \hat{O}_1^{12} \rangle_{\hat{\rho}} = \langle \hat{O}_1 \rangle_{\hat{\rho}'}
\]

On the basis of this definition, the reduced state can be computed by tracing over the degrees of freedom of \( S_2 \), as \( \hat{\rho}_r^{1} = \text{Tr}_2 \hat{\rho} \). As Schlosshauer claims in his well-known book about decoherence, this means that, strictly speaking, a reduced density operator is only “a calculational tool” for computing expectation values (Schlosshauer 2007: 48). For this reason, the author warns us “against a misinterpretation of reduced density matrices as describing a proper mixture of states” (2007: 69).

Although the reduced state of an open system cannot be interpreted as its quantum state, it is quite clear that it does offer a certain description of the involved systems. The claim that reduced states supply coarse descriptions has already appeared in the literature on decoherence (see, e.g., Gell-Mann and Hartle 1993, Omnès 1994, Anastopoulos 2002), but usually without a further elaboration. Here we will support this claim by comparing coarse graining as used in classical statistical mechanics and partial trace as used in quantum mechanics.

5. Coarse graining and partial trace as projections

The intuitive idea of graphical projection – the operation by which a three-dimensional body is projected on two dimensions – is applied in mathematics to the classical case of vectors: as it is well known, the projection \( \vec{a}_b \) of a vector \( \vec{a} \) onto a vector \( \vec{b} \) is a vector computed as \( \vec{a}_b = |\vec{a}| \cos \alpha \hat{b} \), where \( \alpha \) is the angle between \( \vec{a} \) and \( \vec{b} \), and \( \hat{b} \) is the unit vector in the direction of \( \vec{b} \). This simple mathematical notion is generalized in functional analysis by defining a projector \( \Pi \) as an operator that performs a linear transformation from a vector space onto itself, such that \( \Pi \Pi = \Pi \): when \( \Pi \) is applied twice to any vector, it gives the same result as if it were applied only once. From a conceptual viewpoint, a projection supplies a coarse description of the state vector on which it operates, because its action
consists in eliminating some components of that state vector in such a way that only certain components are retained.

As explained in Section 3, in classical statistical mechanics a coarse-grained description arises from a partition of the phase space $\Gamma$ into discrete and disjoint cells $C_j$ of the same volume: this operation defines the coarse-grained distribution $\rho_{cg}$ (eq. (2)). Since both the density function $\rho$ and the coarse-grained distribution $\rho_{cg}$ are defined on the same phase space $\Gamma$, it is not difficult to see that the relationship between $\rho_{cg}$ and $\rho$ can be described in terms of projection$^2$, since applying the same coarse graining operation to $\rho_{cg}$ does not modify the result (see Misra, Prigogine, and Courbage 1979, Misra and Prigogine 1981):

$$\rho_{cg} = \Pi^c \rho = \Pi^c \Pi^c \rho = \Pi^c \rho_{cg} .$$  

(11)

where the classical projector $\Pi^c$ performs the operation described by eq. (2). In other words, the coarse-grained distribution $\rho_{cg}$ supplies a coarse description of the classical system whose statistical state is represented by the density function $\rho$.

In the case of quantum mechanics, let us apply the definition of reduced state of eq. (10) to the case of the open system $S$ and its environment $E$:

$$\langle \hat{O}_{SE} \rangle_{\hat{\rho}} = \langle \hat{O}_S \rangle_{\hat{\rho}_S^{SE}}$$  

