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Hamiltonian Formulation of Statistical Ensembles and Mixed States of Quantum and Hybrid Systems

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Abstract Representation of quantum states by statistical ensembles on the quantum phase space in the Hamiltonian form of quantum mechanics is analyzed. Various mathematical properties and some physical interpretations of the equivalence classes of ensembles representing a mixed quantum state in the Hamiltonian formulation are examined. In particular, non-uniqueness of the quantum phase space probability density associated with the quantum mixed state, Liouville dynamics of the probability densities and the possibility to represent the reduced states of bipartite systems by marginal distributions are discussed in detail. These considerations are used to study ensembles of hybrid quantum-classical systems. In particular, nonlinear evolution of a single hybrid system in a pure state and unequal evolutions of initially equivalent ensembles are discussed in the context of coupled hybrid systems.

Keywords Statistical ensembles · Hybrid systems

1 Introduction

Schrödinger equation of quantum mechanics (QM) on a Hilbert space $\mathcal{H}$ can be written as a Hamiltonian dynamical system on the corresponding phase space [1–5]. This fact enables elegant treatment of quantum dynamical problems, like for example analysis of quantum dynamics with nonlinear constraints [6, 7] and related issues of classical limit [8, 9]. One hopes that full geometrical formulation of QM analogous to that of classical Hamiltonian systems, besides its usefulness in the dynamical issues and its mathematical elegance, will also provide better intuitive understanding of typically quantum phenomena [4, 5]. Furthermore, the Hamiltonian formulation is specially convenient for the treatment of coupling between

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classical and quantum systems, called hybrid systems, [10–13], because it provides a unified mathematical framework for both theories. However, the formal similarity between the Hamiltonian formulation of QM and that of classical systems is only partial, and there are differences in some crucial aspects. The purpose of this paper is to analyze the relation of quantum mixed states with the corresponding statistical ensembles of quantum systems in the Hamiltonian formulation, and to utilize such considerations for an analysis of ensembles of hybrid systems.

The fundamental difference between the Hamiltonian formulation of QM and of classical mechanics (CM) is in the classes of phase space functions which are considered as representing dynamical variables in the two theories. In the Hamiltonian formulation of QM only the quadratic functions on the phase space are interpreted as observables. Functions of more general types generate nonlinear evolution of the quantum states. However, non-quadratic functions and nonlinear evolution of the quantum degrees of freedom appear naturally in the theory of hybrid systems. This fact has profound physical significance, and is reflected in the interpretation of the results of the hybrid theory. Another, but related, type of striking differences and incomplete analogies between Hamiltonian formulations of QM and CM are introduced when states more general than pure are considered. Such considerations reveal, from a new perspective, some well known deep features of quantum mixtures, represented by density operators $\hat{\rho}$, but also point out to some less known differences between quantum and classical ensembles represented by density functions ρ on the quantum phase space. Consequences of these differences in the Hamiltonian formulation of hybrid systems is the main topic of this paper. Thus, our main motivation for the discussion of differences between quantum mixed states and general statistical ensembles in the Hamiltonian formulation of QM, given in Sect. 3, is to better understand the behavior of ensembles of hybrid systems, presented in Sect. 4. In particular, we analyze, in Sect. 3.1, relations between classes of equivalent discrete convex combinations of pure quantum states on one side, and classes of equivalent statistical ensembles in the Hamiltonian formulation of QM on the other side. The well known result of Hughston, Josza and Wooters [14], about the relation between different finite convex representations of a mixed state is generalized to Hamiltonian ensembles represented by general densities. Typical representatives of the equivalence classes of densities representing the same mixed state, such as Gaussian densities, are discussed. Correct interpretation of the phase space function $\langle\psi|\hat{\rho}|\psi\rangle$, where $\hat{\rho}$ is a density matrix, versus a density ρ corresponding to that density matrix $\hat{\rho}$ is stressed. In Sect. 3.2 we briefly describe the formulation of Liouville equation as a Hamiltonian dynamical system. We then analyze, in Sect. 3.3, the relation between the statistical operator obtained by tracing out a subsystem of a quantum system in a pure state on one side, and the statistical ensembles given by marginal distributions in the Hamiltonian formulation on the other side. These considerations are important for proper interpretation of some recently obtained results in the Hamiltonian formulation of hybrid systems [10, 13], which we discuss in Sect. 4.

2 Hamiltonian Formulation

Quantum and classical mechanics might be formulated using the same mathematical framework. Relevant references for the CM case are [15, 16] and for the QM case are [1–5]. This fact suggests to formulate the hybrid theory using the same mathematical framework of Hamiltonian dynamical systems. All three theories will be considered here as dynamical systems $(\mathcal{M}, \omega, g, H)$ on a differentiable manifold $\mathcal{M}$ with a symplectic and Riemannian structures ω and g respectively, with some preferred function, the Hamiltonian, H. The manifold is also assumed to posses a complex structure $J^2 = -I$ such that: $g(x, y) = \omega(x, Jy)$. All problems that we would like to discuss appear already in quantum systems with finite-dimensional Hilbert space, implying a finite-dimensional manifold $\mathcal{M}$. Therefore we shall assume that $\mathcal{M}$ is finite-dimensional.

Formulation of the classical mechanics of isolated conservative systems using $(\mathcal{M}, \omega, H)$ is standard [15, 16]. The formulation of quantum mechanics in terms of $(\mathcal{M}, \omega, g, H)$ is perhaps less well known, but shall not be presented here in any detail since there exist excellent reviews [4, 5]. Very briefly, the basic observation beyond the Hamiltonian formulation of quantum mechanics is that the evolution of a pure quantum state in a Hilbert space $\mathcal{H}$, as given by the Schrödinger equation, can be equivalently described by a Hamiltonian dynamical system on an Euclidean manifold $\mathcal{M}$. The manifold is just the Hilbert space considered as a real manifold, with the symplectic and Riemannian structures given by the real and the imaginary parts of the Hilbert scalar product. Representing a normalized vector $|\psi\rangle \in \mathcal{H}$ in a basis, one can introduce the canonical coordinates $x_j = (c_j^* + c_j)/\sqrt{2}$, $y_j = i(c_j^* - c_j)/\sqrt{2}$, $j = 1, 2 \dots N$. Generic point from $\mathcal{M}$ will also be denoted by X or X^a, where $a = 1, 2 \dots 2N$ is an abstract index. The dimension of the quantum phase space is $2N$ where N is the complex dimension of the system's Hilbert space. It should be stressed, perhaps, that the canonical coordinates x_j, y_j have nothing to do with the canonical coordinates of the classical system that after quantization gives the considered quantum system with the Hilbert space $\mathcal{H}$. The Hamilton's function $H(X)$ is given by the quantum expectation of the Hamiltonian $\hat{H}$ in the state $|\psi_X\rangle \leftrightarrow X$: $H(X) = \langle\psi_X|\hat{H}|\psi_X\rangle$. The Schrödinger dynamical law is that of Hamiltonian mechanics

$$\dot{X}^a = \omega^{ab}\nabla_b H. \tag{1}$$

In the Hilbert space QM and in the Hamiltonian classical mechanics the dynamical variables can be introduced formally as generators of the isomorphisms of the respective relevant structures. In QM these are self-adjoined operators generating unitary transformations that preserve the Hilbert scalar product. In the Hamiltonian formulation of QM the Hilbert scalar product generates the symplectic and Riemannian structure. The symplectic structure is preserved by Hamiltonian vector fields of arbitrary smooth functions, but the metric is preserved only by the Killing vector fields, i.e., by the Hamiltonian vector fields generated by quadratic functions of the canonical variables. In the Hamiltonian formulation of classical systems, the metric of the phase space has no physical relevance and thus all smooth functions generate isomorphic i.e., canonical transformations, and are interpreted as dynamical variables. In the Hamiltonian formulation of QM, only the quadratic functions generate the automorphisms, and only such functions are related to dynamical variables or observables. In fact, all observables are represented by quadratic functions $A(X)$ on $\mathcal{M}$ and are the quantum mechanical expectations of the corresponding quantum observables $A(X) = \langle\psi_X|\hat{A}|\psi_X\rangle$. In particular, the canonical coordinates of the quantum phase space do not have physical interpretation. It is important to observe that the Poisson bracket between two quadratic functions is also a quadratic function and satisfies

$$\{A_1(X), A_2(X)\} = \frac{1}{i\hbar}\langle\psi_X|[\hat{A}_1, \hat{A}_2]|\psi_X\rangle. \tag{2}$$

