

Ehrenfest principle and unitary dynamics of quantum-classical systems with general potential interaction

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Representation of classical dynamics by unitary transformations has been used to develop a unified description of hybrid classical-quantum systems with a particular type of interaction, and to formulate abstract systems interpolating between classical and quantum ones. We solved the problem of a unitary description of two interpolating systems with general potential interaction. The general solution is used to show that with arbitrary potential interaction between the two interpolating systems the evolution of the so-called unobservable variables is decoupled from that of the observable ones if and only if the interpolation parameters in the two interpolating systems are equal.

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I. INTRODUCTION

Koopman–von Neumann (KvN) [1] unitary description of the Liouville equation of classical Hamiltonian dynamical systems was utilized for modeling hybrid quantum-classical systems by Sherry and Sudarshan [2]. They analyzed particular types of interaction between the classical and the quantum parts, and ad hoc prescriptions for definitions of the corresponding Hilbert space operators. It was shown that the premeasurement process can be modeled as an interaction between a classical apparatus and a quantum system within the unitary framework. Sherry and Sudarshan also analyzed the so-called integrity conditions which ought to be satisfied in order that classical variables remain classical during the hybrid unitary evolution in the Heisenberg form. Peres and Terno [3] analyzed consistency of the Koopman–von Neumann–Sudarshan (KNS) hybrid dynamics with the quantum-quantum and the classical-classical limits for the case of linear interaction between harmonic oscillators. Some aspects of the KNS formalism for a hybrid system with specific interaction have also been studied in [4]. The authors investigated the role of unphysical variables which are called unobservables because they do not influence the evolution of the physical observables of the quantum or the classical part if there is no quantum-classical interaction. It was observed, using particular examples of quantum-classical interaction and specific forms of its Hilbert space description, that the evolution of the unobservable and observable variables become coupled.

More recently, KvN formalism and Ehrenfest principle were used to propose a family of abstract unitary systems interpolating between classical system and its quantized counterpart [5]. The problem of hybrid dynamics was not analyzed using the interpolating systems. Our goal is to study the same type of questions, but for the most general potential interaction between the classical and the quantum systems. In fact, we shall obtain unitary dynamical equations for two interpolating abstract systems (IAS) with general potential interaction, and use this to show that generally the evolution

of the unphysical variables is decoupled from that of the physical ones if and only if the interpolation parameters in the two IAS are equal. In particular, unitary dynamics of hybrid systems with potential interaction in general couples the dynamics of the two types of variables. However, there is one special case in the family of general solutions such that the corresponding quantum-classical potential interaction does not couple the physical and the unphysical variables, and implies other properties consistent with this fact.

II. INTERPOLATING ABSTRACT SYSTEMS AND HYBRID MODELS

Dynamical equations for averages of the basic observables of a classical system and that of its quantized counterpart can be mathematically interpolated by an abstract system that depends on a suitable parameter. The first step to achieve this is to rewrite the dynamics of classical and quantum averages using the same mathematical framework. This can be done by rewriting the classical dynamics as a unitary evolution on a suitable Hilbert space, or by rewriting the unitary Schrödinger equation as a (linear) Hamiltonian system on a symplectic manifold. We shall treat here the unitary approach with general potential interaction.

Consider an abstract dynamical system with the basic variables x_j, p_j, χ_j, π_j (hereafter $j = 1, 2$). Properties of the system, expressed through appropriate algebraic relations between the basic variables, are supposed to depend on parameters a_j . The basic variables satisfy commutation relations

$$[x_j, p_j] = i\hbar a_j, \quad [x_j, \pi_j] = [\chi_j, p_j] = i\hbar, \quad (1)$$

with all other commutators being zero. Let us suppose that the algebra (1) is represented by operators acting on a Hilbert space \mathcal{H} . Assume that the dynamical variables x_j, p_j are measurable and that their averages in a state $|\psi\rangle \in \mathcal{H}$ are computed as

$$\langle x_j \rangle_\psi = \langle \psi | \hat{x}_j | \psi \rangle, \quad \langle p_j \rangle_\psi = \langle \psi | \hat{p}_j | \psi \rangle. \quad (2)$$