(12)

where $\hat{O}_{SE} = \hat{O}_S \otimes \hat{I}_E$. In this case, the density operator $\hat{\rho}$ belongs to $\mathcal{H} \otimes \mathcal{H}$, where $\mathcal{H}$ is the Hilbert space of the closed system $SE$, and the reduced state $\hat{\rho}_S^{SE}$ belongs to $\mathcal{H}_S \otimes \mathcal{H}_S$, where $\mathcal{H}_S$ is the Hilbert space of the open system $S$. Therefore, for dimensional reasons the reduced state $\hat{\rho}_S^{SE}$ cannot be expressed as a direct projection of the density operator $\hat{\rho}$. Nevertheless, the expectation value of $\hat{O}_S$ in the reduced state $\hat{\rho}_S^{SE}$ can also be expressed as the expectation value of the observables $\hat{O}_{SE} = \hat{O}_S \otimes \hat{I}_E$ of the closed system $SE$ in a state $\hat{\rho}_S^{SE} \in \mathcal{H} \otimes \mathcal{H}$:

$$\langle \hat{O}_S \rangle_{\hat{\rho}_S^{SE}} = \langle \hat{O}_{SE} \rangle_{\hat{\rho}_S^{SE}} = \langle \hat{O}_S \otimes \hat{I}_E \rangle_{\hat{\rho}_S^{SE}}$$  

(13)

The density operator $\hat{\rho}_S^{SE}$ can be obtained as

$$\hat{\rho}_S^{SE} = \Pi^S \hat{\rho} = \Pi^S \Pi^S \hat{\rho} = \Pi^S \hat{\rho}_S^{SE}$$  

(14)

where the projector $\Pi^S$ performs the following operation:

$$\Pi^S = (Tr_E \hat{\rho}) \otimes \tilde{\delta}^E = \hat{\rho}_S^S \otimes \tilde{\delta}^E$$  

(15)

$^2$ Strictly speaking, the operation of projection is represented by a projector operator when classical statistical mechanics is formulated in the formalism of Koopman (1931) –its Hilbert space formulation--; nevertheless, we will not stress this point since not relevant for our argument.
where $\tilde{\delta}^E \in \mathcal{H}_E \otimes \mathcal{H}_E$ is a normalized identity operator with coefficients $\delta_{a\beta} = \delta_{a\beta} / \sum \delta_{\gamma \gamma}$ (see Fortin and Lombardi 2014). The operator $\Pi^a$ is a projector since

$$\Pi^a \Pi^a \hat{\rho} = \left(\text{Tr}_E \Pi^a \hat{\rho}\right) \otimes \tilde{\delta}^E = \left(\text{Tr}_E \left(\hat{\rho}_S^E \otimes \tilde{\delta}^E\right)\right) \otimes \tilde{\delta}^E = \hat{\rho}_S^E \otimes \tilde{\delta}^E = \Pi^a \hat{\rho} \quad (16)$$

In turn, if we trace off the degrees of freedom of the environment $E$ on $\hat{\rho}_{SE}^r$, we recover the reduced state of the open system $S$:

$$\text{Tr}_E \hat{\rho}_{SE}^r = \text{Tr}_E \left(\hat{\rho}_S^E \otimes \tilde{\delta}^E\right) = \hat{\rho}_S^E \quad (17)$$

This means that the $\hat{\rho}_{SE}^r$, which “erases” the components of the quantum state $\hat{\rho}$ corresponding to the environment $E$, supplies the same information about the open system $S$ as the reduced state $\hat{\rho}_S^E$, but now from the viewpoint of the closed system $SE$ (see Castagnino and Fortin 2013). It is quite clear that $\hat{\rho}_{SE}^r = \Pi^q \hat{\rho}$, although belonging to $\mathcal{H} \otimes \mathcal{H}$, is not the quantum state of the closed system $SE$: it supplies a coarse description of $SE$ that disregards certain information, in particular, that corresponding to the environment $E$. It is interesting to note that, although $\hat{\rho}_{SE}^r$ is not a quantum state, it is a coarse state of the whole closed system $SE$ that may evolve non-unitarily; therefore, it is not the case that non-unitary evolutions are exclusive to open quantum systems.