If one considers the Hilbert space vectors of arbitrary norm, then two vectors $|\psi_1\rangle$ and $|\psi_2\rangle$ from $\mathcal{H}$ are representing the same physical pure state if there is a complex scalar $a \neq 0$ such that $|\psi_2\rangle = a|\psi_1\rangle$. The set of equivalence classes defines the complex projective space $\mathbb{C}P^{N-1} \equiv (\mathbb{C}^N - \{0\})/\sim$. The pure state space $\mathbb{C}P^{N-1}$ is isomorphic with the real manifold S^{2N-1}/S^1 which has compatible complex, Riemannian and symplectic structures. These structures are used to formulate geometric Hamiltonian framework of QM based on the pure state space $\mathbb{C}P^{N-1}$. Almost all formulas that we shall present for the Hamiltonian formulation based on $\mathcal{H}$ are of the same form in the formulation based on $\mathbb{C}P^{N-1}$, with the corresponding understanding of the symbols representing the phase space $\mathcal{M}$, the symplectic structure ω and the Riemannian metric g, and renormalization of the functions representing observables, i.e., $A(X) = \langle\psi_X|\hat{A}|\psi_X\rangle/\|\psi_X\|^2$. In particular, the transition probability $|\langle\psi_1|\psi_2\rangle|^2/(\|\psi_1\|\|\psi_2\|)^2$ is expressed as $\cos^2\theta(X_1, X_2)$ of the geodesic distance $\theta(X_1, X_2)$ between the points $X_1, X_2 \in \mathbb{C}P^{N-1}$. Also the eigenstates ψ_a of an observable $\hat{A}$ are represented by the critical points of the Hamiltonian vector field generated by $A(X)$. In the discussion that follows we shall not need to distinguish explicitly between the formulations based on $\mathcal{H}$ and the one based on $\mathbb{C}P^{N-1}$. Rare cases when a statement is applicable only in one of the formulations, with the non-trivial transcription, will be clearly stated.

The Hamiltonian formulation of QM suggests natural formal generalizations [4]. The most obvious one is to consider a theory where the evolution can be generated by functions which are not quadratic [4, 17, 18]. This would correspond to a nonlinear Schrödinger evolution equation. We shall see that such generalizations are dictated quite naturally in the Hamiltonian framework for a theory of hybrid systems. It has been argued, using particular generalization of the nonlinear evolution with all other aspects of QM unaltered, that such nonlinear evolution would enable superluminal communication between distant systems [19, 20], or violate the second law of thermodynamics [21]. However, other aspects of QM could be altered appropriately, and conveniently using the Hamiltonian framework, as is required in a consistent theory of hybrid systems [10, 12, 13], so that such objections do not apply. These issues will be analyzed after a discussion of ensembles of quantum systems and composite quantum systems in the Hamiltonian framework.

3 Hamiltonian Ensembles and Quantum Mixtures

3.1 Statistical Ensembles of Quantum Systems

Ensembles of quantum Hamiltonian systems are in general described by probability distributions $\rho(X)$ on the phase space $\mathcal{M}$. Average value of a quantum observable $A(X)$ over an ensemble $\rho(X)$ is given by

$$\bar{A} = \int_{\mathcal{M}} \rho(X)A(X)dM, \tag{3}$$

where dM represents the appropriate volume element on $\mathcal{M}$. This expression can be interpreted as unconditional expectation of the conditional expectation of $\hat{A}$ in pure states $|\psi_X\rangle$, the later being distributed according to the probability distribution $\rho(X)$. For a function $A(X) = \langle\psi_X|\hat{A}|\psi_X\rangle/\|\psi_X\|^2$, representing an observable, one has

$$\int_{\mathcal{M}} \rho(X)A(X)dM = \mathrm{Tr}(\hat{\rho}\hat{A}), \tag{4}$$

where the quantum mixed state $\hat{\rho}$ associated with the probability distribution $\rho(X)$ is given by

$$\hat{\rho} = \int_{\mathcal{M}} \rho(X)\hat{\Pi}(X)dM, \tag{5}$$

with $\hat{\Pi}(X) = |\psi_X\rangle\langle\psi_X|/\|\psi_X\|^2$ being the projector corresponding to the pure state represented by the point X. In general, the state vectors $|\psi_X\rangle$ can have arbitrary norm.

Special cases of the above formula are provided by densities with the support on a finite set of points from $\mathcal{M}$, giving finite convex combinations of atomic measures

$$\hat{\rho} = \sum_{i=1}^{M} \rho(X_i)\hat{\Pi}(X_i), \tag{6}$$

where $M \geq \mathrm{Rank}(\hat{\rho})$. Incidentally, this special case of (5) is the most often discussed in the standard Hilbert space QM.

The densities $\rho(X)$ satisfy Liouville equation on $\mathcal{M}$

$$\frac{\partial}{\partial t}\rho(X;t) = \big\{H(X), \rho(X;t)\big\}_{\mathcal{M}}, \tag{7}$$

which differs in sign from the evolution equation of functions on $\mathcal{M}$ representing observables.

One observes that all probability densities with the same second moments give the same values for the expectations (4) of quadratic functions, i.e., quantum observables. Consequently all such densities generate the same statistical operator $\hat{\rho}$ via (5). Furthermore, Liouville evolution of all the densities $\rho(X;t_0)$, yielding the same $\hat{\rho}(t_0)$, generates the same von Neumann evolution $\hat{\rho}(t)$. Indeed, the evolution equation satisfied by $\hat{\rho}(t)$, related by (5) to a solution $\rho(X;t)$ of the Liouville equation, is the von-Neumann equation $i\hbar\partial\hat{\rho}/\partial t = -[\hat{\rho}, \hat{H}]$. This fact is easily obtained from the definition (5) and Eq. (7) by using partial integration. Therefore, a quantum mechanical (mixed) state, described by $\hat{\rho}$, is identified with the equivalence class $\{\rho\}_{\hat{\rho}}$ of densities with the same second moments and generating the same $\hat{\rho}$ via (5). Equivalence of densities with the same second moments is seen as a generalization of standard quantum mechanical statement about the non-uniqueness of the convex decomposition of a statistical operator $\hat{\rho}$.

The most known physical consequence of the equivalence $\{\rho\}_{\hat{\rho}}$ is no-signaling by distant steering (see for example [19] and the references therein). We shall discuss some related issues later in the context of hybrid quantum-classical systems.

