Statistical consistency of quantum-classical hybrids

L. L. Salcedo
Departamento de Física Atómica, Molecular y Nuclear, and Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada, E-18071 Granada, Spain
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After formulating a no-go theorem for perfect quantum-classical hybrid systems, a consistency requirement based on standard statistical considerations is noted. It is shown that such requirement is not fulfilled by the mean-field approach or by the statistical ensemble in configuration space approach. Further unusual features of the latter scheme are pointed out.

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I. INTRODUCTION

The study of the interrelation between classical and quantum dynamics is as old as quantum theory itself. The Copenhagen interpretation invokes a classical measuring device in interaction with the quantum system to be measured [1–4]. However, while classical and quantum dynamics are each internally consistent by themselves and formally similar, their coupling is not straightforward and, in fact, poses a problem of consistency [5–16]. The most immediate approach is the mean-field scheme (or semiclassical or Ehrenfest method), in which the classical system couples to the quantum one through the expectation values. This scheme is robust and elegant but not realistic as it misses the backreaction from the quantum fluctuations [17–19]. For instance, in cosmology it leads to problems in accounting for the local anisotropy in the early universe [20]. Many other coupling schemes for hybrid classical-quantum systems have been proposed in the literature [6,8,12,21–37]. As shown in Ref. [5] (of course, under pertinent assumptions), as soon as a classical degree of freedom couples to a quantum system, a consistent description is only possible if the classical system inherits fluctuations which turn it quantal. (See, however, the critique in Ref. [38].) This type of argument, as well as the accuracy of quantum mechanics in every prediction, would point to the conclusion that only quantum systems exist in nature. While this view is quite extended among the scientific community it is by no means universally accepted, due to the conceptual problems involved in the quantum description [39–42]. Also, the technical and conceptual difficulties encountered in quantum gravity have prompted a certain discussion regarding the necessity or not of treating gravity quantum mechanically [43–54].

In our view the problem of "semiquantization," that is, treating simultaneously classical and quantum observables in interaction and constructing a consistent algebra of such observables, is closely related to the problem of "quantization," that is, how to obtain the quantum version of a system and its algebra of observables, from its classical version. For the latter there are well-known no-go theorems [55–57] and similar negative theorems have been forwarded for the semiquantization problem [9,11–16]. If all physical systems are described by quantum mechanics, both problems would be of technical type, rather than of fundamental type. The quantization program would be to use the classical description as guidance to construct the correct quantum description among the several possible ones with the same classical limit. The semiquantization program would be how to construct a useful approximate description in which some sector of the theory is treated classically to make the treatment accessible to computation. This is actually the situation in many applications in physics and quantum chemistry [17,19,21,58–61].

One goal of the present work is to reanalyze the conditions fulfilled by classical and by quantum systems, conditions which guarantee a consistent description. In Refs. [9,11] it was already shown that a perfect quantum-classical hybrid, that is, sharing all the nice properties of classical and quantum systems is not viable (at least without restrictions on the allowed interactions). A technical limitation was that variables of the position-momentum type were assumed in the quantum sector.[1] More general proofs have been obtained in Refs. [62,63]. Here we present an extremely streamlined proof of this no-go theorem. To have a proof as simple as possible should be of interest for modelers of quantum-classical hybrid dynamics. The failure of perfect hybridization has some consequences if quantum-classical hybrids are taken at the fundamental level, that is, not as approximations. If such hybrid systems would exist in nature they would have emergent properties [64] not shared by the purely classical or the purely quantum dynamics. This is by itself problematic because the prime example of a classical-quantum interacting system, according to the Copenhagen interpretation, would be a quantum measurement. No emergent phenomena have been detected there. Easy or hard to understand from a conceptual point of view, what is seen there is part of the standard quantum mechanics.

However, the main contribution of this work is the introduction of a further consistency requirement to be fulfilled by quantum-classical hybrid dynamics. Essentially, we note that mixed statistical quantum states, a density matrix, can be decomposed in many different ways into pure states. Likewise, a mixed statistical classical state can be decomposed as statistical combinations of other mixed classical states. For either purely classical or purely quantum systems, the concrete decomposition is not relevant; only the statistical mixture is. As it turns out, it is a nontrivial requirement that the evolution of quantum-classical hybrid

[1]This is an important limitation but the proof still covers all degrees of freedom of bosonic type, since the position-momentum pair can be combined to form bosonic creation and annihilation operators and the corresponding bosonic quantum fields.

systems should be independent of the concrete decomposition. This requirement was briefly touched upon in Ref. [13]. Here we analyze it in more detail and show that the mean-field approach and the statistical ensemble scheme in configuration space [65–68] fail to fulfill the requirement. So, for instance, if the violation of this principle were an emergent feature of the hybrid systems, it would be possible to say which is the "true" polarization of the electrons in an unpolarized electron beam. This provides a test for such hybrid schemes. In passing, the hybrid scheme based on statistical ensembles in configuration space is analyzed in some detail. Further emergent features are unveiled for this approach, such as ghost coupling between noninteracting (but entangled) classical and quantum sectors and nonconservation of angular momentum in presence of spin or of internal symmetries in general.

In Sec. II the proof of the no-go theorem for perfect quantum-classical hybrids is presented. In Sec. III the statistical consistency requirement is introduced and applied to the mean-field approach. In Sec. IV the statistical ensemble in configuration space approach is analyzed, in particular regarding its statistical consistency. In Sec. V we present our conclusions.

II. NO-GO THEOREM

A classical system with n_c degrees of freedom can be described using the canonical formalism, that is, by means of the phase-space variables position and momentum, x_i, k_i, $i = 1, \ldots, n_c$. The observables, including the Hamiltonian, are real valued functions of x and k, $A(x,k)$ (for simplicity we disregard an explicit dependence on time in the observables). Their dynamical evolution is described by the Poisson bracket with the Hamiltonian

$$\frac{d}{dt}A = \{A,H\} := \sum_i \left(\frac{\partial A}{\partial x_i}\frac{\partial H}{\partial k_i} - \frac{\partial A}{\partial k_i}\frac{\partial H}{\partial x_i} \right). \tag{2.1}$$

The (classical) canonical formalism seems particularly convenient in a discussion about classical-quantum mixing because it has a parallel in the quantum treatment. Indeed, in the Heisenberg picture quantum observables are Hermitian operators with dynamical evolution dictated by Heisenberg's equation of motion,

$$\frac{d}{dt}A = \frac{1}{i\hbar}[A,H] := \frac{1}{i\hbar}(AH - HA). \tag{2.2}$$

The classical bracket $\{,\}$ and the quantum one $[,]/i\hbar$, share mathematical properties which are essential for the corresponding dynamics. First, they are *Lie brackets*, that is, they are linear, antisymmetric, and fulfilling the Jacobi identity. Lie groups act through Lie algebras, so the Lie bracket property is required in order to implement observables as generators of groups of transformations, including the dynamical evolution. For instance, if the bracket were not antisymmetric, conservation of energy, $dH/dt = 0$, would not be guaranteed [69]. Likewise, if the angular momentum is to generate rotations of the system, the bracket has to carry a representation of the algebra of SO(3), and so this bracket has to enjoy the Jacobi property. Also, this property ensures that a relation like $C = (A,B)$, where $(,)$ denotes the *dynamical bracket*, is preserved under dynamical evolution or other transformations.

