Statistical ensembles in the Hamiltonian formulation of hybrid quantum-classical systems

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General statistical ensembles in the Hamiltonian formulation of hybrid quantum-classical systems are analyzed. It is argued that arbitrary probability densities on the hybrid phase space must be considered as the class of possible physically distinguishable statistical ensembles of hybrid systems. Nevertheless, statistical operators associated with the hybrid system and with the quantum subsystem can be consistently defined. Dynamical equations for the statistical operators representing the mixed states of the hybrid system and its quantum subsystem are derived and analyzed. In particular, these equations irreducibly depend on the total probability density on the hybrid phase space.

Hybrid quantum-classical (QC) systems are neither quantum nor classical. There is no unique generally accepted theory of the QC systems, primarily because each of the suggested theories has some unexpected or controversial features [1–5]. Current technologies are sufficiently developed to enable experimental studies of the interaction between typically quantum and typically classical objects [6]. The choice of the proper hybrid theory will ultimately depend on the experimental tests, but such experiments require detailed preliminary theoretical models. It is plausible to expect that the interaction between the classical and the quantum subsystems might introduce features that are not present either in the quantum or in the classical subsystems without interaction (see for example [1]). In this Brief Report we shall explore some features of the hybrid system theory which is formulated using the framework of Hamiltonian dynamical systems [1,2,7].

The Hamiltonian hybrid theory, as formulated for example in Ref. [1], has many of the properties commonly expected of a good hybrid theory. However, it also has some controversial features concerning the class of mathematical objects that should be interpreted as physical variables of the QC system. Also, what should be mathematical objects that represent the most general statistical ensembles of QC systems and the corresponding mixtures of the quantum subsystems is not trivially obvious and needs a careful discussion. Formally, the problem is inherited from the surplus structure present in the Hamiltonian formulation of the quantum mechanics. It can be argued that what must be considered as nonphysical in the Hamiltonian formulation of the standard linear quantum mechanics might acquire physical meaning for the QC system because of the presence of the classical subsystems and the quantum-classical interaction.

In what follows we shall first briefly recapitulate the Hamiltonian formulation of quantum mechanics and of the hybrid quantum-classical systems. Then we shall discuss possible representation of general statistical ensembles of QC systems within the Hamiltonian formulation. Statistical operator for the QC system as well as conditional and unconditional mixed states of the quantum subsystem corresponding to the general ensembles of the QC systems will be defined and their evolution will be discussed.

Hamiltonian formulation of quantum mechanics. Schrödinger dynamical equation on a Hilbert space $\mathcal{H}$ generates a Hamiltonian dynamical system on an appropriate symplectic manifold [8,9]. The real manifold $\mathcal{M}$ associated with the Hilbert space $\mathcal{H}$ in fact has Riemannian and symplectic structure, provided by the real and the imaginary parts of the scalar product, and can be viewed as a phase space of a Hamiltonian dynamical system, additionally equipped with the Riemannian metric which reflects its quantum origin. A vector $|\psi\rangle$ from $\mathcal{H}$, associated with a pure quantum state, is represented by the corresponding point in the phase space $\mathcal{M}$ denoted by X_ψ or simply by X.

Real coordinates $\{(x_j, y_j), \ j = 1, 2, \dots\}$ of a point $\psi \in \mathcal{H} \equiv \mathcal{M}$ are introduced using expansion coefficients $\{c_j, \ j = 1, 2, \dots\}$ in some basis $\{|j\rangle, \ j = 1, 2, \dots\}$ of $\mathcal{H}$ as follows:

$$|\psi\rangle = \sum_j c_j |j\rangle, \quad x_j = \sqrt{2}\,\mathrm{Re}\,c_j, \quad y_j = \sqrt{2}\,\mathrm{Im}\,c_j. \quad (1)$$

The coordinates (x_j, y_j) represent canonical coordinates of a Hamiltonian dynamical system on $\mathcal{M}$. Consequently, the Poisson bracket between two functions F_1 and F_2 on $\mathcal{M}$ in the canonical coordinates (x_j, y_j) is given by

$$\{F_1, F_2\}_\mathcal{M} = \frac{1}{\hbar} \sum_j \left(\frac{\partial F_1}{\partial x_j} \frac{\partial F_2}{\partial y_j} - \frac{\partial F_2}{\partial x_j} \frac{\partial F_1}{\partial y_j} \right). \quad (2)$$