On the basis of the above presentation, the classical and the quantum cases, with their corresponding states and observables, can be viewed from a unified perspective (see Table 1). In the two cases, a state $\rho_{CD}$ that supplies a coarse description of the closed system can be defined, in such a way that it can be obtained as a projection of the “fine description” $\rho_{FD}$:

$$\rho_{CD} = \Pi \rho_{FD} \quad \rho_{CD} = \Pi \rho_{FD}$$

The fine description is given by the statistical state, represented by the density function $\rho$, in classical statistical mechanics, and by the quantum state, represented by the density operator $\hat{\rho}$, in quantum mechanics. In turn, the coarse state acquires different forms in classical statistical mechanics and in quantum mechanics: in the first case, it is a function $\rho_{cg}(r)$ on the phase space $\Gamma$; in the second case, it is an operator $\hat{\rho}_{SE}^r$ belonging to $\mathcal{H} \otimes \mathcal{H}$. Therefore, the corresponding projections are expressed as

$$\rho_{cg} = \Pi^q \rho \quad \text{and} \quad \hat{\rho}_{SE}^r = \Pi^q \hat{\rho} \quad (18)$$

The difference between the two cases relies on what is disregarded in each one of them. As clearly expressed by Michael Mackey (1989):

- **Coarse graining implies the loss of some information about the exact values of all the dynamical variables.** This fact is formally expressed in classical statistical mechanics by the definition of “gross”, coarse-grained observables $O_{cg}$ corresponding to the dynamical observables of the system, whose expectation values can be computed as (see eq. (5)):

$$\left\langle O_{cg}\right\rangle_\rho = \left\langle O\right\rangle_{\rho_{cg}} = \left\langle O_{cg}\right\rangle_{\rho_{cg}} \quad . (19)$$
Partial trace implies the loss of all the information about the exact value of some dynamical variables, in particular, the dynamical variables of the environment. This fact is formally expressed in quantum mechanics by retaining only the observables \( \hat{O}^SE \) of the open system, whose expectation values are computed as (see eq. (12) and eq. (13)):

\[
\langle \hat{O}^SE \rangle_{\hat{\rho}} = \langle \hat{O}^SE \rangle_{\hat{\rho}^{SE}} = \langle \hat{O} \rangle_{\hat{\rho}^{SE}}
\]  

(20)

<table>
<thead>
<tr>
<th>CSM</th>
<th>QM</th>
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<tr>
<td>( \rho(r,t) ; O(r) )</td>
<td>( \hat{\rho}(t) ; \hat{O} )</td>
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<tr>
<td>( \partial \rho / \partial t = -{H, \rho} )</td>
<td>( \partial \hat{\rho} / \partial t = -i/\hbar [\hat{H}, \hat{\rho}] )</td>
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<tr>
<td>( \langle O(r) \rangle_{\rho(r)} = \int_{\Gamma} \rho(r) O(r) , dr )</td>
<td>( \langle \hat{O} \rangle_{\hat{\rho}} = \text{Tr} (\hat{\rho} \hat{O}) )</td>
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Let us define a coarse description \( \rho_{CD} \) such that

\( \rho_{CD} = \Pi \rho_{FD} \)

\( \rho_{FD} \equiv \hat{\rho} \quad \rho_{CD} \equiv \rho_{cg} \)

\( \rho_{cg} = \Pi^5 \rho \)

Loss of some information about the exact values of all the dynamical variables

\( \rho_{FD} \equiv \hat{\rho} \quad \rho_{CD} \equiv \hat{\rho}_r^{SE} \)

\( \hat{\rho}_r^{SE} = \Pi^q \hat{\rho} \)

Loss of all the information about the exact values of some dynamical variables

Table 1: Comparison between the classical statistical case and the quantum case regarding fine and coarse descriptions.

Up to this point, we have considered the most used strategies to account for irreversible behavior by disregarding degrees of freedom: coarse graining in classical statistical mechanics and partial trace in quantum mechanics. In the following section, we will complete the parallel between the two cases by considering coarse graining in quantum mechanics and partial trace in classical statistical mechanics.

6. Coarse graining and partial trace in the classical and the quantum cases

6.1. Coarse graining

Let us recall that coarse graining implies the loss of some information about the exact values of all the dynamical variables. As explained in Section 3, in classical statistical mechanics this is formalized by defining some gross observables (see eq. (4)) that do not
discriminate below a certain precision, and whose expectation values can be computed as in eq. (19).