Throughout we consider dynamics of "universal" type, rather than of restricted type, so we really need the bracket between any two observables to be defined (and to be itself an observable) since any observable can be regarded as a possible Hamiltonian, or any observable can be added to the Hamiltonian as a perturbation.

Another conspicuous property of the dynamical brackets is that they are a *derivation*; that is, they fulfill Leibniz's rule:

$$(A,BC) = (A,B)C + B(A,C). \tag{2.3}$$

This property ensures that a relation like $C = AB$ is preserved under dynamical evolution. For instance, if $\boldsymbol{p}$ is the momentum operator, the kinetic energy $\boldsymbol{p}^2/2m$ evolves as $\boldsymbol{p}^2(t)/2m$. This avoids the odd scenario in which the expression of the kinetic energy would be different at different times, and similarly for any other observable without intrinsic time dependence.

A further property refers to the structure of systems composed of different sectors, that is, different independent sets of degrees of freedom, for instance, two different particles or spin and position of a single particle. In this case, the observables of the full system have the structure of *tensor product* over the various sectors. This is true in classical and in quantum mechanics. An immediate consequence of the tensor product construction is that observables of two different quantum sectors commute, and furthermore the product of two such observables is also an observable (the product of two Hermitian commuting operators being automatically Hermitian). The bracket of two observables of the same sector remains in that same sector and, moreover, the bracket of observables in two *different* sectors vanishes. This property is important. It ensures that the two different sectors evolve independently unless an interaction term is present in the Hamiltonian. Indeed, if the Hamiltonian takes the form $H = H_1 + H_2$, with H_1 and H_2 acting in the two different sectors, and the observable A_1 belongs to the first sector, its evolution will not depend on H_2.

The fact that the two canonical structures, classical and quantal, have common properties is, of course, no accident. As is well known, using, for example, the Wigner representation [70–72], the Poisson bracket can be obtained as an $\hbar \to 0$ limit of the commutator. The above-mentioned properties are preserved by the limiting procedure as they do not explicitly depend on $\hbar$.

A rather natural approach suggests itself to describe systems having simultaneously quantum and classical degrees of freedom, namely, to start with a quantum-quantum system and somehow take the classical limit in just one of the two sectors. (For instance, one could start with operators defined in the tensor product Hilbert space of the two quantum sectors, apply a Wigner transformation in just one of the spaces, and take the classical limit there.) In that description observables would be Hermitian operators in the Hilbert space of the quantum sector and also functions of the phase-space variables of the classical sector.

Dynamical brackets have been proposed for the hybrid quantum-classical systems in this approach, most notably by Aleksandrov and by Boucher and Traschen [6,24]:

$$(A,B) = \frac{1}{i\hbar}[A,B] + \frac{1}{2}\{A,B\} - \frac{1}{2}\{B,A\}. \tag{2.4}$$

[Here the Poisson bracket is applied as defined in Eq. (2.1) to the operators A and B, which in general do not commute.] This bracket has some good properties (certainly better than the bracket proposed in Ref. [26]; see [9,69,73]) but it is not a derivation and does not fulfill the Jacobi identity. In addition, it does not preserve positivity of the density matrix [6].

In fact, no bracket can provide a dynamics with all the nice properties common to the purely quantum or purely classical cases. (We refer to that hypothetic dynamics as perfect hybridization.) This is shown in Ref. [9]. The key point is that, although the properties hold for any value of $\hbar$, they require $\hbar$ to take the same value in all sectors [9,11]. Elaborated proofs based on this idea can be found in Refs. [62,63]. Here we present a simple proof. Let A_1, B_1 be two observables in one sector and A_2, B_2 in another sector. Let us assume that the bracket $(\,,\,)$ in the total space enjoys all the above-mentioned properties and in particular, that in each sector they are quantum brackets with two different Planck constants,

$$(A_1,B_1)=\frac{1}{i\hbar_1}[A_1,B_1],\quad (A_2,B_2)=\frac{1}{i\hbar_2}[A_2,B_2]. \tag{2.5}$$

By assumption we can form the new observables A_1A_2 and B_1B_2. Then, applying Leibniz's rule twice,

$$\begin{aligned}(A_1A_2,B_1B_2)&=(A_1A_2,B_1)B_2+B_1(A_1A_2,B_2)\\&=A_1(A_2,B_1)B_2+(A_1,B_1)A_2B_2\\&\quad+B_1A_1(A_2,B_2)+B_1(A_1,B_2)A_2\\&=(A_1,B_1)A_2B_2+B_1A_1(A_2,B_2).\end{aligned} \tag{2.6}$$

In the last equality it has been used that the bracket vanishes for different sectors. On the other hand, due to antisymmetry of the bracket, the expression is antisymmetric under exchange of labels A and B:

$$(A_1A_2,B_1B_2)=-(B_1B_2,A_1A_2); \tag{2.7}$$

therefore,

$$\begin{aligned}&(A_1,B_1)A_2B_2+B_1A_1(A_2,B_2)\\&\quad=-(B_1,A_1)B_2A_2-A_1B_1(B_2,A_2)\\&\quad=(A_1,B_1)B_2A_2+A_1B_1(A_2,B_2).\end{aligned} \tag{2.8}$$

This implies the compact relation

$$(A_1,B_1)[A_2,B_2]=[A_1,B_1](A_2,B_2). \tag{2.9}$$

This relation for generic operators, combined with Eq. (2.5), leaves only the possibility

$$\hbar_1=\hbar_2. \tag{2.10}$$

Hence, there is no quantum-classical mixing (which would require $\hbar_1=\hbar$, $\hbar_2=0$) with all the nice properties shared by the purely classical or purely quantum cases, no perfect quantum-classical mixing. Note that the Jacobi identity has not been used. Also, the Leibniz rule has not been applied at its full power. We have only assumed that A_1A_2 evolves into $A_1(t)A_2(t)$, that is, only for the product of two observables in different sectors.