A quantum observable $\hat{H}$ is represented by the corresponding function of the form

$$H(X_\psi) = \langle \psi | \hat{H} | \psi \rangle. \quad (3)$$

Hamiltonian flows with the Hamilton's function of the form (3) generate isometries of the Riemannian metric. More general Hamiltonian flows on $\mathcal{M}$, corresponding to the Hamilton's function which are not of the form (3), do not generate isometries and do not have the physical interpretation of quantum observables. It can be seen easily that

$$\{H_1, H_2\}_\mathcal{M} = \frac{1}{i\hbar} \langle [\hat{H}_1, \hat{H}_2] \rangle. \quad (4)$$

The Schrödinger evolution equation

$$i\hbar |\dot{\psi}\rangle = \hat{H} |\psi\rangle \quad (5)$$

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is equivalent to the Hamilton equations on $\mathcal{M}$ assuming the standard form in the canonical coordinates (x_j, y_j),

$$\dot{x}_j = \frac{\partial H}{\partial y_j}, \quad \dot{y}_j = -\frac{\partial H}{\partial x_j}, \tag{6}$$

with H given by Eq. (3).

The Hamiltonian formulation of the Schrödinger equation on $\mathcal{H}$ automatically preserves the constraints imposed by the physical equivalence of Hilbert space vectors. In fact, Hamiltonian formulations based on $\mathcal{H}$ and on the projective Hilbert space as the space of physical states are equivalent. We use the formulation in which points of the quantum phase space are identified with the vectors from $\mathcal{H}$ since it is sufficient for our main purpose.

Mixed states of a quantum system in the Hamiltonian formulation. A quantum state is in general represented by the corresponding density operator $\hat{\rho}$ on $\mathcal{H}$. On the other hand every positive function $\rho(x, y)$ with unit integral on $\mathcal{M}$ represents a density of some probability theory on $\mathcal{M}$. Expectation of a function $F(x, y)$ with respect to $\rho(x, y)$ is given by

$$\bar{F} = \int_{\mathcal{M}} \rho(x, y) F(x, y) dM, \tag{7}$$

where dM is the Lebesque measure on $\mathcal{M}$. The densities satisfy Liouville equation on $\mathcal{M}$,

$$\frac{\partial}{\partial t} \rho(x, y; t) = \{H(x, y), \rho(x, y; t)\}_{\mathcal{M}}. \tag{8}$$

Quantum-mechanical average of the observable $\hat{F}$ in the state $\hat{\rho}$, $\mathrm{Tr}(\hat{\rho}\hat{F})$, is reproduced with the formula (7) using any of the probability densities $\rho(x, y; t)$ with the same first moment fixed by the requirement

$$\hat{\rho}(t_0) = \int_{\mathcal{M}} \rho(x, y; t_0) \hat{\Pi}(x, y) dM, \tag{9}$$

where $\hat{\Pi}(x, y) = |\psi_{x,y}\rangle\langle\psi_{x,y}|$ and the state $|\psi_{x,y}\rangle \in \mathcal{H}$ corresponds to the coordinates (x, y) of $\mathcal{M}$. Liouville evolution of the densities $\rho(x, y; t)$ yielding the same $\hat{\rho}(t_0)$ generates the same von Neumann evolution $\hat{\rho}(t)$. The fact that the quantum mixed state $\hat{\rho}$ determines only an equivalence class of densities, those with the appropriate first moment, is equivalent to the nonuniqueness of the expansion of the quantum mixed state in terms of convex combinations of pure state projectors.

Hamiltonian theory of hybrid systems. Hamiltonian theory of hybrid quantum-classical 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 [7]. The result in the macro limit imposed on the classical subsystem turns out to be equivalent to a Cartesian product of two Hamiltonian systems as in Ref. [1]. One of these Hamiltonian systems corresponds to the quantum and the other one to the classical subsystem of the hybrid. However, the interaction between the two subsystems has crucial influence on their properties.