In quantum mechanics an analogous strategy can be developed. Let us consider a closed system whose Hilbert space \( \mathcal{H} \) is spanned by the eigenstates \( |r\rangle \) of an observable \( R \) of continuous spectrum; so, any state \( \hat{\rho} \) and any observable \( \hat{O} \) can be expressed, respectively, as

\[
\hat{\rho} = \int \rho(r,r') |r\rangle\langle r'| drdr'.
\]

(21)

\[
\hat{O} = \int O(r,r') |r\rangle\langle r'| drdr'.
\]

(22)

In this case, coarse graining is the result of partitioning the space \( \mathcal{H} \otimes \mathcal{H} \) into regions corresponding to \( (r,r') \in C_i \). On the basis of this partition, coarse-grained states and coarse-grained observables can be defined as follows. First, certain coarse-grained functions that average the components of states and observables in the regions \( C_i \) are defined:

\[
\rho_{cg}(r,r') = \int \rho(r,r') |r\rangle\langle r'| drdr' \quad \text{if} \ (r,r') \in C_i.
\]

(23)

\[
O_{cg}(r,r') = \int O(r,r') |r\rangle\langle r'| drdr' \quad \text{if} \ (r,r') \in C_i.
\]

(24)

Second, the corresponding operators are obtained as

\[
\hat{\rho}_{cg} = \int \rho_{cg}(r,r') |r\rangle\langle r'| drdr'.
\]

(25)

\[
\hat{O}_{cg} = \int O_{cg}(r,r') |r\rangle\langle r'| drdr'.
\]

(26)

This leads to a situation completely analogous to the classical case: the coarse-grained description can be obtained both by averaging the fine-grained observables in the coarse-grained state or by averaging the coarse-grained observables in the fine-grained state (see eq. (19):

\[
\langle \hat{O} \rangle_{\hat{\rho}_{cg}} = \langle \hat{O}_{cg} \rangle_{\hat{\rho}}
\]

(27)

It is interesting to recall that this coarse-graining procedure was the strategy followed in certain early attempts to explain the classical limit of quantum mechanics, during a period that can be considered as the pre-history of the decoherence program. In the 1950s and the early 1960s, the emergence of classical macroscopic features from quantum microscopic descriptions was treated in the context of the study of irreversibility in closed systems (van Kampen 1954, van Hove 1957, 1959, Daneri, Loinger, and Prosperi 1962). From this perspective, the states indistinguishable from the viewpoint of certain “gross” observables were described by the same coarse-grained state, whose evolution was proved to reach equilibrium in a certain relaxation time. The main problem of this period was that the
relaxation times so obtained turned out to be too long to account for experimental results (see Omnès 2005).

Summing up, although coarse graining is a traditional procedure to explain irreversibility in classical statistical mechanics, it can be appealed to when the issue is quantum irreversibility; see Table 2 for the analogy between the two cases.

<table>
<thead>
<tr>
<th>CSM</th>
<th>QM</th>
</tr>
</thead>
<tbody>
<tr>
<td>( r \in \Gamma ; \rho(r) ; O(r) )</td>
<td>( R ) with (</td>
</tr>
<tr>
<td>Coarse graining in variable ( r )</td>
<td>Coarse graining in variable ( r )</td>
</tr>
</tbody>
</table>
| \( \rho_{cg}(r) = \left\{ \begin{array}{ll} 1 \over \mu(C_i) \int_{C_i} \rho(r) \, dr & \text{if } r \in C_i \\
0 & \text{otherwise} \end{array} \right. \) | \( \rho_{cg}(r, r') = \left\{ \begin{array}{ll} \int_{C_r} \rho(r, r') \, dr \, dr' & \text{if } (r, r') \in C_i \\
0 & \text{otherwise} \end{array} \right. \) |
| \( O_{cg}(r) = \left\{ \begin{array}{ll} 1 \over \mu(C_i) \int_{C_i} O(r) \, dr & \text{if } r \in C_i \\
0 & \text{otherwise} \end{array} \right. \) | \( O_{cg}(r, r') = \left\{ \begin{array}{ll} \int_{C_r} O(r, r') \, dr \, dr' & \text{if } (r, r') \in C_i \\
0 & \text{otherwise} \end{array} \right. \) |
| \( \langle O \rangle_{\rho_{cg}} = \langle O_{cg} \rangle_{\rho} \) | \( \langle \hat{O} \rangle_{\hat{\rho}_{cg}} = \langle \hat{O}_{cg} \rangle_{\hat{\rho}} \) |

Table 2: Coarse graining in classical statistical mechanics and in quantum mechanics.