Quantum-classical hybrids can be considered at two levels, a practical one and a fundamental one. If quantum-classical hybrid systems are regarded as an approximation to a full quantum system, the previous no-go theorem just shows that such approximation will always meet some intrinsic limitations. This is not particularly surprising and it does not prevent these kind of approximations from being useful ones. On the other hand, if the aim is to describe hypothetical quantum-classical hybrids truly existing in nature, the no-go result implies that such hybrid systems will have *emergent* features, not present in any of the two sectors separately. This is because a hybrid with just the standard features has been shown not to be consistent. In this scenario there are at least two alternatives. First, that quantum and classical mechanics are just limit cases of a larger theory [74], and in this case the emergent features were already present from the beginning. Second, whenever the two sectors, classical and quantal, are not coupled by any interaction term in the Hamiltonian, they behave precisely as expected from standard classical mechanics and from standard quantum mechanics, being that only their coupling would yield new emergent properties. To be practical, we adopt the latter possibility as our working assumption. Let us remark that the assumption refers not only to the case of classical and quantum sectors which are never coupled, but also to the cases in which the coupling acts occasionally. In support of this assumption is the empirical fact that quantum mechanics is verified to work very accurately for systems for which the previous history is not known (and so they may include a previous interaction with hypothetic classical sectors). Also, assuming that a quantum measurement requires a truly classical apparatus, the assumption is supported by the fact that quantum mechanics works accurately also after measurements have taken place.

III. STATISTICAL CONSISTENCY AND MEAN-FIELD SCHEME

In this section we assume a system with truly quantum and truly classical sectors, as described by their corresponding standard dynamics when they do not interact. We show that *nonlinear* hybrid dynamics are in conflict with quantum mechanics as we understand it.[2]

The simplest and most intuitive description of the quantum-classical mixing follows from the well-known *mean-field* dynamics. In this dynamics the classical sector and the quantum sector remain (or can remain) always in pure states. That is, at any time, and with or without interaction switched on, the position and momentum of the classical particles are well defined, and the quantum state is described by a wave function rather than a density matrix. The dynamics is as follows:

$$\begin{aligned}&\frac{dx_i}{dt}=\frac{\partial}{\partial k_i}\langle H(x,k)\rangle_\psi,\quad \frac{dk_i}{dt}=-\frac{\partial}{\partial x_i}\langle H(x,k)\rangle_\psi,\\&i\hbar\frac{d}{dt}|\psi\rangle=H(x,k)|\psi\rangle.\end{aligned} \tag{3.1}$$

The Hamiltonian of the system is a function defined on the classical phase space that takes values on operators of the Hilbert space of the quantum system. Such dynamics contains

[2]Obviously, from the beginning there has been much debate about interpretation and other details of quantum mechanics. Here we refer to quantum mechanics as found in textbooks, for example, [75].

a backreaction of the quantum sector on the classical sector, but misses the "quantum backreaction," that is, the effect of quantum fluctuation around the expectation value, that presumably should also be present [18].

A nice reformulation of the mean-field approach has recently been presented in Ref. [37] (see also [76,77]). This is based on the well-known observation that the wave function can be regarded as a classical field, and the Schrödinger equation can be regarded as the corresponding classical field equation of motion. Quantum observables can be represented by their expectation value, $\mathcal{A}(\psi) = \langle A \rangle_\psi$, so that the commutator is represented by the Poisson bracket, with ψ_q and $i\hbar\psi_q^*$ as the canonical conjugate variables. Here $\psi_q = \langle q|\psi\rangle$ and $|q\rangle$ is any orthonormal basis of the Hilbert space of the quantum sector. In the hybrid case these variables are augmented with the phase-space variables of the classical sector, and $\mathcal{A}(\psi,x,k) = \langle A(x,k)\rangle_\psi$,

$$\{\mathcal{A},\mathcal{B}\} = \frac{1}{i\hbar}\sum_q \left(\frac{\partial\mathcal{A}}{\partial\psi_q}\frac{\partial\mathcal{B}}{\partial\psi_q^*} - \frac{\partial\mathcal{A}}{\partial\psi_q^*}\frac{\partial\mathcal{B}}{\partial\psi_q}\right) + \sum_i \left(\frac{\partial\mathcal{A}}{\partial x_i}\frac{\partial\mathcal{B}}{\partial k_i} - \frac{\partial\mathcal{A}}{\partial k_i}\frac{\partial\mathcal{B}}{\partial x_i}\right). \tag{3.2}$$

The hybrid dynamics given by

$$\dot{X} = \{X, \langle H(x,k)\rangle_\psi\}, \quad X = \psi_q, \psi_q^*, x_i, k_i, \tag{3.3}$$

is easily shown to be equivalent to that in Eq. (3.1).

In this formulation there is a Lie bracket which is also a derivation, so this approach would seem to bypass the no-go theorem. The caveat is that the dynamical bracket of two observables should be itself an observable, and this is not the case here. In the scheme of [37] observables are expectation values of operators $A(x,k)$ and so are bilinear in ψ and ψ^*. This property is not preserved by the classical part of the bracket (which, in general, will be quadratic in ψ and quadratic in ψ^*). This implies that the time derivative of an observable, $\dot{\mathcal{A}}$, is not an observable, that is, of the form $\mathcal{B} = \langle B(x,k)\rangle_\psi$, for some operator valued $B(x,k)$.

Now we come to the main argument of this work. We introduce a consistency condition to be added to others considered up to now in the literature. In quantum mechanics, as commonly understood, the state of a system is described, in the most general case, by a density matrix [75,78] (interpreted in the usual sense of "proper mixtures" [79]). This represents a statistical mixture of pure states, pure states themselves being a particular case. The key observation is the well-known fact that, in general, density matrices can be realized in many different ways as mixtures of pure states. A simple example is that of an unpolarized electron beam. Such a state can be attributed to an equiprobable mixture of up and down spins, but the same mixture is obtained regardless of the quantization axis chosen. For another example, let

$$\hat{\rho} = \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|, \quad p_\alpha \geqslant 0, \quad \sum_\alpha p_\alpha = 1, \tag{3.4}$$

where the $|\psi_\alpha\rangle$ are normalized but not orthogonal. Because $\hat{\rho}$ is Hermitian and positive it can be diagonalized into orthonormal states with positive weights,

$$\hat{\rho} = \sum_\nu w_\nu |\phi_\nu\rangle\langle\phi_\nu|, \quad w_\nu \geqslant 0, \qquad \sum_\nu w_\nu = 1, \quad \langle\phi_\nu|\phi_{\nu'}\rangle = \delta_{\nu\nu'}. \tag{3.5}$$

The new states (eigenstates of $\hat{\rho}$) are linear combination of the old ones, but different from them (unless all the $|\psi_\alpha\rangle$ are the same state).