A pure state $\hat{\rho}_0 = |\psi_{X_0}\rangle\langle\psi_{X_0}|$, where $X_0 \in S^{2N-1}/S^1$, is uniquely represented by the corresponding delta function $\delta(X - X_0)$ on S^{2N-1}/S^1. The equivalence class $\{\rho\}_{\hat{\rho}_0}$ indeed contains a single element, i.e., $\delta(X - X_0)$, as can be seen by the following reasoning. Let $\rho_0(X)$ belong to $\{\rho\}_{\hat{\rho}_0}$, i.e.,

$$\hat{\rho}_0 = \int_{\mathcal{M}} \rho_0(X)\hat{\Pi}(X)dM. \tag{8}$$

Choose an arbitrary state $|\psi^{\perp}\rangle$ orthogonal to the state $|\psi_{X_0}\rangle$. Now, one has

$$0 = \langle\psi^{\perp}|\hat{\rho}_0|\psi^{\perp}\rangle = \int_{\mathcal{M}} \rho_0(X)\big|\langle\psi_X \mid \psi^{\perp}\rangle\big|^2 dM. \tag{9}$$

This means that $\rho_0(X)$ is nonzero only when $\langle\psi_X|\psi^{\perp}\rangle = 0$. Because of the arbitrariness of $|\psi^{\perp}\rangle$, the density $\rho_0(X)$ is nonzero only at $X = X_0$ leading to $\rho_0(X) = \delta(X - X_0)$. Thus, a pure state is uniquely represented by single δ-density, i.e., by a single trivial convex combination on S^{2N-1}/S^1.

Each equivalence class $\{\rho\}_{\hat{\rho}}$ of densities over $\mathcal{M} = \mathbb{R}^{2N}$ based on the Hilbert space $\mathcal{H}$, corresponding to a mixed state $\hat{\rho}$, contains a distribution of a unique form and with fixed normalized second moments. Indeed, consider a statistical operator $\hat{\rho}$ which matrix elements in the abstract (arbitrary) basis satisfy

$$\begin{aligned} \mathrm{Re}(\hat{\rho}_{ij}) &= \int_{\mathcal{M}} \rho(X)\frac{x_i x_j + y_i y_j}{\|X\|^2} dM, \\ \mathrm{Im}(\hat{\rho}_{ij}) &= \int_{\mathcal{M}} \rho(X)\frac{y_i x_j - x_i y_j}{\|X\|^2} dM, \end{aligned} \tag{10}$$

where (x_i, y_i) $(i, j = 1, 2 \dots N)$ i.e., X^a $(a = 1, 2 \dots 2N)$ are the components of the Hilbert space vector in the same abstract basis, while $\|X\|^2 = 2\,\|\psi_X\|^2$ holds. All densities from the equivalence class $\{\rho\}_{\hat{\rho}}$ give the same $\hat{\rho}_{ij}$ by definition. The form of $\hat{\rho}_{ij}$ implies that the expectation of any normalized quadratic function $A_{ab}X^a X^b/\|X\|^2$ $(a, b = 1, 2 \dots 2N)$ on $\mathcal{M} = \mathbb{R}^{2N}$ is computable once one finds the normalized covariance matrix of the density ρ

$$\sigma_{\rho}^{ab} = \int_{\mathcal{M}} \rho(X)\frac{X^a X^b}{\|X\|^2} dM \equiv \sigma_{\hat{\rho}}^{ab}, \tag{11}$$

which is the same for any density from the equivalence class $\{\rho\}_{\hat{\rho}}$, and is thus equivalently denoted by $\sigma_{\hat{\rho}}^{ab}$. Next we observe that the following distribution, fixed by (11), over $\mathcal{M} = \mathbb{R}^{2N}$

$$\tilde{\rho}(X) = \frac{\|X\|^2}{(2\pi)^N (\det \sigma_{\hat{\rho}})^{1/2}} \exp\left[-\frac{1}{2}\left(\sigma_{\hat{\rho}}^{-1}\right)_{ab} X^a X^b\right], \tag{12}$$

is a member of the equivalence class $\{\rho\}_{\hat{\rho}}$ because it reproduces the matrix elements (10). Therefore, the only distributions on $\mathcal{M} = \mathbb{R}^{2N}$ that are needed to represent all possible mixed quantum states are of the form (12).

Each equivalence class corresponding to a mixed state could also be represented by other types of distributions. In fact, the distribution given by finite discrete convex combination of delta functions

$$\rho(X) = \sum_{i=1}^{N} \rho_i \delta(X - X_i), \tag{13}$$

where ρ_i are the eigenvalues and X_i correspond to the eigenvectors of the density matrix $\hat{\rho}$, also satisfies (5).

Assume now that the state vectors are normalized, as is customary in the Hamiltonian form of QM. One should be careful with the interpretation of distributions $\rho(X)$ satisfying (5), the function $\langle\psi_X|\hat{\rho}|\psi_X\rangle$ and the quantum mechanical expression $|\langle\psi|\psi'\rangle|^2$. A statistical operator $\hat{\rho}$ is Hermitian and therefore can be formally considered as an observable. The later are represented by the general rule as $\langle\psi_X|\hat{\rho}|\psi_X\rangle$, which we shall denote by $\langle\hat{\rho}\rangle(X)$ in order to distinguish it from the function $\rho(X)$ defined as to satisfy (5). The relation between the two functions is given by

$$\langle\hat{\rho}\rangle(X) = \int_{\mathcal{M}} \rho\left(X'\right) |\langle\psi_{X'}|\psi_X\rangle|^2 dM'. \tag{14}$$

In case of the pure state ensemble $|\psi_{X_0}\rangle\langle\psi_{X_0}|$ uniquely represented by the density $\delta(X - X_0)$, the function $\langle\hat{\rho}\rangle(X)$ is everywhere nonzero except at X corresponding to vectors orthogonal to $|\psi_{X_0}\rangle$. Note that the function $\langle\hat{\rho}\rangle(X)$ cannot be considered as a density on $\mathcal{M}$, representing the quantum ensemble $\hat{\rho}$, because when substituted in (5) it does not give the correct result (4), $\mathrm{Tr}(\hat{\rho}\hat{A})$. In the case $\mathcal{M} = \mathbb{C}P^{N-1}$, the substitution gives [22]

$$\int_{\mathcal{M}} \langle\hat{\rho}\rangle(X) A(X) dM = \frac{V_N}{N(N+1)}\left(\mathrm{Tr}(\hat{\rho}\hat{A}) + \mathrm{Tr}(\hat{A})\right), \tag{15}$$

where V_N is the volume of $\mathbb{C}P^{N-1}$. However, modified function $P(X) = (\langle\hat{\rho}\rangle(X) - 1/(N+1))N(N+1)/V_N$, gives the correct averages [22]. Nevertheless, $P(X)$ is not non-negative for all X even though $\langle\hat{\rho}\rangle(X)$ is. Therefore, $P(X)$ can be used to compute the quantum expectation $\mathrm{Tr}(\hat{\rho}\hat{A})$, but it cannot be considered as a probability density on $\mathbb{C}P^{N-1}$.

Fallacy of the interpretation of the function $\langle\hat{\rho}\rangle(X)$ as a probability distribution for given $\hat{\rho}$ is best seen in the case of a pure state $\hat{\rho}$. Let us be permitted to stress the basic postulate of quantum mechanics concerning the interpretation of the expression $|\langle\psi|\psi'\rangle|^2$. This gives a probability that a system prepared in the state $|\psi\rangle$ with certainty, will transform during measurement of an observable with an eigenvector $|\psi'\rangle$

precisely into the state $|\psi'\rangle$. It is a probability distribution over the eigenbasis of the measured observable and is not a probability distribution over the space of all pure states. Therefore a pure state $|\psi_{X_0}\rangle$ is not represented by function $|\langle\psi_X|\psi_{X_0}\rangle|^2$, but by the probability distribution $\delta(X - X_0)$. Similarly the ensemble $\hat{\rho}$ is represented by some $\rho(X)$ satisfying (5) and not by $\langle\hat{\rho}\rangle(X)$ or $P(X)$.