6.2. Partial trace

Let us recall that partial trace implies the loss of all the information about the exact value of some dynamical variables. As explained in Section 4 and Section 5, in quantum mechanics the operation of partial trace is extensively used for the account of decoherence through the definition of the reduced state of the open system (see eq. (8)), which disregards the degrees of freedom of the environment. This amounts to retaining only the observables \( \hat{O}_{SE} \) of the open system, whose expectation values are computed as in eq. (20).

In classical statistical mechanics an analogous strategy can be developed. Let us consider a closed system \( SE \) of \( N \) particles described in a phase space \( \Gamma \) of \( 6N \) dimensions. The states and observables of the system are functions of the \( 3N \) positions \( q_i \) and the \( 3N \) momenta \( p_i \) of the \( N \) particles:

\[
\rho(r) = \rho(q_1, p_1, \ldots, q_{3N}, p_{3N}) .
\]  
\[
O(r) = O(q_1, p_1, \ldots, q_{3N}, p_{3N}) .
\]
If the purpose is to describe an open subsystem $S$ of $s$ particles, the interest is centered on the observables $O_S(q_1, p_1, ..., q_{3s}, p_{3s})$. In order to compute the expectation values of these observables, a reduced state $\rho_S^r(t)$ can be computed by means of a partial trace:

$$\rho_S^r(q_1, p_1, ..., q_{3s}, p_{3s}) = \int ... \int \rho(q_1, p_1, ..., q_{3N}, p_{3N}) dq_{3s+1} dp_{3s+1} ... dq_{3N} dp_{3N}.$$  (30)

The reduced state $\rho_S^r(q_1, p_1, ..., q_{3s}, p_{3s})$ disregards the degrees of freedom of the environment $E$ composed by the remaining $N - s$ particles. In turn, the observable of the open system $S$ can be expressed from the viewpoint of the closed system of $N$ particles as a function on the phase space $\Gamma$:

$$O_S(q_1, p_1, ..., q_{3s}, p_{3s}) = O_{SE}^S(q_1, p_1, ..., q_{3N}, p_{3N}).$$  (31)

The reduced state $\rho_S^r(q_1, p_1, ..., q_{3s}, p_{3s})$ can also be expressed from the viewpoint of the closed system as a function on $\Gamma$:

$$\rho_S^r(q_1, p_1, ..., q_{3s}, p_{3s}) = \rho_{SE}^S(q_1, p_1, ..., q_{3N}, p_{3N}).$$  (32)

Therefore, the expectation values of the observables of the subsystem of $s$ particles can be computed alternatively from the perspective of the closed system $SE$ of $N$ particles or from the perspective of the open subsystem $S$ of $s$ particles:

$$\langle O_{SE}^S \rangle_\rho = \langle O_{SE}^S \rangle_{\rho_S^r} = \langle O_S \rangle_{\rho_S^r}.$$  (33)

It is interesting to recall that, in the quantum domain, the operation of partial-trace was implicit in what Schrödinger (1926) called “density of electricity” or “electric charge density”, a quantity defined in the space of three dimensions, which he considered the quantum magnitude with direct physical meaning (see Przibram 1967). At present, the partial-trace procedure is the strategy used in quantum chemistry in the so-called “independent electron approximation”, which consists in thinking of each electron as occupying its “own” orbital, in such a way that the total wavefunction of the $N$-electron system is written in the form of an antisymmetrized product of single-electron wavefunctions (see, e.g., Atkins and de Paula 2006).