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Suppose that the dynamics of these averages is given by the Ehrenfest principle

$$\frac{d}{dt} \langle \psi(t) | \hat{x}_j | \psi(t) \rangle = \langle \psi(t) | \frac{\hat{p}_j}{m_j} | \psi(t) \rangle, \quad (3a)$$

$$\frac{d}{dt} \langle \psi(t) | \hat{p}_j | \psi(t) \rangle = \langle \psi(t) | -V'_j(\hat{x}_j) | \psi(t) \rangle, \quad (3b)$$

and that the state evolution is unitary $i\hbar|\dot{\psi}\rangle = \hat{H}_{\text{IAS}}|\psi\rangle$. The corresponding evolution equations for the dynamical variables in the Heisenberg form are $i\hbar d\hat{x}_j/dt = [\hat{x}_j, \hat{H}_{\text{IAS}}]$ and analogously for $\hat{p}_j, \hat{\chi}_j, \hat{\pi}_j$. The operator \hat{H}_{IAS} is the evolution generator and might depend on all dynamical variables $\hat{H}_{\text{IAS}} = H_{\text{IAS}}(\hat{x}_j, \hat{p}_j, \hat{\chi}_j, \hat{\pi}_j)$. It is not necessarily interpreted as the physical energy. It should be remarked that the relations (2) and (3) are treated as axioms in the general abstract formulation [5], expressing the conservative nature of the dynamics. Following the approach of [5], one can obtain the class of evolution generators yielding (3),

$$\hat{H}_{\text{IAS}} = \sum_{j=1,2} \frac{1}{a_j} \left(\frac{\hat{p}_j^2}{2m_j} + V_j(\hat{x}_j) \right) + F_j(\hat{x}_j - a_j \hat{\chi}_j, \hat{p}_j - a_j \hat{\pi}_j), \quad (4)$$

where F_j are arbitrary functions of the indicated arguments. Observe that, consistent with (3), there are no terms coupling observables with different subscripts, so that the abstract system (4) can be interpreted as a compound system with two noninteracting components.

Explicit representation of the operator \hat{H}_{IAS} depends on the representation space \mathcal{H} , and is not important in our analysis. Nevertheless, it should be remarked that the Hilbert space \mathcal{H} is determined as a space of an irreducible representation of the algebra (1), and is the same space for any value of the parameters a_j . In particular, it is seen that in the case we want to represent two quantum systems, the Hilbert space needed to accommodate (1) with $a_1 = a_2 = 1$ is larger than the space $L_2(x_1) \otimes L_2(x_2) \equiv L_2(x_1, x_2)$, which is relevant in the standard quantum mechanics without the additional variables χ_j, π_j . It can be shown that one irreducible representation of the algebra is provided with the Hilbert space of operators on $L_2(x_1, x_2)$ [6]. Thus, the vectors from \mathcal{H} can be considered as density matrices or mixed states of the quantum-quantum system [5]. Similarly, if the abstract systems represent two classical systems, i.e., when $a_1 = a_2 = 0$ so that \hat{x}_j, \hat{p}_j all commute, the interpretation of the state $|\psi\rangle$ is that of the amplitude of a probability density $\rho(x_1, x_2, p_1, p_2) = |\langle x_1, x_2, p_1, p_2 | \psi \rangle|^2$ on the corresponding phase space $\mathcal{M}(x_1, x_2, p_1, p_2)$ [5]. The scalar product in (2) coincides with the ensemble average $\int_{\mathcal{M}} \rho x_j dM$ or $\int_{\mathcal{M}} \rho p_j dM$. Observe that the classical Hilbert space can be partitioned into equivalence classes $|\psi\rangle \sim e^{i\phi}|\psi\rangle$, where each class corresponds to a single density ρ . The evolution equations preserve the equivalence classes because there is no interaction [4].