For further comparison with the Hilbert space formulation one should observe that the set of combinations of delta functions centered at discrete set of points is dense in the space of functionals on the space of continuous functions on $\mathcal{M}$. In other words, any density $\rho(X)$ can be arbitrary well approximated by a finite discrete convex combination of δ-functions

$$\rho(X) = \int_{\mathcal{M}} \rho(X')\delta(X - X')dM' \approxeq \sum_i \rho_{X_i}\, \delta(X - X_i). \tag{16}$$

Approximation of $\rho(X)$ by finite discrete convex combination of delta functions corresponds to a well known ensemble decomposition $\{\rho_{X_i}, |\psi_{X_i}\rangle\}$ of a density matrix in terms of finite convex combination of pure state projectors. We will call such density *discrete*. $\rho(X)$ and $\rho'(X)$ from the same equivalence class $\{\rho\}_{\hat{\rho}}$ correspond to equivalent ensemble decompositions $\{\rho_{X_i}, |\psi_{X_i}\rangle\}$ and $\{\rho'_{X'_i}, |\psi_{X'_i}\rangle\}$ of the density matrix $\hat{\rho}$. They are related by the Hughston-Jozsa-Wooters formula [14]

$$(\rho_{X_i})^{1/2}|\psi_{X_i}\rangle = \sum_j u_{ij}\, (\rho'_{X'_j})^{1/2}|\psi_{X'_j}\rangle, \tag{17}$$

where $[u_{ij}]$ is unitary matrix of appropriate (not necessary equal) dimensions.

The preceding analysis implies the following generalization of (17) to the case of arbitrary equivalent continuous densities $\rho(X)$ and $\rho'(X)$ from the same equivalence class $\{\rho\}_{\hat{\rho}}$

$$(\rho(X))^{1/2}|\psi_X\rangle = \int_{\mathcal{M}} u(X|X')\, (\rho'(X'))^{1/2}|\psi_{X'}\rangle dM', \tag{18}$$

where $u(X|X')$ is a complex integral kernel satisfying

$$\int_{\mathcal{M}} u(X|X')\, u^*(X|X'')\, dM = \delta(X' - X''), \tag{19}$$

and * denotes complex conjugation.

3.2 Hamiltonian Dynamics of Densities

Since this paper is about applications of the theory of Hamiltonian dynamical systems in QM and in hybrid theories, let us mention in passing that von-Neumann and Liouville equations themselves can be presented in the form of appropriate Hamiltonian dynamical systems [16]. Considerations of these issues reveal from another perspective the importance and the consequences of the QM restriction on the class of functions generating the structure isomorphisms.

The Lie algebra g of the infinite Lie group $\mathcal{G}$ of canonical transformations on some finite dimensional symplectic phase space $\mathcal{M}$ consists of the Hamiltonian vector fields on $\mathcal{M}$, and is isomorphic with the Lie algebra of smooth functions $C^\infty(\mathcal{M})$. The dual of $C^\infty(\mathcal{M})$ is the coadjoint algebra g^* isomorphic with the space of densities $\rho \in S(\mathcal{M})$. The paring is given by $\int_\mathcal{M} \rho(X)H(X)dM$. In order to present the Liouville equation $\dot{\rho} = -\{\rho, H\}_\mathcal{M}$ as a Hamiltonian dynamical system one follows the standard construction of the symplectic structure on a coadjoint orbit O_ρ of the Lie group $\mathcal{G}$ [16]. First, a Poisson structure is defined on S as

$$\{\mathcal{H}_1(\rho), \mathcal{H}_2(\rho)\}_S = \int_\mathcal{M} \rho \left\{\frac{\delta\mathcal{H}_1}{\delta\rho}, \frac{\delta\mathcal{H}_2}{\delta\rho}\right\}_\mathcal{M} dM = \int_\mathcal{M} \rho\{H_1, H_2\}_\mathcal{M} dM, \tag{20}$$

where $\mathcal{H}_i(\rho) = \int_\mathcal{M} \rho H_i dM$. Hamiltonian vector fields on S are given by $X_\mathcal{H}(\rho) = -\{\rho, \frac{\delta\mathcal{H}}{\delta\rho}\}_S$. The Poisson structure (20) on S is degenerate, but its restriction on an orbit of $\mathcal{G}$ in S

$$O_\rho = \{\rho \circ \lambda \,|\, \lambda \in \mathcal{G}\} \tag{21}$$

gives the desired symplectic structure on O_ρ.

The Liouville equation appears as a Hamiltonian system on O_ρ with the corresponding Hamiltonian $\mathcal{H}(\rho) = \int_\mathcal{M} \rho H dM$ and the Hamiltonian equations

$$\dot{\rho} = -\{\rho, \mathcal{H}\}_{O_\rho} = \{H, \rho\}_\mathcal{M}. \tag{22}$$

The Hamiltonian system (22) is linear and therefore integrable.

Consider now the above formalism appropriate for QM, where the preservation of the Riemannian structure of $\mathcal{M}$ introduces the corresponding restrictions on $\mathcal{G}$, g and g^*. The structure isomorphism group $\mathcal{G}_q$ is the finite subgroup of canonical transformations generated by quadratic functions on $\mathcal{M}$. This is isomorphic to the unitary group $U(N)$. The group Lie algebra g_q is the Lie algebra of quadratic functions, and the coadjoint algebra g_q^* is formed by the equivalence classes $\rho_{\hat{\rho}}$. The coadjoint orbit through $\hat{\rho}$ is isomorphic with finite-dimensional manifold

$$U(N)/U(k_1) \otimes U(k_2) \otimes \cdots \otimes U(k_m),\ k_1 + k_2 + \cdots + k_m = N, \tag{23}$$

where $k_1, k_2, \ldots, k_m$ are dimensions of the eigenspaces of $\hat{\rho}$. The orbit $O_{\hat{\rho}}$, given by (23), is a finite-dimensional symplectic manifold, whose dimension depends on the spectrum of $\hat{\rho}$. The symplectic structure on $O_{\hat{\rho}}$ may be introduced as in the general case, and the von Neumann equation for $\hat{\rho}$ is seen as the Hamilton dynamical equation (22).

3.3 Mixtures as States of Subsystems

Consider a quantum system composed of two subsystems, with Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ of the components and $\mathcal{H}_{12} = \mathcal{H}_1 \otimes \mathcal{H}_2$ of the total system. Partial trace $\mathrm{Tr}_2(\hat{\rho})$ of a pure $\hat{\rho} = |\psi_{12}\rangle\langle\psi_{12}|$ over the space $\mathcal{H}_2$ gives a density operator $\hat{\rho}_1$ on $\mathcal{H}_1$. The operator $\hat{\rho}_1$ is a projector corresponding to a pure state $|\psi_1\rangle \in \mathcal{H}_1$ if an only if the pure state of the total system $\hat{\rho} = |\psi_{12}\rangle\langle\psi_{12}|$ is separable, i.e., of the form $|\psi_1\rangle \otimes |\psi_2\rangle$ for some $|\psi_1\rangle \in \mathcal{H}_1$ and $|\psi_2\rangle \in \mathcal{H}_2$. In this case $\hat{\rho}_1 = |\psi_1\rangle\langle\psi_1|$ does not depend on the particular $|\psi_2\rangle$ in $|\psi_{12}\rangle\langle\psi_{12}|$. In the case of a more general non-entangled state, i.e., for a convex mixture of separable states of the form $\hat{\rho} = \sum_i p_i \hat{\rho}_1^i \otimes \hat{\rho}_2^i$, the partial trace $\mathrm{Tr}_2(\hat{\rho})$ gives a convex mixture of the first subsystem states $\hat{\rho}_1^i$ with the same coefficients p_i.