The phase space 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 $\mathcal{M}_q$. Denoting the local coordinates on the product as (p, q, x, y), where $(p, q) \in \mathcal{M}_c$ and $(x, y) \in \mathcal{M}_q$,

one can write the evolution equations of the QC system as Hamiltonian dynamical equations on the phase space $\mathcal{M}$ with the Hamilton's function comprised of three terms,

$$H_t(p, q, x, y) = H_c(p, q) + H_q(x, y) + V_{\mathrm{int}}(p, q, x, y), \tag{10}$$

where H_c is the Hamilton's function of the classical subsystem, $H_q(x, y)$ of the form (3) is the Hamilton's function of the quantum subsystem and $V_{\mathrm{int}}(p, q, x, y) = \langle\psi_{x,y}|\hat{V}_{\mathrm{int}}(p, q)|\psi_{x,y}\rangle$, where $\hat{V}_{\mathrm{int}}(p, q)$ is an operator in the Hilbert space of the quantum subsystem which depends on the classical coordinates (p, q) and describes the interaction between the subsystems. The Poisson bracket on $\mathcal{M}$ of arbitrary functions of the local coordinates (p, q, x, y) is defined as

$$\{f_1, f_2\}_{\mathcal{M}} = \sum_{i=1}^{k} \left(\frac{\partial f_1}{\partial q_i}\frac{\partial f_2}{\partial p_i} - \frac{\partial f_2}{\partial q_i}\frac{\partial f_1}{\partial p_i} \right)$$
$$+ \frac{1}{\hbar} \sum_j \left(\frac{\partial f_1}{\partial x_j}\frac{\partial f_2}{\partial y_j} - \frac{\partial f_2}{\partial x_j}\frac{\partial f_1}{\partial y_j} \right). \tag{11}$$

Thus, the Hamiltonian form of the QC dynamics on $\mathcal{M}$ as the phase space reads

$$\dot{q} = \{q, H_t\}_{\mathcal{M}}, \quad \dot{p} = \{p, H_t\}_{\mathcal{M}}, \tag{12}$$

$$\dot{x} = \{x, H_t\}_{\mathcal{M}}, \quad \dot{y} = \{y, H_t\}_{\mathcal{M}}, \tag{13}$$

where the Hamilton's function $H_t(p, q, x, y)$ in local coordinates on $\mathcal{M}$ is given by Eq. (10).

Statistical ensembles of QC systems and quantum subsystems. Consider a general probability density $\rho(p, q, x, y)$ on the total hybrid phase space $\mathcal{M} = \mathcal{M}_c \times \mathcal{M}_q$. There is no reason to require such probability density to represent a physical quantity or an observable of the QC system. If such $\rho(p, q, x, y)$ is a quadratic function of x, y then it is equal to the quantum expectation in the corresponding state $|\psi_{x,y}\rangle$ of an operator function $\hat{f}_\rho(p, q)$, i.e., $\rho(p, q, x, y) = \langle\psi_{x,y}|\hat{f}_\rho(p, q)|\psi_{x,y}\rangle$, where for each fixed p, q the operator $\hat{f}_\rho(p, q)$ is a statistical operator on the Hilbert space of the quantum subsystem. However, in general a probability density of an arbitrary form $\rho(p, q, x, y)$ describes a perfectly legitimate statistical ensemble of QC systems. In general, following the Hamiltonian formulation of the QC system dynamics, the evolution of $\rho(p, q, x, y; t)$ considered as a statistical ensemble on $\mathcal{M}$ is given by the Liouville equation with the Hamilton's function (10) and the Poisson bracket (11),

$$\frac{\partial}{\partial t} \rho(p, q, x, y; t) = \{H_t(p, q, x, y), \rho(p, q, x, y; t)\}_{\mathcal{M}}, \tag{14}$$

i.e., $\rho(p(t), q(t), x(t), y(t); t) = \mathrm{const}$ when $(p(t), q(t))$ and $(x(t), y(t))$ are determined from the Hamilton equations (12) and (13), respectively. However, Liouville evolution of an ensemble which is at $t = t_0$ of the form $\langle\psi_{x,y}|\hat{f}_\rho(p, q; t_0)|\psi_{x,y}\rangle$ will in general result in some probability density $\rho(p, q, x, y; t)$ which is not quadratic in x, y, i.e., cannot be expressed as expectation of an operator. Therefore, it can be argued that the most general statistical ensembles of QC systems need to be represented by general probability densities $\rho(p, q, x, y; t)$. We shall therefore assume, in accordance with the Hamiltonian theory, that an arbitrary probability density $\rho(p, q, x, y; t)$

describes a statistical ensemble of QC systems, that is, a mixed state of the hybrid, and that the evolution of such mixed states is given by the corresponding Liouville equation.