Convenient choices of the arbitrary functions F_j can reproduce the evolution equations for noninteracting classical-classical (C-C) ($a_1 = a_2 = 0$), quantum-quantum (Q-Q) ($a_1 = a_2 = 1$), and classical-quantum systems (C-Q) ($a_1 = 0, a_2 = 1$). The relevant choice of functions F_j and the corresponding

equations can be obtained as the special case from the general equations, that will be given later, with interaction set to zero.

For arbitrary $a_1, a_2 \neq 0, 1$ the dynamical equations describe the evolution of an abstract system interpolating between the quantum and the classical systems (hence the notation \hat{H}_{IAS}). Because there is no interaction between the two systems, the evolution of \hat{x}_j, \hat{p}_j is also independent of $\hat{\chi}_j, \hat{\pi}_j$. The system has $2 + 2$ degrees of freedom, and each of the degrees of freedom evolves independently of the others. If the abstract system (4) is meant to represent two quantum or two classical systems, the variables \hat{x}_j, \hat{p}_j are interpreted as physical observables of coordinates and momenta. The variables $\hat{\chi}_j, \hat{\pi}_j$, similarly as \hat{H}_{IAS} , do not represent physical observables. They are dynamically separated from the physical observables and appear because the family of systems (4) must interpolate between the classical and the quantum dynamics [5].

III. IAS WITH GENERAL POTENTIAL INTERACTION

Potential interaction between two quantum systems or between two classical systems appears in the equations of motion in the form of gradients of the corresponding scalar potential. In the extended Hilbert space formalism, which is required for the formulation of the IAS, such potential Q-Q or C-C interaction can be represented by an operator expression in terms of all variables with the role of coordinates $\hat{W} = W(\hat{x}_1, \hat{x}_2, \hat{\chi}_1, \hat{\chi}_2)$. We assume that in the dynamical equations for the corresponding momenta \hat{W} should appear as a gradient with respect to the corresponding coordinate.

We shall now consider dynamics of two abstract systems with arbitrary values of a_1, a_2 and with an arbitrary potential interaction between them. Like in the Q-Q and C-C cases, we demand that the following relations hold:

$$\frac{d}{dt} \langle \Psi(t) | \hat{x}_j | \Psi(t) \rangle = \langle \Psi(t) | \frac{\hat{p}_j}{m_j} | \Psi(t) \rangle, \quad (5a)$$

$$\frac{d}{dt} \langle \Psi(t) | \hat{p}_j | \Psi(t) \rangle = \langle \Psi(t) | -V'_j(\hat{x}_j) - \frac{\partial \hat{W}}{\partial \hat{x}_j} | \Psi(t) \rangle. \quad (5b)$$

Notice that the potential interaction can be completely general. Particular examples of interaction which do not necessarily satisfy (5) have been assumed in a somewhat ad hoc manner and studied in [2–4]. Our goal is to determine the unitary evolution generator $\hat{H}_{\text{IAS}} = H_{\text{IAS}}(\hat{x}_1, \hat{p}_1, \hat{x}_2, \hat{p}_2, \hat{\chi}_1, \hat{\pi}_1, \hat{\chi}_2, \hat{\pi}_2)$ such that $i\hbar|d\Psi(t)/dt\rangle = \hat{H}_{\text{IAS}}|\Psi(t)\rangle$ holds. The unitary evolution and (5) give the following relations:

$$\frac{1}{i\hbar} [\hat{x}_j, \hat{H}_{\text{IAS}}] = \frac{\hat{p}_j}{m_j}, \quad -\frac{1}{i\hbar} [\hat{p}_j, \hat{H}_{\text{IAS}}] = V'_j(\hat{x}_j) + \frac{\partial \hat{W}}{\partial \hat{x}_j}, \quad (6)$$

and the related system of partial differential equations (PDEs) for the function H_{IAS} ,

$$a_j \frac{\partial H_{\text{IAS}}}{\partial p_j} + \frac{\partial H_{\text{IAS}}}{\partial \pi_j} = \frac{p_j}{m_j}, \quad (7a)$$

$$a_j \frac{\partial H_{\text{IAS}}}{\partial x_j} + \frac{\partial H_{\text{IAS}}}{\partial \chi_j} = V'_j(x_j) + \frac{\partial W}{\partial x_j}. \quad (7b)$$