In classical statistical mechanics, the reduced densities are used to compute the expectation values of the observables (phase functions) that depend on the dynamical variables of a subset of the particles of the system, such as, for instance, the kinetic energy of a single particle, or the potential energy of two particles. The evolution of the reduced densities is described by the set of equations known as BBGKY hierarchy due to the name of its authors: Nicolái Bogoliubov (1946), Max Born and Herbert Green (1946), John Kirkwood (1946), and Jacques Yvon (1935).
Summing up, although partial trace is a traditional procedure to account for the behavior of open systems in quantum mechanics, it is also extensively used in classical statistical mechanics when the interest is focused on certain particular magnitudes; see Table 3 for the analogy between the two cases.

<table>
<thead>
<tr>
<th>CSM</th>
<th>QM</th>
</tr>
</thead>
<tbody>
<tr>
<td>System $SE : \Gamma (N \text{ particles}) ; \rho ; O$</td>
<td>System $SE : \mathcal{H} \otimes \mathcal{H} ; \hat{\rho} ; \hat{O}$</td>
</tr>
<tr>
<td>Subsystem $S$ ($s$ particles)</td>
<td>Subsystem $S$ (open system)</td>
</tr>
<tr>
<td>$\mathcal{O}_s (q_1, p_1, \ldots, q_s, p_s)$</td>
<td>$\hat{\mathcal{O}}_S \in \mathcal{H}_S \otimes \mathcal{H}_S$</td>
</tr>
<tr>
<td>$\mathcal{O}<em>s^{SE} (q_1, p_1, \ldots, q</em>{3N}, p_{3N})$</td>
<td>$\hat{\mathcal{O}}_S^{SE} = \hat{\mathcal{O}}_S \otimes \hat{I}_E$</td>
</tr>
<tr>
<td>$\rho_s^S = \int \ldots \int \rho dq_{3s+1} dp_{3s+1} \ldots dq_{3N} dp_{3N}$</td>
<td>$\hat{\rho}_s^S = \text{Tr}_E \hat{\rho}$</td>
</tr>
<tr>
<td>$\langle \mathcal{O}<em>s \rangle</em>{\rho_s^S} = \langle \mathcal{O}<em>s^{SE} \rangle</em>{\rho}$</td>
<td>$\langle \hat{\mathcal{O}}<em>S \rangle</em>{\hat{\rho}_s^S} = \langle \hat{\mathcal{O}}<em>S^{SE} \rangle</em>{\hat{\rho}}$</td>
</tr>
</tbody>
</table>

Table 3: Partial trace in classical statistical mechanics and in quantum mechanics.

7. Final remarks: consequences for the interpretation of quantum decoherence

When these results are considered together, a unified view of the emergence of irreversibility can be proposed, which turns out to be applicable both to the classical and to the quantum cases. According to this unified view, the relation between the irreversible macro-level and the reversible micro-level is that of a generalized coarse description, mathematically defined as a projection.

From this perspective, it is very difficult to confuse the system’s states, which evolve according to the dynamical postulate of the considered theory, with a coarse-grained state or a reduced state, which offer a coarse description of the system. Once it is accepted that $\rho_{cg}$ and $\rho_r^S$ are not statistical states, it must be admitted that $\hat{\rho}_{cg}$ and $\hat{\rho}_r^S$ are not quantum states. This is particularly relevant for the interpretation of quantum mechanics, since some interpretive difficulties are the result of endowing reduced states with the same interpretation as quantum states. In particular, conceiving reduced states as the quantum states of open systems represents an obstacle for no-collapse interpretations to explain consecutive measurements (see detailed discussion in Ardenghi, Lombardi, and Narvaja 2012).
This unified view supplies an understanding of the phenomenon of decoherence different from that implicit in most presentations: since the reduced state is not the quantum state of the open system, but a coarse description of the closed composite system, decoherence should not be conceived as a phenomenon resulting from the interaction between an open system and its environment (Castagnino, Fortin, and Lombardi 2010a); by contrast, decoherence is the consequence of a coarse evolution that emerges from disregarding certain degrees of freedom of the whole closed system (Castagnino, Laura, and Lombardi 2007, Lombardi, Fortin, and Castagnino 2012). Ignoring this fact led the orthodox approach to decoherence, which insists on the essential role played by the openness of the system in the emergence of classicality, to a serious difficulty, explicitly recognized by Zurek: “one issue which has been often taken for granted is looming big as a foundation of the whole decoherence program. It is the question of what are the ‘systems’ which play such a crucial role in all the discussions of the emergent classicality” (Zurek 1998: 22).