Suppose a QC system is in a general mixed state $\rho(p,q,x,y;t)$. The density $\rho(p,q,x,y;t)$ generates a unique positive operator valued function (POVF):

$$\hat{\rho}(p,q;t) = \int_{\mathcal{M}_q} \rho(p,q,x,y;t)\hat{\Pi}(x,y)dM_q, \qquad (15)$$

which can be called the hybrid statistical operator. $\hat{\rho}(p,q;t)$ contains less information about the hybrid system state than the density $\rho(p,q,x,y;t)$, and plays a secondary role in the hybrid theory presented here. The corresponding mixed state of the quantum subsystem conditional on the classical subsystem being in the state (p,q) is uniquely represented by

$$\hat{\rho}_{p,q}(t) = \hat{\rho}(p,q;t)/\int_{\mathcal{M}_q} \rho(p,q,x,y;t)dM_q. \qquad (16)$$

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

$$\hat{\rho}(t) = \int_{\mathcal{M}} \rho(p,q,x,y;t)\hat{\Pi}(x,y)dM. \qquad (17)$$

At time t the previous formula defines positive, trace 1 operator, i.e., a statistical operator representing the mixed state of the quantum subsystem. At any t the statistical operator $\hat{\rho}(t)$ depends on the value of the subintegral expression at the same time t. The Liouville evolution of $\rho(p,q,x,y;t)$ is certainly continuous in t and the dependence on t of $\hat{\rho}(t)$ given by Eq. (17) is also continuous. Thus, the formula (17) defines a continuous one-parameter family of statistical operators on $\mathcal{H}$.

Analogously to the relation (9) valid for a purely quantum system, many hybrid ensembles represented by different $\rho(p,q,x,y;t)$ have the quantum subsystem in the same conditional or unconditional mixed state. The crucial difference between the purely quantum and the hybrid systems is that we have assumed that each different $\rho(p,q,x,y;t)$ describes physically different ensembles of QC systems with the quantum subsystem in the same mixed state. This will be reflected in the evolution of (15) or (17). Recall that all different $\rho(x,y;t)$ in Eq. (9) with the same first moment correspond to the physically equivalent quantum mixture $\hat{\rho}(t_0)$, and generate unique von Neumann evolution of $\hat{\rho}(t)$ which is obtained from the Liouville evolution of any such $\rho(x,y;t)$. Therefore, all such $\rho(x,y;t)$ are equivalent in the purely quantum case. In the hybrid case, different $\rho(p,q,x,y;t)$ which give the same $\hat{\rho}(p,q;t_0)$ [or $\hat{\rho}(t_0)$], as we shall see, generate different evolution of $\hat{\rho}(p,q;t)$ [or $\hat{\rho}(t)$] and thus must be considered as physically different.

The evolution equation satisfied by $\hat{\rho}(p,q;t)$ can be obtained from (14) and (15) using partial integration over (x_j,y_j) and the identities $\partial F/\partial x_j = (\langle\psi_{x,y}|\hat{F}|j\rangle + \langle j|\hat{F}|\psi_{x,y}\rangle)/\sqrt{2}$, $\partial F/\partial y_j = i(\langle\psi_{x,y}|\hat{F}|j\rangle - \langle j|\hat{F}|\psi_{x,y}\rangle)/\sqrt{2}$, where $F = \langle\psi_{x,y}|\hat{F}|\psi_{x,y}\rangle$. The resulting equation is

$$\frac{\partial\hat{\rho}(p,q;t)}{\partial t} = \frac{1}{i\hbar}[\hat{H}_q + \hat{V}_{int}(p,q),\hat{\rho}(p,q;t)] + \{H_c(p,q),\hat{\rho}(p,q;t)\}_{p,q}$$

$$+ \int_{\mathcal{M}_q} \{V_{int}(p,q,x,y),\rho(p,q,x,y;t)\}_{p,q}$$

$$\times \hat{\Pi}(x,y)dM_q. \qquad (18)$$

The solution of Eq. (18) remains a well defined statistical operator on $\mathcal{H}$ for all t, which is a desirable property not shared by some other hybrid system theories [4,5]. The equation for the statistical operator of the quantum subsystem $\hat{\rho}(t)$ follows after the integration over (p,q),

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

$$+ \int_{\mathcal{M}_c} \{H_c(p,q),\hat{\rho}(p,q;t)\}_{p,q}dM_c$$

$$+ \int_{\mathcal{M}} \{V_{int}(p,q,x,y),\rho(p,q,x,y;t)\}_{p,q}$$

$$\times \hat{\Pi}(x,y)dM. \qquad (19)$$

The first term on the right side of Eq. (19) generates the unitary part of the evolution. The other terms do not preserve the norm of $\hat{\rho}(t)$, and are responsible for nonunitary 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 $\rho(p,q,x,y;t)$.