The commutation relations (6), i.e., the PDEs (7), are not consistent for an arbitrary choice of the interaction potential \hat{W} . Jacobi identity $[\hat{H}_{\text{IAS}}, [\hat{p}_1, \hat{p}_2]] + [\hat{p}_1, [\hat{p}_2, \hat{H}_{\text{IAS}}]] + [\hat{p}_2, [\hat{H}_{\text{IAS}}, \hat{p}_1]] = 0$ and the commutation relation $[\hat{p}_1, \hat{p}_2] = 0$ imply that $[\hat{p}_1, [\hat{p}_2, \hat{H}_{\text{IAS}}]] = [\hat{p}_2, [\hat{p}_1, \hat{H}_{\text{IAS}}]]$, so that

$$\left[a_1 \frac{\partial}{\partial x_1} + \frac{\partial}{\partial \chi_1}, a_2 \frac{\partial}{\partial x_2} + \frac{\partial}{\partial \chi_2} \right] H_{\text{IAS}} = 0 \quad (8)$$

must be satisfied. Invoking the second relation of (7), we get the consistency requirement

$$\left(a_1 \frac{\partial}{\partial x_1} + \frac{\partial}{\partial \chi_1} \right) \frac{\partial W}{\partial x_2} - \left(a_2 \frac{\partial}{\partial x_2} + \frac{\partial}{\partial \chi_2} \right) \frac{\partial W}{\partial x_1} = 0. \quad (9)$$

The general solution of (9) is

$$W = \int_{-\infty}^{\infty} \mathcal{W}(x_1 + (\alpha - a_1)\chi_1, x_2 + (\alpha - a_2)\chi_2, \alpha) d\alpha, \quad (10)$$

where \mathcal{W} is an arbitrary function such that the previous integral is defined. Note that when $a_1 \neq a_2$, i.e., when the systems are of different type, the interaction potential \hat{W} will depend on at least one of the unobservables $\hat{\chi}_1, \hat{\chi}_2$. This conclusion remains valid in the particular case of a hybrid classical-quantum system, where $a_1 = 0$ corresponds to the classical part and $a_2 = 1$ is related to the quantum part. Let us stress that this fact is proved here for quite general potential interaction and not just observed for some special choices of the interaction [3,4].

Consider a particular choice of $\mathcal{W} \propto \delta(\alpha - a)$ yielding the interaction potential $\hat{W} = W(\hat{x}_1 + (a - a_1)\hat{\chi}_1, \hat{x}_2 + (a - a_2)\hat{\chi}_2)$. The related solution of the PDEs (7) gives

$$\begin{aligned} \hat{H}_{\text{IAS}} = & \sum_{j=1,2} \frac{1}{a_j} \left(\frac{\hat{p}_j^2}{2m_j} + V_j(\hat{x}_j) \right) \\ & + \frac{1}{a} W(\hat{x}_1 + (a - a_1)\hat{\chi}_1, \hat{x}_2 + (a - a_2)\hat{\chi}_2) \\ & + F(\hat{x}_1 - a_1\hat{\chi}_1, \hat{p}_1 - a_1\hat{\pi}_1, \hat{x}_2 - a_2\hat{\chi}_2, \hat{p}_2 - a_2\hat{\pi}_2), \end{aligned} \quad (11)$$