We now consider statistical ensembles in the Hamiltonian formulation of composite systems. The phase space $\mathcal{M}_{12}$ of a bipartite quantum system with the Hilbert space $\mathcal{H}_{12}$ is constructed directly from $\mathcal{H}_{12}$ (or $P\mathcal{H}_{12}$) without any reference to the components $\mathcal{H}_1$ and $\mathcal{H}_2$ with the corresponding phase spaces $\mathcal{M}_1$ and $\mathcal{M}_2$. Of course, the dimensionality of $\mathcal{M}_{12}$ is much larger than that of $\mathcal{M}_1 \times \mathcal{M}_2$. In fact, $\mathcal{M}_1 \times \mathcal{M}_2$ is an embedded submanifold of $\mathcal{M}_{12}$. In the case $\mathcal{M}_1 = \mathbb{C}P^{N-1}$, $\mathcal{M}_2 = \mathbb{C}P^{M-1}$ and $\mathcal{M}_{12} = \mathbb{C}P^{MN-1}$ the embedding $\mathbb{C}P^{N-1} \times \mathbb{C}P^{M-1} \to \mathbb{C}P^{MN-1}$ is known as Segre embedding [5, 23]. We shall denoted the coordinates $\{X^a\}$ adapted to the Segre embedding by (X_1, X_2, X_3) where X_1 and X_2 are the sets of coordinates on $\mathcal{M}_1 \times \mathcal{M}_2$. The set of coordinates denoted by X_3 assume zero values iff the state is separable.

A statistical ensemble of bipartite systems is described by a probability density $\rho(X) \in S(\mathcal{M}_{12})$. A density on $\mathcal{M}_{12}$ gives a statistical operator on $\mathcal{H}_{12}$ according to the general prescription:

$$\hat{\rho}_{12} = \int_{\mathcal{M}_{12}} \rho_{12}(X_{12})\, \hat{\Pi}(X_{12})\, dM_{12}. \tag{24}$$

Mixed state $\hat{\rho}_{12}$ is separable if there exists a convex mixture representation (24) of $\hat{\rho}_{12}$ in terms of separable pure states. If each of the equivalent convex representations contains at least one entangled pure state then $\hat{\rho}_{12}$ is entangled. Therefore, it makes sense to call a density ρ_{12} separable if $\rho_{12}(X_1, X_2, X_3)$ is zero when $X_3 \neq 0$, that is when it's support is contained in $\mathcal{M}_1 \times \mathcal{M}_2$. Such densities will be denoted by $\rho(X_1, X_2)$. If any of the densities in the equivalence class $\{\rho_{12}\}_{\hat{\rho}_{12}}$ is separable then $\hat{\rho}_{12}$ is by definition separable. On the other hand, if $\hat{\rho}_{12}$ is entangled then none of the densities in the equivalence class $\{\rho_{12}\}_{\hat{\rho}_{12}}$ is separable, and each must have an entangled state in its support. However, notice that some of the densities from a single equivalence class, corresponding to a separable mixed state $\hat{\rho}_{12}$, might be separable and some might not. In one word, it is misleading to talk about entangled densities, but the notion of a separable density is perfectly consistent with the standard terminology.

Let us demonstrate the standard relations between the state of a compound system and the state of the first subsystem using the representation (24). We perform a partial trace over the second subsystem

$$\hat{\rho}_1 = \mathrm{Tr}_2(\hat{\rho}_{12}) = \int_{\mathcal{M}_{12}} \rho_{12}(X_{12}) \mathrm{Tr}_2\big(\hat{\Pi}(X_{12})\big) dM_{12}. \tag{25}$$

Let $\mathcal{D}_1$ denotes the manifold of the density matrices $\hat{\sigma}_1$ of the first subsystem and let $\delta_\sigma^{(1)}$ and $dM_\sigma^{(1)}$ be delta function and Lebesgue measure on $\mathcal{D}_1$. By inserting the identity[1]

$$\int_{\mathcal{D}_1} \delta_\sigma^{(1)}\bigl(\hat{\sigma}_1 - \mathrm{Tr}_2\bigl(\hat{\Pi}(X_{12})\bigr)\bigr) dM_\sigma^{(1)} = 1, \tag{26}$$

into (25) we express $\hat{\rho}_1$ as a convex combination of density matrices of the first subsystem

$$\hat{\rho}_1 = \int_{\mathcal{D}_1} \rho_1(\hat{\sigma}_1)\hat{\sigma}_1 dM_\sigma^{(1)}, \tag{27}$$

where the distribution ρ_1 over $\mathcal{D}_1$ is normalized to unity and obeys

$$\rho_1(\hat{\sigma}_1) = \int_{\mathcal{M}_{12}} \rho_{12}(X_{12})\delta_\sigma^{(1)}\bigl(\hat{\sigma}_1 - \mathrm{Tr}_2\bigl(\hat{\Pi}(X_{12})\bigr)\bigr) dM_{12}. \tag{28}$$

In the case of a pure state $\hat{\rho}_{12} = \hat{\Pi}(\bar{X}_{12})$ which is represented by the delta density $\rho_{12}(X_{12}) = \delta(X_{12} - \bar{X}_{12})$, one obtains

$$\rho_1(\hat{\sigma}_1) = \delta_\sigma^{(1)}\bigl(\hat{\sigma}_1 - \mathrm{Tr}_2(\hat{\rho}_{12})\bigr), \tag{29}$$

which is expected.

The result (28) can be further analyzed. Let $\hat{\Pi}(X_{12}) = |\psi_{X_{12}}\rangle\langle\psi_{X_{12}}|$ in terms of normalized state vectors. Using the Schmidt decomposition $|\psi_{X_{12}}\rangle = \sum_{i=1}^{R_{12}} \sqrt{p_i}\,|\phi_i^{(1)}\rangle \otimes |\chi_i^{(2)}\rangle$, with $p_i > 0$, one obtains mixed state $\mathrm{Tr}_2(\hat{\Pi}(X_{12})) = \sum_{i=1}^{R_{12}} p_i |\phi_i^{(1)}\rangle\langle\phi_i^{(1)}|$, where $R_{12} = \mathrm{Rank}(\mathrm{Tr}_2(\hat{\Pi}(X_{12})))$. Any other state $|\psi_{X_{12}^\lambda}\rangle$ such that $\mathrm{Tr}_2(\hat{\Pi}(X_{12}^\lambda)) = \mathrm{Tr}_2(\hat{\Pi}(X_{12}))$ has the form $|\psi_{X_{12}^\lambda}\rangle = \sum_{i=1}^{R_{12}} \sqrt{p_i}\,|\phi_i^{(1)}\rangle \otimes |\chi_{i,\lambda}^{(2)}\rangle$, and can be obtained as a result of unitary transformation acting non-trivially on the second subsystem $|\psi_{X_{12}^\lambda}\rangle = \hat{U}_\lambda|\psi_{X_{12}}\rangle$. Such transformation induces the corresponding action $X_{12}^\lambda = U_\lambda X_{12}$ on $\mathcal{M}_{12}$ and yields the following equivalent form of (28)

$$\rho_1(\hat{\sigma}_1) = \int_{\Lambda(\hat{\sigma}_1)} \rho_{12}(U_\lambda \widetilde{X}_{12}) d\lambda, \tag{30}$$

where λ parameterizes the space $\Lambda(\hat{\sigma}_1) \cong U(M)/U(M - \mathrm{Rank}(\hat{\sigma}_1))$ and $\widetilde{X}_{12} \in \mathcal{M}_{12}$ is an arbitrary state satisfying $\mathrm{Tr}_2(\hat{\Pi}(\widetilde{X}_{12})) = \hat{\sigma}_1$.