In general, we can consider that in Eq. (3.4) the label α runs through the set of *all* pure states $|\psi_\alpha\rangle$ (normalized vectors, and modulo a phase) each pure state with some weight p_α. Note that we mean all states, not just a linear basis of states. This is an infinite number even for a qubit. A configuration $\{p_\alpha\}$ will produce a density matrix, but the number of possible different density matrices is much smaller than that of configurations. All the configurations $\{p_\alpha\}$ yielding the same density matrix represent precisely the same quantum state. In quantum mechanics there is no way to distinguish between two mixtures producing the same density matrix. Not only will the expectation value of every observable be the same, $\mathrm{tr}\,(\hat{\rho}A)$, but also the results of any measurement will be identical, as also the probabilities can be written using the density matrix only, $P(A = a) = \langle a|\hat{\rho}|a\rangle$ [75]. This means that, in quantum mechanics, the precise decomposition of a density matrix into pure states has no physical meaning.

In the classical theory there is the probability density function on phase space $\rho(x,k)$ and in this case the decomposition into pure states $\delta(x-a)\delta(k-b)$ is unique,

$$\rho(x,k) = \int d^n a\, d^n b\, \rho(a,b)\delta(x-a)\delta(k-b). \tag{3.6}$$

A classical-quantum hybrid scheme like the mean-field one does not directly dictate an evolution for statistical mixtures of classical or quantal pure states. However, nothing prevents us from applying the hybrid scheme for pure states and take the statistical mixing at any time. The basis for this procedure follows from the meaning of the statistical mixture and from standard probability theory. It does not rely on quantum mechanics. This implies a stringent consistency condition on any hybrid scheme. We may not know how things work in a hybrid system when they interact, but we know that in the absence of interaction each sector behaves in the standard way. Therefore, let the interaction be switched off for $t < t_0$, and let the state at t_0 be $(x,k) = (x_0,k_0)$ in the classical sector and $|\psi_\alpha\rangle$ in the quantum sector. The interaction is connected for $t > t_0$ and the evolution depends on the hybrid scheme adopted. In fact, we can consider all such evolutions for all possible initial $|\psi_\alpha\rangle$ [but the same (x_0,k_0)]. Let $\mathcal{A}_\alpha(t)$ be the expectation value of any hybrid observable A for each α at time t. Whenever two mixtures $\{p_\alpha\}$ and $\{p'_\alpha\}$ produce the same density matrix at $t = t_0$,

$$\hat{\rho} = \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha| = \sum_\alpha p'_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|, \tag{3.7}$$

we should demand that

$$\sum_\alpha p_\alpha \mathcal{A}_\alpha(t) = \sum_\alpha p'_\alpha \mathcal{A}_\alpha(t) \quad \text{for } t \geqslant t_0 \text{ and for any observable } A. \tag{3.8}$$

The reason is that for $t \leqslant t_0$ the two states described by $\{p_\alpha\}$ and $\{p'_\alpha\}$ are identical, if quantum mechanics is correct and complete for the isolated quantum sector. Therefore, the evolution at later times of the two states should also be identical, regardless of the nature of the hybrid dynamics.

A hybrid scheme violating the condition contained in Eq. (3.8) would automatically provide an experimental way to discriminate between two mixtures which, according to quantum mechanics, are indistinguishable, and presumably would provide, for any mixture, its true decomposition into pure states. Such true pure states would be a type of hidden variables in quantum mechanics, as quantum mechanics is blind to them. This possibility should be rejected: If such hybrid scheme is applied to describe the measurement process in quantum mechanics, the measurement apparatus being classical, the fact that the scheme distinguishes mixtures with the same density matrix would be in contradiction with what is known about expectation values and measurements in quantum mechanics. So a hybrid system violating Eq. (3.8) is either inconsistent or of limited applicability. For want of a better name, we refer to the requirement just introduced as *statistical consistency*.[3]

The mean-field scheme violates this condition. To see this, consider a collection of alternative pure states $|\psi_\alpha\rangle$ at t_0 in the quantum sector with a common state (x_0,k_0) in the classical sector, and let each hybrid state have its evolution. In the mean-field dynamics, the evolution of the expectation of an observable takes the form

$$\frac{d}{dt}\langle A\rangle_\alpha = \frac{1}{i\hbar}\langle [A,H]\rangle_\alpha + \{\langle A\rangle_\alpha, \langle H\rangle_\alpha\}. \tag{3.9}$$

Multiplying by p_α, summing over α, and taking $t = t_0$, we can see that the last term cannot be expressed in terms of $\sum_\alpha p_\alpha |\psi_\alpha(t)\rangle\langle\psi_\alpha(t)|$, due to the lack of linearity in the dynamics. Hence, statistical consistency is lost.

For instance, for a classical particle with quantum spin and Hamiltonian $H = \frac{\lambda}{2}\boldsymbol{x}^2\boldsymbol{k}\cdot\boldsymbol{\sigma}$, let the state at t_0 be $(\boldsymbol{x}_0,\boldsymbol{k}_0)$, and unpolarized spin. To implement this, let us choose an arbitrary axis $\hat{\boldsymbol{n}}$ and let the pure spin states be $|\uparrow\rangle$ and $|\downarrow\rangle$, each with probability one half. At t_0 one finds $\frac{d}{dt}\langle \boldsymbol{k}\cdot\boldsymbol{\sigma}\rangle = -\lambda\hat{\boldsymbol{n}}\cdot\boldsymbol{x}_0\hat{\boldsymbol{n}}\cdot\boldsymbol{k}_0$. The dependence on $\hat{\boldsymbol{n}}$ breaks statistical consistency.[4]

The mean-field evolution in Eq. (3.9) can be also written as

$$\frac{d}{dt}\mathrm{tr}\,(\hat\rho A) = \frac{1}{i\hbar}\mathrm{tr}\,(\hat\rho[A,H]) + \{\mathrm{tr}\,(\hat\rho A), \mathrm{tr}\,(\hat\rho H)\}, \tag{3.10}$$

where $\hat\rho = |\psi_\alpha(t)\rangle\langle\psi_\alpha(t)|$ (no sum over α). The equation written in this form suggests to propose this very dynamics but now inserting in $\hat\rho$ a general density matrix. In this case $\hat\rho$ would evolve according to

$$\begin{aligned} \frac{dx_i}{dt} &= \frac{\partial}{\partial k_i}\mathrm{tr}\,(\hat\rho H), \\ \frac{dk_i}{dt} &= -\frac{\partial}{\partial x_i}\mathrm{tr}\,(\hat\rho H), \quad i\hbar\frac{d}{dt}\hat\rho = [H,\hat\rho]. \end{aligned} \tag{3.11}$$