Observe that taking different $\rho'(p,q,x,y;t)$ yielding the same $\hat{\rho}'(p,q;t_0) = \hat{\rho}(p,q;t_0)$ via (15) will in general generate different $\hat{\rho}'(p,q;t) \neq \hat{\rho}(p,q;t)$. In other words, the states of the quantum subsystem of a hybrid in different states $\rho(p,q,x,y;t)$ and $\rho'(p,q,x,y;t)$ might be the same at some moment t_0, but will inevitably evolve differently. This is natural since the corresponding evolution equation (18) for $\hat{\rho}(p,q;t)$ must depend on the evolution of the entire QC system. In particular, one might adjust the total initial ensemble of the hybrid so that the evolution of the quantum subsystem from a fixed initial mixture $\hat{\rho}(t_0)$ has different properties, without altering the Hamiltonian. Experimental observation of different evolutions of the same initial quantum state $\hat{\rho}(p,q;t_0)$, obtained from multiple $\rho(p,q,x,y;t)$ that are different functions of (x,y), would provide a confirmation of our main assumption concerning the class of physically distinguishable ensembles of hybrid QC systems.

Summary and discussion. In summary, we have explored some of the consequences of the assumption that in the Hamiltonian formulation the set of ensembles of hybrid quantum-classical systems is mathematically represented by the space of probability densities on the hybrid system phase space. Each such ensemble uniquely determines a conditional and an unconditional mixed state of the quantum subsystem represented by the corresponding density operators on the quantum subsystem Hilbert space. Evolution of the quantum subsystem mixtures is defined using the evolution of the hybrid probability density. Different hybrid ensembles might give the same quantum subsystem mixture at some time t_0, but that quantum mixture obtained from different hybrid ensembles will evolve differently. The evolution equations for the hybrid statistical operator $\hat{\rho}(p,q;t)$ (18) and for the quantum subsystem unconditional mixture $\hat{\rho}(t)$ (19) have been derived and inevitably involve the full density $\rho(p,q,x,y;t)$.

The initial assumption about the mathematical objects needed to represent all physically possible ensembles of hybrid systems in fact assumes that the ensembles of possibly interacting quantum-classical systems are more general than ensembles of quantum-classical systems without the interaction between the subsystems. In the latter situation a set of densities on the hybrid phase space that is invariant under the evolution can be chosen to contain only functions that are necessary of quadratic dependence on the quantum degrees of freedom. However, if the quantum and the classical subsystem interact then the invariant set of densities is in general the full set of probability densities on the hybrid phase space.

We have shown how such a general set of hybrid ensembles generates consistently defined quantum-mechanical mixtures of the quantum subsystem with the corresponding evolution equations reflecting the quantum-classical interaction. The interaction implies that the evolution of the quantum subsystem statistical operator shows explicit dependence on the equivalent representations of the initial density operator.

[1] H-T. Elze, Phys. Rev. A **85**, 052109 (2012).

[2] Q. Zhang and B. Wu, Phys. Rev. Lett. **97**, 190401 (2006).

[3] M. J. W. Hall, Phys. Rev. A **78**, 042104 (2008); L. L. Salcedo, Phys. Rev. Lett. **90**, 118901 (2003); A. Peres and D. R. Terno, Phys. Rev. A **63**, 022101 (2001); L. Diósi, N. Gisin, and W. T. Strunz, *ibid.* **61**, 022108 (2000).

[4] A. Anderson, Phys. Rev. Lett. **74**, 621 (1995).

[5] I. V. Aleksandrov, Z. Naturforsch. **36A**, 902 (1981).

[6] M. Wallquist, K. Hammerer, P. Rabl, M. Lukin, and P. Zoller, Phys. Scr. T **137**, 014001 (2009); G. De Chiara, M. Paternostro, and G. M. Palma, Phys. Rev. A **83**, 052324 (2011).

[7] M. Radonjić, S. Prvanović, and N. Burić, Phys. Rev. A **85**, 064101 (2012).

[8] T. W. B. Kibble, Commun. Math. Phys. **64**, 73 (1978); A. Heslot, Phys. Rev. D **31**, 1341 (1985); D. C. Brody and L. P. Hughston, J. Geom. Phys. **38**, 19 (2001); N. Burić, Ann. Phys. (NY) **233**, 17 (2008).

[9] M. Radonjić, S. Prvanović, and N. Burić, Phys. Rev. A **84**, 022103 (2011); **85**, 022117 (2012).