We now want to consider a possible analog of the partial trace formulated entirely in terms of the Hamiltonian densities and marginal distributions. We shall first consider the cases when the total quantum state $\hat{\rho}_{12}$ is separable pure or mixed. General ensembles are represented by densities on $\mathcal{M}_{12}$ denoted by $\rho_{12}(X)$. In the coordinates X_1, X_2, X_3 adapted to the Segre embedding the densities are written as $\rho_{12}(X) = \rho_{12}(X_1, X_2, X_3)$. In order to treat the separable states it is enough to consider probability densities with the support on $\mathcal{M}_1 \times \mathcal{M}_2$ i.e., densities dependent only on X_1, X_2. This is obvious if the state is pure, and if the state is mixed then there

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[1] We are grateful to the referee for this observation and its consequences.

is at least one convex representation of it with the density having the stated property. Ensemble of pure states X_0, corresponding to the pure $\hat{\rho}_{12} = \hat{\Pi}(X_0)$, is represented by the delta function centered at X_0. In the coordinates X_1, X_2, X_3 adapted to the Segre embedding, the ensemble of pure separable states X_0 is represented by $\rho_{12}(X_1, X_2) = \delta(X_1 - X_{01})\delta(X_2 - X_{02})$. If the state is mixed separable then it can be represented by a density of the form $\rho(X) = \rho(X_1, X_2)$. Integration over X_2 in the pure separable case gives

$$\begin{aligned} &\int_{\mathcal{M}_2} \delta(X_1 - X_{01})\delta(X_2 - X_{02})dM_2 = \delta(X_1 - X_{01}), \\ &\qquad \text{separable pure } \hat{\rho}_{12} = \hat{\Pi}(X_0). \end{aligned} \tag{31}$$

The result is a delta density on $\mathcal{M}_1$ which reproduces, via the general formula (5), the reduced matrix $\mathrm{Tr}_2(\hat{\Pi}(X_0))$. Similarly, in the mixed separable case the integration over X_2 gives a density on $\mathcal{M}_1$

$$\rho_1(X_1) = \int_{\mathcal{M}_2} \rho(X_1, X_2)dM_2, \quad \text{separable mixed } \hat{\rho}_{12}, \tag{32}$$

which reproduces $\mathrm{Tr}_2(\hat{\rho}_{12})$ if $\rho(X_1, X_2)$ reproduces $\hat{\rho}_{12}$. We see that the analog of the partial trace in the case of separable state, pure or mixed, is provided by taking the marginal distribution of the appropriate distribution on the total phase space.

However, the analogy does not work for entangled states. In fact, consider a pure entangled state, represented by the delta density $\rho_{12}(X; X_0) = \delta(X_1 - X_{01})\delta(X_2 - X_{02})\delta(X_3 - X_{03})$. Integration over X_2, X_3 gives, up to a function dependent on X_0, the delta function of $X_1 - X_{01}$

$$\begin{aligned} &\rho_1(X_1; X_0) = \int_{X_2, X_3} \rho_{12}(X_1, X_2, X_3; X_0)dX_2dX_3 = \delta(X_1 - X_{01})g(X_0) \\ &\qquad \text{entangled pure } \hat{\rho}_{12} = \hat{\Pi}(X_0), \end{aligned} \tag{33}$$

which is proportional to the density that represents a pure state in $\mathcal{H}_1$, and not the reduced mixed state.

The general conclusion of this analysis is that if the state of the total system is separable then the marginal distribution of a specific probability distribution reproducing the state of the total system, reproduces the reduced density matrix of the subsystem. Evolution of such reduced density will preserve this property if the Hamiltonian does not entangle the two subsystems. In this case, arbitrary transformations or approximations of the second subsystem density do not effect the evolution of the first subsystem. The case of separable bipartite states is specially important for hybrid systems, when one of the parts is treated as a classical system, since in the Hamiltonian hybrid theory, presented in the next Section, there can be no entanglement between the classical and the quantum parts. On the other hand, if the initial total state of a bipartite quantum system is entangled, or becomes entangled due to the evolution, then the states of the subsystems are not given simply in terms of the marginal distributions.

4 Ensembles of Hybrid Systems

There is no unique generally accepted theory of interaction between micro and macro degrees of freedom, where the former are described by quantum and the later by classical theory. The reason is primarily because each of the suggested theories has some unexpected or controversial features (see [10] for an informative review). Partial selection of hybrid theories can be found in [24–29]. Some of the suggested hybrid theories are mathematically inconsistent, and "no go" type theorems have been formulated [30], suggesting that no consistent hybrid theory can be formulated. Nevertheless, mathematically consistent but inequivalent hybrid theories exist [10, 28, 29]. Even the proper conceptual status and putative domains of application of hybrid theories need not be unique and are not generally agreed upon. Hybrid theories that attempt to describe the quantum measurement process or serve as approximate but consistent models in quantum chemistry or model the interaction between classical gravity and quantized matter might be fundamentally different or differ only in some additional details. Usually, it is not claimed that macroscopic systems are composed of something other that microscopic parts well described by quantum theory. However it is legitimate to assume that dynamics of at least some of the observable degrees of freedom of a macroscopic system are correctly described by classical mechanics, and that the classical mechanical description need not be reduced or derived from quantum description of all the microscopic components. Neither quantum nor classical theory is designed to describe the dynamics of systems consisting of micro and macro subparts, as separately described by the quantum and the classical mechanics respectively.

The Hamiltonian hybrid theory, as formulated and discussed for example in [10–13, 31], has many of the properties commonly expected of a good hybrid theory. In fact, the dynamical formulas of the Hamiltonian theory are equivalent to the well known mean field approximation, the main novelty being that the theory is formulated entirely in the framework of the theory of Hamiltonian dynamical systems. In particular, this demonstrates that the theory is mathematically consistent. However, the theory also has some controversial features concerning the class of mathematical objects that should be interpreted as physical variables and the most general type of states of the hybrid system. In what follows we shall first briefly recapitulate the Hamiltonian formulation of the hybrid systems and present the dynamical laws for pure states and for ensembles of hybrid systems. Unlike the purely quantum case, the dynamics of hybrids in pure states is nonlinear and the dynamics of densities involves the most general class of statistical ensembles. Therefore, one needs to discuss the possibility of superluminal communication between hybrid systems.

Hamiltonian theory of hybrid systems can be developed starting from the Hamiltonian formulation of a composite quantum system and imposing a constraint that one of the components is behaving as a classical system [12]. The result, in the macro-limit imposed on the constrained subsystem, turns out to be equivalent to a Cartesian product of two Hamiltonian systems as in [10]. One of these Hamiltonian systems corresponds to the quantum and one to the classical subsystem of the hybrid. However, the interaction between the two subsystems has crucial influence on their properties.