Unfortunately, such evolution is not consistent with the meaning of statistical mixture. That meaning implies that, given two alternative situations $\hat\rho_1$ and $\hat\rho_2$ with probabilities p_1 and p_2, the mixture $\hat\rho = p_1\hat\rho_1 + p_2\hat\rho_2$ at $t = t_0$ should remain so at any other time. Each alternative represents a possible different history and, by definition of expectation value, one should have a weighted average of the two histories, $\langle A\rangle_\rho = p_1\langle A\rangle_{\rho_1} + p_2\langle A\rangle_{\rho_2}$, at any time. So, in practice, linearity in $\hat\rho$ is required and this constraint is not fulfilled by Eq. (3.10).[5]

Hybrid schemes like those considered in Sec. II, where observables are operator valued functions in the classical phase space, meet the requirement of statistical consistency. They can be formulated using the combined density matrix of quantum and classical sectors, $\hat\rho(x,k)$, with the following linear evolution:

$$\frac{d}{dt}\hat\rho(x,k) = [\hat H(x,k),\hat\rho(x,k)]. \tag{3.12}$$

Therefore, the issue of the manifold decomposition of the density matrix into pure states is never raised. (However, these dynamics are subject to the no-go theorem of Sec. II.) On the other hand, hybrid schemes which do not preserve the linearity of quantum mechanics are likely to have trouble with the requirement of statistical consistency. Conflicts with the principle of locality have been also observed [7,29], one again rooted in the nonlinearity of the scheme. The critique in this latter reference applies also to the nonlinear models considered in Ref. [81], and presumably these models are also in conflict with statistical consistency.

IV. STATISTICAL ENSEMBLE IN CONFIGURATION SPACE

A. The scheme

In the statistical ensemble approach in configuration space (SECS) of [65,66], the basic state of a quantum-classical hybrid system is described by two real functions, $P(x,q)$ and $S(x,q)$, defined on configuration space, x being the classical coordinates and q the quantum ones. $P(x,q)$ represents the probability density function of the state (x,q) and so it is non-negative and normalized.[6]

When the quantum sector is missing, the pair $P(x)$ and $S(x)$ represents a particular type of mixed

[3]The name "mixture independence" would be also suitable to emphasize that a scheme can be mathematically consistent even if it does not enjoy this property [80].

[4]This example suggests restoring statistical consistency in the mean-field approach by making a suitable average over all possible decompositions of a given density matrix into pure states, $\hat\rho = \sum_\alpha p_\alpha|\psi_\alpha\rangle\langle\psi_\alpha|$. In the example above, a rotational average over $\hat{\boldsymbol{n}}$ seems appropriate. It is not clear to us whether, in the general case, there is a natural density probability function defined on the set of choices p_α, and to what extent this procedure would be an improvement regarding consistency.

[5]Strictly speaking, linearity means preservation of the relation $\hat\rho = \lambda_1\hat\rho_1 + \lambda_2\hat\rho_2$, for any real weights $\lambda_{1,2}$, while we only need non-negative weights $p_{1,2}$.

[6]Following [65,66], we use x, q, $\int dx\,dq$, etc., although x and q represent sets of several coordinates.

state, namely, that with phase-space probability density function

$$\rho(x,k) = P(x)\delta(k - \nabla S(x)). \tag{4.1}$$

This form is preserved by the purely classical dynamics. Using Hamilton's equations to evolve x and k, one finds the evolution of P and S. For a classical particle with mass M in presence of a potential $V(x,t)$,

$$\frac{\partial P}{\partial t} = -\frac{1}{M}\nabla(P\nabla S), \quad \frac{\partial S}{\partial t} = -\frac{1}{2M}(\nabla S)^2 - V. \tag{4.2}$$

The first relation is the continuity equation and the second one is the Hamilton-Jacobi equation. They can be derived from a canonical bracket. For two functionals of P and S, $\mathcal{A}$ and $\mathcal{B}$,

$$\{\mathcal{A},\mathcal{B}\} = \int dx \left(\frac{\delta\mathcal{A}}{\delta P(x)}\frac{\delta\mathcal{B}}{\delta S(x)} - \frac{\delta\mathcal{A}}{\delta S(x)}\frac{\delta\mathcal{B}}{\delta P(x)}\right). \tag{4.3}$$

Hence, $d\mathcal{A}/dt = \{\mathcal{A},\mathcal{H}\}$, with Hamiltonian

$$\mathcal{H} = \int dx P \left(\frac{1}{2M}(\nabla S)^2 + V\right). \tag{4.4}$$

Likewise, when the classical sector is missing, the quantum state is a pure state with wave function

$$\psi(q) = P(q)^{1/2}e^{iS(q)/\hbar}. \tag{4.5}$$

For a quantum particle with mass m in a potential $V(q,t)$, the Schrödinger equation evolves the pair $P(q)$ and $S(q)$ as

$$\begin{aligned}\frac{\partial P}{\partial t} &= -\frac{1}{m}\nabla(P\nabla S),\\ \frac{\partial S}{\partial t} &= -\frac{1}{2m}(\nabla S)^2 + \frac{\hbar^2}{2m}\frac{\nabla^2 P^{1/2}}{P^{1/2}} - V.\end{aligned} \tag{4.6}$$

This evolution derives from a bracket similar to the classical one (with q instead of x), this time with Hamiltonian

$$\mathcal{H} = \int dq\ P\left(\frac{1}{2m}(\nabla S)^2 + \frac{\hbar^2}{8m}(\nabla \ln P)^2 + V\right). \tag{4.7}$$

So in this approach the quantum description differs from the classical one just by the term with explicit $\hbar$ in $\mathcal{H}$.