where F is arbitrary real-valued smooth function that commutes with the observables $O(\hat{x}_1, \hat{p}_1, \hat{x}_2, \hat{p}_2)$. Let us observe that when the two systems are of the same type, the unobservables do not influence the evolution of the physical observables for the choice $a_1 = a_2 = a$. The result (11) can be extended, although with some care, to the limit $a \rightarrow 0$, which will turn out to be interesting for the hybrid Q-C system. Namely, one can take a part of the function F to be of the suitable form $-\frac{1}{a} W(\hat{x}_1 - a_1\hat{\chi}_1, \hat{x}_2 - a_2\hat{\chi}_2)$ that yields in the $a \rightarrow 0$ limit,

$$\begin{aligned} \hat{H}_{\text{IAS}} = & \sum_{j=1,2} \frac{1}{a_j} \left(\frac{\hat{p}_j^2}{2m_j} + V_j(\hat{x}_j) \right) \\ & + \partial_1 W(\hat{x}_1 - a_1\hat{\chi}_1, \hat{x}_2 - a_2\hat{\chi}_2) \hat{\chi}_1 \\ & + \partial_2 W(\hat{x}_1 - a_1\hat{\chi}_1, \hat{x}_2 - a_2\hat{\chi}_2) \hat{\chi}_2 \\ & + F(\hat{x}_1 - a_1\hat{\chi}_1, \hat{p}_1 - a_1\hat{\pi}_1, \hat{x}_2 - a_2\hat{\chi}_2, \hat{p}_2 - a_2\hat{\pi}_2), \end{aligned} \quad (12)$$

where $\partial_j W$ denotes partial derivative of the potential with respect to the j th argument.

The limit of (11) when $a_j \rightarrow 0$ can also be obtained by choosing a part of the function F in the form $-\frac{1}{a_j} \left[\frac{(\hat{p}_j - a_j\hat{\pi}_j)^2}{2m_j} + V_j(\hat{x}_j - a_j\hat{\chi}_j) \right]$, as in [5]. In particular, this yields the Hamiltonian, as the dynamics generator, of a hybrid classical-quantum system ($a_1 \rightarrow 0, a_2 = 1$)

$$\begin{aligned} \hat{H}_{\text{hyb}} = & \frac{\hat{p}_1}{m_1} \hat{\pi}_1 + V_1'(\hat{x}_1) \hat{\chi}_1 + \frac{\hat{p}_2^2}{2m_2} + V_2(\hat{x}_2) \\ & + \frac{1}{a} W(\hat{x}_1 + a\hat{\chi}_1, \hat{x}_2 + (a - 1)\hat{\chi}_2) \\ & + F(\hat{x}_1, \hat{p}_1, \hat{x}_2 - \hat{\chi}_2, \hat{p}_2 - \hat{\pi}_2), \end{aligned} \quad (13)$$

where the first four terms describe a noninteracting hybrid system. As already mentioned, the interaction potential depends on at least one of the unobservables $\hat{\chi}_1, \hat{\chi}_2$. The appearance of the unphysical variables in the Hamiltonian is not a problem *per se*, because the Hamiltonian is anyway interpreted as the dynamics generator and not as the physical energy. Additionally, in the purely C-C case ($a_1 = a_2 = a \rightarrow 0$) one gets

$$\begin{aligned} \hat{H}_{\text{C-C}} = & \frac{\hat{p}_1}{m_1} \hat{\pi}_1 + V_1'(\hat{x}_1) \hat{\chi}_1 + \frac{\hat{p}_2}{m_2} \hat{\pi}_2 + V_2'(\hat{x}_2) \hat{\chi}_2 \\ & + \partial_1 W(\hat{x}_1, \hat{x}_2) \hat{\chi}_1 + \partial_2 W(\hat{x}_1, \hat{x}_2) \hat{\chi}_2, \end{aligned} \quad (14)$$

with the unobservables being present, but not within the arguments of the interaction potential. However, in the C-C case the unphysical variables do not appear in the evolution equations of the physical observables. We may remark in passing that \hat{W} is not interpreted as the potential energy of the hybrid, but as a term in the generator of dynamics corresponding to the potential interaction. However, the crucial property of hybrid Q-C systems is that the equations of motion for the physical and unphysical variables become coupled. Those equations are easily obtained from the generator (13). Thus, we have shown that the dynamical equations couple physical and unphysical variables in the case of a potential Q-C interaction in general, that is with the Hamiltonian of the general hybrid form (13).