The space of pure states of the hybrid system $\mathcal{M}$ is considered as a Cartesian product $\mathcal{M} = \mathcal{M}_c \times \mathcal{M}_q$ of the classical subsystem phase space $\mathcal{M}_c$ and of the quantum subsystem phase space $\mathcal{M}_q$. Local coordinates on the product are denoted $\{p, q, x, y\}$, where $(p, q) \in \mathcal{M}_c$ will be called the classical degrees of freedom (CDF) and $(x, y) \in \mathcal{M}_q$ will be called the quantum degrees of freedom (QDF). The constraint that CDF behave as a classical system implies that there is no entanglement between QDF and CDF, but no restriction on the entanglement in QDF is imposed. The evolution equations of the hybrid system are of the Hamiltonian form with the Hamilton's function comprised of three terms

$$H_t(p, q, x, y) = H_c(p, q) + H_q(x, y) + V_{int}(p, q, x, y), \tag{34}$$

where H_c is the Hamilton's function of the classical subsystem, $H_q(x, y) = \langle\psi_{x,y}|\hat{H}_q|\psi_{x,y}\rangle$ is the Hamilton's function of the quantum subsystem and $V_{int}(p, q, x, y) = \langle\psi_{x,y}|\hat{V}_{int}(p, q)|\psi_{x,y}\rangle$ describes the interaction between the subsystems, where $\hat{V}_{int}(p, q)$ is an operator in the Hilbert space of the quantum subsystem which depends on the classical coordinates (p, q). The state vectors $|\psi_{x,y}\rangle$ are normalized by assumption. The Poisson bracket on $\mathcal{M}$ of arbitrary functions of the local coordinates (p, q, x, y) is defined as

$$\{F_1, F_2\}_{\mathcal{M}} = \sum_{i=1}^{n_c}\left(\frac{\partial F_1}{\partial q_i}\frac{\partial F_2}{\partial p_i} - \frac{\partial F_2}{\partial q_i}\frac{\partial F_1}{\partial p_i}\right) + \sum_{j=1}^{n_q}\left(\frac{\partial F_1}{\partial x_j}\frac{\partial F_2}{\partial y_j} - \frac{\partial F_2}{\partial x_j}\frac{\partial F_1}{\partial y_j}\right), \tag{35}$$

where n_c and n_q are numbers of CDF and QDF respectively. Of course, if the Hilbert space of the quantum part is of infinite dimension then n_q is infinite. Thus, the Hamiltonian form of the hybrid dynamics on $\mathcal{M}$ as the phase space reads

$$\dot{q} = \{q, H_t\}_{\mathcal{M}}, \qquad \dot{p} = \{p, H_t\}_{\mathcal{M}}, \tag{36}$$

$$\dot{x} = \{x, H_t\}_{\mathcal{M}}, \qquad \dot{y} = \{y, H_t\}_{\mathcal{M}}, \tag{37}$$

where H_t is given by (34).

In particular, the evolution of QDF can be stated in the form of the Schrödinger equation

$$i\hbar\partial_t|\psi_{x,y}\rangle = \hat{H}_{qc}(p, q)|\psi_{x,y}\rangle, \tag{38}$$

with the Hamiltonian operator $\hat{H}_{qc}(p, q) = \langle p, q|\hat{H}|p, q\rangle$ acting on the Hilbert space of quantum subsystem and depending parametrically on the CDF (p, q) through the coherent states $|p, q\rangle$. The evolution of the state vectors (38) is norm-preserving, but nonlinear.

It is worth noticing that the state of QDF in a hybrid system might have nonzero entanglement. We tested this using as an example a pair of 1/2-spins in interaction with a 2D classical oscillator. The interaction between QDF and CDF couples the classical coordinates with the spins components $\sigma^{1,2}_{x,y,z,}$. It turns out that the concurrence of the pure state of the two spins displays nontrivial dynamics and is often nonzero.

Thus, QDF of the hybrid model display some typically quantum properties and evolve nonlinearly in the same time. Furthermore, the Poisson bracket (35) of two functions $F_1(p,q,x,y)$ and $F_2(p,q,x,y)$ which are both quadratic in QDF and depend on CDF, is not a function quadratic in the QDF. However, the proper interpretation of this fact is nontrivial. Let us first reexamine the situation in the purely quantum case with linear evolution and normalized state vectors. There, a quadratic function $A(x,y)=\langle\psi_{x,y}|\hat{A}|\psi_{x,y}\rangle$ was considered as mathematical representative of a dynamical variable, and the set of quadratic functions is invariant under the evolution. Thus, in the purely quantum case, the evolution of a quadratic function can be interpreted as the Heisenberg picture of the evolution of a dynamical variable or as the Schrödinger picture of the expectation of the variable in an evolving state. On the other hand, in the Hamiltonian hybrid theory one can stick to the original interpretation of $A(x,y)$ as the expectation of the observable $\hat{A}$ in the state $|\psi_{x,y}\rangle$. One could then argue that the Heisenberg picture of the hybrid evolution is not defined, and the non-quadratic expression $A(x,y;t)=\langle\psi_{x,y}(t)|\hat{A}|\psi_{x,y}(t)\rangle$ should be interpreted as the expectation value of the standard Schrödinger quantum variable in the state $|\psi_{x,y}(t)\rangle$ at time t. Nevertheless, the nonlinear evolution of the QDF shows that QDF of a hybrid system do not have all the properties of a purely quantum system. Hybrid systems appear to be qualitatively different from a simple union of classical and quantum systems [10, 12, 13, 31]. This is further illustrated by studying the evolution of ensembles of hybrid systems.

The most general ensemble of hybrid systems is represented by some probability density $\rho(p,q,x,y)$. As pointed out in Sect. 3.1, the function ρ should not be considered as an expectation $\langle\hat{\rho}(q,p)\rangle$ of some density operator $\hat{\rho}(q,p)$ parametrically dependent on (q,p). The densities evolve according to the Liouville equation with a solution $\rho(p,q,x,y;t)$. As in Sect. 3.2, this Liouville equation for the hybrid system is itself a Hamiltonian dynamical system. The density $\rho(p,q,x,y;t)$ for any fixed t generates a unique positive operator valued function (POVF):

$$\hat{\rho}(p,q;t)=\int_{\mathcal{M}_q}\rho(p,q,x,y;t)\hat{\Pi}(x,y)dM_q, \tag{39}$$

which can be called the hybrid statistical operator. The unconditional mixed state of the quantum subsystem of the hybrid in the state $\rho(p,q,x,y;t)$ is also uniquely obtained as

$$\hat{\rho}(t)=\int_{\mathcal{M}}\rho(p,q,x,y;t)\hat{\Pi}(x,y)dM\equiv\int_{\mathcal{M}_q}\rho_q(x,y;t)\hat{\Pi}(x,y)dM_q, \tag{40}$$

where the marginal distribution $\rho_q(x,y;t)$

$$\rho_q(x,y;t)=\int_{\mathcal{M}_c}\rho(p,q,x,y;t)dM_c \tag{41}$$

can be considered as the probability density on $\mathcal{M}_q$ associated with the state $\hat{\rho}(t)$ of QDF. Due to the properties of the Liouville evolution of $\rho(p,q,x,y;t)$, the formula (40) defines for all t a continuous one-parameter family of statistical operators on $\mathcal{H}$. Like in the purely quantum case, $\hat{\rho}(t)$ and $\rho(p,q,x,y;t)$ give the same expectation

$\mathrm{Tr}(\hat{\rho}(t)\hat{A}) = \int \rho A(x, y) dM$ of quantum observables $\hat{A}$ represented by $A(x, y)$. All that was said about many-to-one relation between ρ and $\hat{\rho}$ in the quantum case applies also in the hybrid case.