The guiding principle to introduce hybrid quantum-classical systems is that new degrees of freedom are to be added exactly in the same way as is done in the purely classical or purely quantum cases, namely, by adding new coordinates in the functions P and S. The hybrid case is then described by $P(x,q)$ and $S(x,q)$, and the dynamical bracket is

$$\{\mathcal{A},\mathcal{B}\} = \int dx\, dq \left(\frac{\delta\mathcal{A}}{\delta P(x,q)}\frac{\delta\mathcal{B}}{\delta S(x,q)} - \frac{\delta\mathcal{A}}{\delta S(x,q)}\frac{\delta\mathcal{B}}{\delta P(x,q)}\right). \tag{4.8}$$

For classical and quantum particles interacting through a potential $V(x,q,t)$,

$$\mathcal{H} = \int dx\, dq\ P \times \left(\frac{1}{2M}(\nabla_x S)^2 + \frac{1}{2m}(\nabla_q S)^2 + \frac{\hbar^2}{8m}(\nabla_q \ln P)^2 + V\right), \tag{4.9}$$

and this produces the hybrid evolution equations

$$\begin{aligned}\frac{\partial P}{\partial t} &= -\frac{1}{M}\nabla_x(P\nabla_x S) - \frac{1}{m}\nabla_q(P\nabla_q S),\\ \frac{\partial S}{\partial t} &= -\frac{1}{2M}(\nabla_x S)^2 - \frac{1}{2m}(\nabla_q S)^2 + \frac{\hbar^2}{2m}\frac{\nabla_q^2 P^{1/2}}{P^{1/2}} - V.\end{aligned} \tag{4.10}$$

The scheme extends straightforwardly to more general quantum systems (e.g., with spin degrees of freedom).

In this approach observables are represented by their expectation value, as real valued functionals of P and S. (The Hamiltonians above follow this rule.) So a classical observable $f(x,k)$ is represented by the functional

$$\mathcal{F} = \int dx\, dq\ P f(x,\nabla_x S), \tag{4.11}$$

whereas a quantum observable $\hat{A}$ is represented by the functional

$$\begin{aligned}\mathcal{A} &= \int dx\ \langle\psi(x)|\hat{A}|\psi(x)\rangle,\\ \psi(x,q) &= \langle q|\psi(x)\rangle = P(x,q)^{1/2}e^{iS(x,q)/\hbar}.\end{aligned} \tag{4.12}$$

The Hamiltonian and equations of motion of the SECS approach in Eqs. (4.9) and (4.10) are written in terms of the classical-like variables P and S. It is also instructive to write them using the quantumlike wave function $\psi(x,q)$. In this case ψ and $i\hbar\psi^*$ are the canonical variables. In the new variables, the equations read

$$\begin{aligned}\mathcal{H} = \int dx\, dq \Big(&\frac{\hbar^2}{2M}|\nabla_x\psi|^2 + \frac{\hbar^2}{2m}|\nabla_q\psi|^2\\ &+ V|\psi|^2 - \frac{\hbar^2}{2M}(\nabla_x|\psi|)^2\Big),\end{aligned} \tag{4.13}$$

$$i\hbar\frac{\partial}{\partial t}\psi = \left(-\frac{\hbar^2}{2M}\nabla_x^2 - \frac{\hbar^2}{2m}\nabla_q^2 + \frac{\hbar^2}{2M}\frac{\nabla_x^2|\psi|}{|\psi|} + V\right)\psi. \tag{4.14}$$

The equation of motion is similar to the Schrödinger equation except for the nonlinear term introduced by the effective potential

$$V_{\rm eff}(x,q) = \frac{\hbar^2}{2M}\frac{\nabla_x^2|\psi|}{|\psi|}. \tag{4.15}$$

This term renders the x degree of freedom into a classical one and is responsible for the nonlinearity with respect to $\psi(x,q)$ in the SECS approach.

The SECS approach passes a number of tests listed in Refs. [65–67]. However, it has some limitations too.[7]

There is a problem in the definition of which functionals $\mathcal{A}[P,S]$ are acceptable as observables. The statistical interpretation of P requires the observables to be homogeneous functionals of degree one in P. Some further constraints are

[7]Let us emphasize from the outset that the no-go theorem of Sec. II does not directly apply to the SECS approach for two reasons to be discussed below: First, the product of two general observables is not defined, and second, the dynamical bracket between different sectors is not always zero.

noted in Refs. [65,66] to ensure positivity of P during the dynamical evolution and global phase invariance of the wave function (this is required to implement gauge invariance and so a consistent electromagnetic coupling[8]). However, these conditions still leave an enormous set of functionals. To see that restrictions are needed to select true observables out of this set of functionals, consider a purely classical system. There, a term

$$\mathcal{H}_1 = \int dx\, P(x) \frac{\hbar^2}{8M} [\nabla \ln P(x)]^2 \tag{4.16}$$

added to the Hamiltonian passes all the noted conditions, but still it is not acceptable as a genuine observable, because in classical mechanics we already know which functionals correspond to true observables, to wit, those of the form

$$\mathcal{F} = \int dx\, P f(x, \nabla_x S). \tag{4.17}$$

Note that $\mathcal{H}_1$ in Eq. (4.16) is identical to the term in the Hamiltonian of Eq. (4.9) which distinguishes the quantum degree of freedom from the classical one; that is, the "interaction" $\mathcal{H}_1$ would turn the classical particle (one that obeys the Hamilton-Jacobi equation) into a quantum particle (one that obeys the Schrödinger equation). Likewise, a quantum particle could be turn into a classical one by switching on a suitable interaction term, namely, by subtracting the term analogous to $\mathcal{H}_1$ in the q sector. Any such functionals should be rejected as genuine observables in the purely classical or, respectively, in the purely quantum cases.

The previous argument suggests that also in the hybrid case most functionals are completely unrelated to observables. In the purely classical or purely quantum cases, the growth in the number of observables when new degrees of freedom are added is limited. As noted above, new observables in the full system are obtained by tensor product of the observables in the subsectors. However, the product of a classical observable with a quantum observable is not automatically defined in the SECS approach to hybrid systems: The blocks $f(x, \nabla_x S)$ and $\hat{A}$ do not commute in general ($\hat{A}$ acts on q and S contains q). Of course, one could introduce some symmetrization prescription [plus possible $O(\hbar)$ terms], thus defining a set of hybrid observables.[9] However, this is not sufficient because it should be verified that such set is closed upon application of the dynamical bracket, and this condition is far from trivial.

Another problem of the SECS approach is that the bracket of a generic quantum observable with a generic classical observable is not zero [66]. This is a serious problem because, as noted above, it implies that the classical Hamiltonian induces an evolution in the quantum sector and vice versa, even when no interaction is taking place between both sectors. Such a bracket vanishes only for particular observables or for particular configurations [66]. An instance of such special configuration is the separable one:

$$P(x,q,t) = P(x,t)P(q,t), \quad S(x,q,t) = S(x,t) + S(q,t). \tag{4.18}$$

(Of course, the various functions P and the various functions S are different; we let their arguments distinguish them.) The separable case represents sectors which never interact. It is easy to verify that, in the absence of interaction between sectors, the separable form is preserved by the evolution. In the separable case the classical sector does not act on the quantum one and vice versa. However, this is not sufficient for a consistent dynamics. If the interaction between sectors is switched on during a certain time interval and then set to zero, the configuration will no longer be separable; the two sectors are *entangled*. Then one would find that, even though the two sectors are no longer connected, what happens to one sector affects the other.