This problem is dissolved when the above results are taken into account. In fact, the coarse description –both under the coarse-graining form and under the partial-trace form– depends on how the relevant information is selected. Coarse graining depends on which information about the exact values of the dynamical variables we accept to lose (which “gross” observables we select to study). Partial trace depends on which dynamical variables we choose in order to lose all the information about them (which observables we disregard as the “environment”). As a consequence, decoherence is relative to the observables selected to be studied. In turn, since there is no privileged or essential decomposition of the closed system, there is no need of an unequivocal criterion for identifying the systems involved in decoherence. Therefore, the looming big issue that threatens the whole decoherence program dissolves in the light of the relativity of decoherence (see detailed discussion in Castagnino, Fortin, and Lombardi 2010b, Lombardi, Fortin, and Castagnino 2012).

The closed-system perspective proposed here allows us to take a step further: instead of thinking in the decoherence of systems and their states, it is possible to focus on observables and to consider the time behavior of their expectation values. This perspective centered on the observables is in resonance with the algebraic formalism of quantum mechanics (Haag 1993), according to which a quantum system is mathematically characterized by the space $\mathcal{O}$ of the self-adjoint elements of an algebra of operators representing observables, and states are represented by functionals on $\mathcal{O}$. In this theoretical framework, the observables are the basic elements of the theory, and states are secondary elements, defined in terms of the basic ones as mere tools to compute expectation values. Therefore, instead of saying that the open system behaves as if it were classical or that the states of the pointer basis become classical, it is be more accurate to say that certain observables of the closed system decohere and behave as if they were classical observables; this happens when their expectation values tend very rapidly to certain values that can be computed as classical expectation values.
This observable-centered view dissolves certain perplexities that arise from conceiving the emergence of classicality according to the orthodox approach. In fact, certain many-particle models show that, although some particles decohere and may behave classically, the subsystem composed by all of them does not decohere and retains its quantum nature; in particular, it may be the case that all the particles of a closed system decohere and may behave classically when considered independently, although the closed system certainly does not decohere and, therefore, retains its quantum character (see Castagnino, Fortin, and Lombardi 2010a). The perplexity disappears when decoherence is no longer a process of systems but a process of the expectation values of observables. The closed-system and observable-centered perspective proposed here leads to the unambiguous identification, among all the observables of the closed system, of those that will have a classical-like behavior because their expectation values acquire a classical form (Fortin and Lombardi 2016).

Summing up, the phenomenon of decoherence gains objectivity when understood from the perspective of the closed system’s observables. If the term ‘decoherence’ denotes a system’s process, represented by the time evolution of the system’s state, then it refers to a coarse-grained process that is relative to the observables selected to be studied, that is, to how the “open system” of interest is defined. If, by contrast, the term ‘decoherence’ applies to the system’s observables, then it is endowed with a non-relative meaning: an observable decoheres when it acquires a classical-like behavior because its expectation value tends to a classical form.

This closed-system observable-centered view of decoherence and the classical limit naturally fits into a top-down view of quantum mechanics, according to which the only legitimate quantum systems are the unitary evolving closed systems. This approach finds a significant affinity with the so called “quantum structural studies”, which focus on the different ways in which a quantum system can be decomposed into subsystems (quantum structures) (Jeknæ-Dugiæ, Arsenijeviæ, and Dugiæ 2013, Arsenijeviæ, Jeknæ-Dugiæ and Dugiæ 2016, Harshman 2016). But this topic is beyond the limits of the present article and will be the subject of a future work.

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References


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