However, contrary to the purely quantum case, different $\rho(p, q, x, y; t_0)$ that give the same $\hat{\rho}(t_0)$ generate different evolution of $\hat{\rho}(p, q; t)$ (or $\hat{\rho}(t)$) and thus must be considered as physically different (for a related analysis please see [30, 31]). Indeed, the evolution equation satisfied by $\hat{\rho}(p, q; t)$ [13] is

$$\begin{aligned} \frac{\partial \hat{\rho}(p, q; t)}{\partial t} &= \frac{1}{i\hbar}\big[\hat{H}_q + \hat{V}_{int}(p, q), \hat{\rho}(p, q; t)\big] + \big\{H_c(p, q), \hat{\rho}(p, q; t)\big\}_{p,q} \\ &\quad + \int_{\mathcal{M}_q} \big\{V_{int}(p, q, x, y), \rho(p, q, x, y; t)\big\}_{p,q} \hat{\Pi}(x, y) dM_q. \end{aligned} \tag{42}$$

The dynamical equation for $\hat{\rho}(t)$ is

$$\frac{d\hat{\rho}(t)}{dt} = \frac{1}{i\hbar}\big[\hat{H}_q, \hat{\rho}(t)\big] + \frac{1}{i\hbar}\int_{\mathcal{M}_c} \big[\hat{V}_{int}(p, q), \hat{\rho}(p, q; t)\big] dM_c. \tag{43}$$

The first term of (43) generates the unitary part of the evolution and the second term does not preserve the norm of $\hat{\rho}$ and is responsible for non-unitary effects. Notice that the evolution of $\hat{\rho}(p, q; t)$ ($\hat{\rho}(t)$) cannot be expressed only in terms of $\hat{\rho}(p, q; t)$ ($\hat{\rho}(t)$), but irreducibly involves the probability density $\rho(p, q, x, y; t)$. At this point we might remark that the von Neumann entropy of $S_{vN} = \mathrm{Tr}(\hat{\rho} \ln \hat{\rho})$ of (40) can increase and decrease during the evolution (43) starting from a general initial ensemble. However, this is not an instance of the Peres objection [21] against nonlinear evolution of a quantum system since the QDF form an open dynamical system. On the other hand the Gibbs entropy $S(\rho) = \int_{\mathcal{M}} \rho \ln \rho \, dM$ is conserved by the Liouville evolution of the total density.

The evolution equation for $\hat{\rho}(t)$ is reduced to (36) and (37) if the initial $\rho(p, q, x, y; t_0)$ is a pure state in $\mathcal{M}$. This is intuitively clear since there can be no entanglement between QDF and CDF. Formally, pure initial state is represented as a delta function on the total phase space and the Liouville equation is reduced to the Hamilton equations for pure states. If however, the initial density is of the form $\delta(x - x_0)\delta(y - y_0)\rho(q, p)$ the pure state $\hat{\rho}(t_0) = |\psi(t_0)\rangle\langle\psi(t_0)|$ might evolve according to (43) into a non-pure mixture. Quantum-classical interaction with the classical part in the initially mixed state can transform an initially pure state of the quantum part into a mixed state. This is an important observation.

The evolution of QDF of a hybrid system is fundamentally different from the linear evolution of a quantum subsystem of a quantum system. The reason for this qualitative difference is that dynamical influences of many degrees of freedom corresponding to the entangled states and to the non-classical states of the classical subsystem are completely neglected in the derivation of the hybrid dynamics.

The characteristic main features of the QDF evolution in the hybrid case are expressed by the nonlinearity of the pure state evolution, or by the dynamically induced differences of $\hat{\rho}(t)$ with different convex mixture representations. It is well known [19, 20], that the linearity of the Schrödinger equation and the equivalence of different convex mixtures, are both necessary in order to prevent superluminal communication in ordinary quantum mechanics of bipartite systems. If either of the two properties is violated, without further modification of the quantum formalism, superluminal communication between entangled parts of a bipartite system is possible. The nonlinear pure state evolution and the evolution dependence on the initially equivalent different ensembles appear quite naturally in the Hamiltonian description of hybrid systems, and in the same time the QDF of the hybrid might be in an entangled state. Therefore, superluminal communication can be avoided only by some further modification of the hybrid theory. It has been argued that the direct product might not be the natural type of coupling between systems with nonlinear evolution [19], and that nonlinear evolution might suggest non-standard computation of correlations [32]. Alternatively, one might consider the model of hybrid systems presented here as insufficient to describe fully the true features of coupled real quantum and macroscopic classical systems. One might resort to *ad hoc* modifications of the hybrid evolution by introducing dissipation and stochastic terms [33, 34] or one might explore the possibilities opened up by replacing a simple classical system by truly complex classical systems with many degrees of freedom [10, 34].

Finally, we would like to stress that the presented theory of quantum-classical interaction does not provide a description of the quantum measurement process (for a discussion of this opinion see [35]) if the total system is initially in a pure state. The Hamiltonian system (36) and (37) with, for example $H_q(x,y)=0$ and $H_c(p,q)=0$, but with a nonzero interaction, for example $H_{int}(p,q,x,y)=cx^2p$, where c is a coupling constant, can describe "classical measurement" of a quantity $A(x)=x^2$ by the meter given by the variable conjugate to p, that is by q. In fact $q(t)$ and the initial x_0 get correlated as $q(t)=cx_0^2t$ and thus reading of $q(t)$ at some t is a measurement of x_0^2. However, the result of such "classical measurement", i.e., $A(x,y)$, is the expectation of the observable $\hat{A}$, and not one of its eigenvalues, as it should be in ideal quantum measurement on a single system. Only if the initial state of the QDF is an eigenstate of $\hat{A}$ with eigenvalue a_1, the quantum-classical interaction can give the eigenvalue a_1. An arbitrary initial state of the QDF, for example a superposition of a_1 and a_2 eigenstates would lead to $q(t)$ corresponding to the average of the eigenvalues. In conclusion, the proper quantum measurement process seems to involve dynamical entanglement between the quantum system and the apparatus, which, once entangled with the system, must be considered in some sense complex and classical. The initial entanglement is impossible in the present model of quantum-classical interaction, which treats the macroscopic apparatus as completely described by the classical theory from the beginning. On the other hand, in order to reproduce the results of ideal quantum measurement by quantum-classical interaction one could contemplate the hybrid systems as effectively dissipative, supplementing the Hamiltonian model with the attractors indicating the eigenvalues of the quantum observable.

5 Summary

We have explored relations between properties of quantum mixed states as represented by statistical operators or by density distributions on the phase space in the Hamiltonian formulation of quantum mechanics and hybrid systems. Some consequences of the fact that in general many density functions correspond to a single statistical operator are discussed. Liouville and von Neumann evolution equations are seen as Hamiltonian dynamical systems. This perspective additionally illustrates the restriction imposed on a general Hamiltonian system if it is to represent a physical system with quantum mechanical properties. We then explored representation of the partial trace operation in terms of partial integration over the relevant variables in the Hamiltonian formulation. Our main objective was to analyze ensembles of hybrid quantum-classical systems in the Hamiltonian formulation. In this context relation between the evolution of the quantum degrees of freedom in a pure state and in a mixed state is explored. The quantum degrees of freedom of a hybrid in a pure state evolve nonlinearly and if the hybrid is in a mixed state different convex representations must be considered as nonequivalent because they evolve differently.

Linear evolution of QM, and invariance of the evolution of $\hat{\rho}$ on different convex representations, need to be abandoned if the effects of interaction with CDF, like those occurring during measurements, are to be described dynamically. On the other hand, QM treatment of composite systems is adapted to the linear evolution, and if the later is replaced by a nonlinear one, the kinematic properties of the composite QM systems have to be modified as well. The needed modification of the kinematic properties of quantum composite systems is not supplied by the presented Hamiltonian hybrid theory. Furthermore, the theory does not describe the measurement process. It is fair to say that the Hamiltonian hybrid theory, in its presented form, does not describe the quantum-classical interaction successfully. In fact the QC interaction is treated in an oversimplified manner, because the macro-object in interaction with QDF is considered as fully described by a small subset of distinguished degrees of freedom which are described classically. A large number of degrees of freedom of the macroscopic object which also interact with the quantum system are completely neglected. The presented form of the Hamiltonian hybrid theory must be modified in order to incorporate the effects of these degrees of freedom. It is our belief that such modifications will result in a hybrid theory which is consistent and whose predictions are closer to the experimentally observed facts.

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