A very special case of (13) is obtained in the limit $a \rightarrow 0$ with the appropriate choice of the function F yielding the Hamiltonian

$$\begin{aligned} \hat{H}_{\text{hyb}} = & \frac{\hat{p}_1}{m_1} \hat{\pi}_1 + V_1'(\hat{x}_1) \hat{\chi}_1 + \frac{\hat{p}_2^2}{2m_2} + V_2(\hat{x}_2) \\ & + \partial_1 W(\hat{x}_1, \hat{x}_2 - \hat{\chi}_2) \hat{\chi}_1 + \partial_2 W(\hat{x}_1, \hat{x}_2 - \hat{\chi}_2) \hat{\chi}_2, \end{aligned} \quad (15)$$

with the corresponding equations of motion of the variables

$$\frac{d\hat{x}_j}{dt} = \frac{\hat{p}_j}{m_j}, \quad (16a)$$

$$\frac{d\hat{p}_j}{dt} = -V_j'(\hat{x}_j) - \partial_j W(\hat{x}_1, \hat{x}_2 - \hat{\chi}_2), \quad (16b)$$

$$\frac{d}{dt}(\hat{x}_2 - \hat{\chi}_2) = 0. \quad (16c)$$

This solution describes the situation when the evolution of the classical system depends on the quantum system only through a constant of motion $\hat{x}_2 - \hat{\chi}_2$. In this very special case of the general hybrid solution, the classical variables see only a quite coarse-grained effect of the quantum evolution. On the other hand, the dynamics of the quantum sector is influenced by the details of the dynamics of the classical physical variables \hat{x}_1, \hat{p}_1 . In addition, this is the only case of the potential Q-C interaction which satisfies the integrity principle of Sudarshan [2]. Namely, the terms $\partial_j W(\hat{x}_1, \hat{x}_2 - \hat{\chi}_2)$ in this form of the Hamiltonian commute with the momenta \hat{p}_1, \hat{p}_2 , which assures commutation of the classical variables at different times.

IV. SUMMARY

We have studied the type of theory of hybrid quantum-classical systems where the evolution is described by unitary transformations on an appropriate Hilbert space. The fact that both classical and quantum mechanics can be formulated on the same Hilbert space makes it possible to introduce a parameter dependent family of abstract systems interpolating between a classical system and its quantized counterpart [5]. The variables involved in the formulation of the abstract interpolating model can be divided into two groups, one with the standard physical interpretation and one with no physical interpretation. In the limits of the classical or the quantum system the two groups of variables are dynamically separated. We have studied two such abstract interpolating systems with quite arbitrary potential interaction between them. General solution for the problem of constructing dynamical equations

for such a pair of systems is provided. It is shown that, with the most general type of potential interaction, the dynamics of the two groups of variables is separated if and only if the two abstract interpolating systems have the same value of the interpolation parameter. On the other hand, if the interpolation parameters of the two system are different, the two groups of variables dynamically influence each other. The variables which can be considered as unphysical and cannot be observed in the purely quantum or in the purely classical case, do have an observable effect in the hybrid quantum-classical system. Our results demonstrate this fact for arbitrary potential interaction, in line with the previous special cases [3,4]. Analogous conclusions are obtained in the symplectic approach to the conservative hybrid dynamics [7,8], and the analogy is worth further investigation. We have also analyzed the particular case of the general solution corresponding to the situation when the classical part is influenced by the quantum part only through a particular combination of the variables from the quantum system that remains constant during the evolution. This, rather special case, is the only possible dynamics of the hybrid system within the framework of unitary dynamics with potential interaction, when the physical and the unphysical variables can be considered as decoupled, and also when the Sudarshan integrity condition of the classical system is satisfied.

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