A concrete observable affected by such ghost coupling induced by "hybrid entanglement" is the kinetic energy [66]. For instance, according to the SECS approach, if a neutral *free* classical particle is "entangled" with a charged quantum one, an electromagnetic wave acting upon the quantum particle would induce a variation with the same frequency in the energy of the classical particle. By all accounts, the kinetic energy of a (hypothetical) classical particle would be a *bona fide* observable quantity and so the ghost coupling seems odd. (See, however, the discussion in Ref. [66] for a different opinion.) The roles of quantum and classical can be exchanged with a similar conclusion. It should be noted that the entanglement does not produce such effect in the quantum-quantum case or in the classical-classical case. In those cases the bracket of different sectors vanishes, as one would expect.

Instead of using the nonvanishing of the bracket, the same effect can be seen from the evolution of the marginal probability distribution of (x,k)

$$\rho(x,k) = \int dq\, P(x,q)\, \delta(k - \nabla_x S(x,q)). \tag{4.19}$$

In the separable case this reduces to $P(x)\,\delta(k - \nabla_x S(x))$, so what happens to the quantum sector has no effect on the classical sector. However, in the general entangled case it would seem that the evolution of q will produce some effect even if there is no interaction. In fact, this is not so straightforward as it would seem. Note that the same naive argument would apply in the classical-classical case. However, in that case, using the evolutions of $P(x,q)$ and $S(x,q)$ (with $\hbar \to 0$) it can be shown that the net effect vanishes because it comes in the form of a total derivative with respect to q. In the quantum-classical case a similar cancellation occurs for the marginal distribution of x (hence for observables depending only on x and not on k) and also for the special case of $\langle k \rangle$ [66], but not for the full $\rho(x,k)$, due to the extra term $\hbar^2/(2m)\nabla_q^2 P^{1/2}/P^{1/2}$ in the evolution of $S(x,q)$.

There is a related difficulty with conservation of angular momentum in the presence of spin. The simplest setting to

[8]For classical and quantum particles with charge Q_1 and Q_2, minimal coupling is achieved by the replacements $\nabla_x S \to \nabla_x S - Q_1 A(x,t)$, $\nabla_q S \to \nabla_q S - Q_2 A(q,t)$, $V \to V + Q_1\phi(x,t) + Q_2\phi(q,t)$ in $\mathcal{H}$. The dynamics is invariant under the gauge transformations: $P(x,q,t) \to P(x,q,t)$, $S(x,q,t) \to S(x,q,t) + Q_1\Lambda(x,t) + Q_2\Lambda(q,t)$, $A \to A + \nabla\Lambda$, $\phi \to \phi - \partial_t\Lambda$. Observe that the electromagnetic field is not dynamical here.

[9]Note that once the product of a classical observable, A_1, with a quantum observable, A_2, is defined, the product of general observables is straightforwardly defined by $(A_1A_2)(B_1B_2) = (A_1B_1)(A_2B_2)$.

show this is a classical particle $(\boldsymbol{x},\boldsymbol{k})$ with quantum spin $\frac{1}{2}$.[10] The wave function of the hybrid system [analogous to $\psi(x,q)$ in Eq. (4.12)] is

$$\psi_a(\boldsymbol{x}) = P_a^{1/2}(\boldsymbol{x})e^{iS_a(\boldsymbol{x})/\hbar}. \tag{4.20}$$

In the present case $q = a = \pm\frac{1}{2}$ is a discrete label, so we put it as a subindex. $\hbar a$ is the projection of the spin along some quantization axis. In order to define the angular momentum, we should specify the action of the rotation group. The obvious way is to regard $\psi_a(\boldsymbol{x})$ as a bispinor with respect to a (since this is the only choice when the classical sector is not present). Hence, for a rotation R with axis $\hat{\boldsymbol{n}}$ and angle ϕ,

$$\psi_a(\boldsymbol{x}) \to (e^{-i\phi\hat{\boldsymbol{n}}/2}\psi)_a(R^{-1}\boldsymbol{x}). \tag{4.21}$$

This procedure correctly defines a representation of the rotation group, and the generator can be realized (using the dynamical bracket) by means of an observable:

$$\begin{aligned}\boldsymbol{J} &= \boldsymbol{L} + \boldsymbol{S} \\ &= \int d^3x \sum_{a,b} \psi_a^*(\boldsymbol{x}) \left(-i\hbar\, \boldsymbol{x}\times\boldsymbol{\nabla}\delta_{ab} + \frac{\hbar}{2}\boldsymbol{\sigma}_{ab}\right)\psi_b(\boldsymbol{x}).\end{aligned} \tag{4.22}$$

Note that the orbital (classical) part can be written equivalently in the form

$$\boldsymbol{L} = \int d^3x \sum_a P_a(\boldsymbol{x})\, \boldsymbol{x}\times\boldsymbol{\nabla}S_a(\boldsymbol{x}). \tag{4.23}$$

So $\boldsymbol{L}$ and $\boldsymbol{S}$ are the angular momenta observables to be expected for the classical and for the quantum systems. In the present case, the symmetry group guarantees that the bracket of $\boldsymbol{L}$ with $\boldsymbol{S}$ vanishes and that $\boldsymbol{J}$, $\boldsymbol{L}$, $\boldsymbol{S}$ are all of them angular momenta; that is, they fulfill the commutation relations of the so(3) algebra. The bracket of $\boldsymbol{J}$ with an observable yields the effect of an infinitesimal rotation on the observable.

Let the hybrid particle be free. The Hamiltonian contains just the kinetic energy,

$$\mathcal{H} = \int d^3x \sum_a \frac{1}{2M} P_a(\boldsymbol{x})[\boldsymbol{\nabla}S_a(\boldsymbol{x})]^2. \tag{4.24}$$

Note that everything is fixed and there is no freedom to change anything. Unfortunately, $\mathcal{H}$ is not at all an invariant functional under spin rotations. $P_a(\boldsymbol{x})$ and $S_a(\boldsymbol{x})$ do not have good transformation properties under rotations. In particular, they are not bispinors. This means that for each choice of quantization axis, $\mathcal{H}$ represents a different functional.[11] As can be shown in detail, the bracket $\{\boldsymbol{J},\mathcal{H}\}$ is not zero, so the Hamiltonian is not rotationally invariant, and conversely, the angular momentum is not conserved. ($\boldsymbol{L}$ is conserved but $\boldsymbol{S}$ is not.) Of course, if $(\boldsymbol{x},\boldsymbol{k})$ and a are not entangled, $P_a(\boldsymbol{x}) = P(\boldsymbol{x})P_a$, $S_a(\boldsymbol{x}) = S(\boldsymbol{x}) + S_a$, these problems do not arise. It is instructive to note that the free *quantum-quantum* Hamiltonian,

$$\begin{aligned}&\int d^3x \sum_a \frac{\hbar^2}{2M}|\boldsymbol{\nabla}\psi_a(\boldsymbol{x})|^2 \\ &= \int d^3x \sum_a \left(\frac{1}{2M}P_a(\boldsymbol{x})[\boldsymbol{\nabla}S_a(\boldsymbol{x})]^2 + \frac{\hbar^2}{8M}\frac{[\boldsymbol{\nabla}P_a(\boldsymbol{x})]^2}{P_a(\boldsymbol{x})}\right),\end{aligned} \tag{4.25}$$

is rotationally invariant but the two terms in the right-hand side are not separately invariant. [The first term, without $\hbar$, is the Hamiltonian of Eq. (4.24).]

The problem seems to be ubiquitous for the implementation of internal symmetries in the quantum sector, due to the nonlinear nature of the approach. This can be seen from the modified Schrödinger equation obeyed by the extended wave function $\psi_a(x,q)$ of the hybrid system, a being a generic internal index,

$$i\hbar\frac{\partial}{\partial t}\psi_a = \left(-\frac{\hbar^2}{2M}\nabla_x^2 - \frac{\hbar^2}{2m}\nabla_q^2 + \frac{\hbar^2}{2M}\frac{\nabla_x^2|\psi_a|}{|\psi_a|} + V\right)\psi_a. \tag{4.26}$$

The effective potential $V_a(x,q) = (\hbar^2/2M)\nabla_x^2|\psi_a|/|\psi_a|$, which turns x into a classical degree of freedom, tends to break any internal symmetry carried by the index a. This is also an impediment to describing relativistic particles with spin. The same problem pointed out for spin-$\frac{1}{2}$ particles reappears if one tries to couple the electromagnetic field to classical charged particles, if the photon is a quantum dynamical degree of freedom.

All the difficulties noted for the SECS have a common root. They stem from the hybrid description

$$\psi(x,q) = P(x,q)^{1/2}e^{iS(x,q)/\hbar}. \tag{4.27}$$

Here q represents the configuration label of a basis $|q\rangle$ of the Hilbert space of the quantum system. The separable case describes two sectors that never interact. This case is of limited interest, so we consider the entangled case. If x and q are entangled, a change of basis $|q\rangle$ affects in a nontrivial way the other sector: It modifies the marginal distribution of the classical sector and in particular its kinetic energy.

Formally, the pair $[P(x,q),S(x,q)]$ carries the same information as $\psi(x,q)$, but the former description is better suited for the purely classical case and the second description is better suited for purely quantum case [just consider how linear superposition of quantum states reflects on the pair (P,S)]. Using a common language for the quantum and classical sectors, by means of any of these two descriptions for the classical-quantum case, does not by itself solve the problem of quantum-classical hybridization. A canonical transformation in the classical-classical case acts naturally on $[P(x,q),S(x,q)]$, but a unitary transformation in q acts awkwardly. Likewise, a classical canonical transformation on x acts in an unnatural way on $\psi(x,q)$ regarded as a wave function.

If q does not have a classical limit, as happens for the spin or other internal labels, there is no natural choice of basis $|q\rangle$ and each choice produces different evolution even with

[10] Everything can be repeated, with the same conclusions, for a classical particle interacting with a quantum particle having spin $\frac{1}{2}$. In this case we would have $\psi_a(x,q)$. The case considered in the text would follow by assuming that the motion of the quantum particle can be neglected.

[11] Once again one could consider taking an average over all choices of axis, hence restoring the rotational invariance. However, the resulting Hamiltonian would contain $\boldsymbol{\sigma}$ and so it would represent an interaction between the two sectors rather than a free particle.

no interaction present between (entangled) sectors. However, even when it seems that there is a privileged choice of basis, like q labeling the position of a quantum particle, the problem remains. Indeed, the dynamical evolution is nothing else than a continued canonical transformation, produced by the dynamical bracket. In the quantum case this is a continued change of orthonormal basis. In the classical case it is a continued change of canonical coordinates. Hence, the root of the difficulties is that the two types of canonical transformations are not compatible because the two sectors carry two different values of $\hbar$.

B. Statistical consistency of the scheme

In this section we examine the statistical consistency of the configuration space ensemble approach to hybrid systems. As discussed in Sec. III a nonlinear scheme is unlikely to fulfill statistical consistency. This is the case of the SECS approach, and in fact the situation is even worse than that found for the mean-field approach. For the mean-field dynamics the failure came from the *quantum* version of the statistical consistency requirement; that is, different evolutions were obtained from different decompositions of a single quantum density matrix. In the SECS approach the failure takes place even for the *classical* version of the requirement (as well as for the quantum one). This means the following. The SECS is based on the evolution of classical ensembles of the type $[P(x),S(x)]$ in Eq. (4.1). This by no means represents the most general classical ensemble, $\rho(x,k)$. In turn, a generic $\rho(x,k)$ can be decomposed in many different ways as a combination of ensembles (P,S),

$$\rho(x,k) = \sum_\alpha p_\alpha P_\alpha(x)\,\delta(k - \nabla S_\alpha(x)). \tag{4.28}$$

This follows from the fact that α runs over the set of all possible pairs $[P(x),S(x)]$ and so the number of possible p_α is much larger than that of possible probability density functions $\rho(x,k)$. Because only $\rho(x,k)$ is meaningful, it should be demanded that different decompositions produce the same evolution. This requirement is, of course, true in the purely classical case [$\rho(x,k,t)$ fulfills the autonomous Liouville equation which is consistent because it is linear] but it fails to hold for the hybrid evolution.[12]

To show this, we take the noncontroversial case of a classical particle and a quantum particle without internal degrees of freedom, interacting through a potential $V(x,q,t)$. To test statistical consistency we can consider the expectation value of observables of the form $\mathcal{A}(t) = \int dx\,dq\; P(x,q,t)\,A(x,q,t)$. These are hybrid observables and should be admissible since the potential belongs to this class. Of course, we can trade the information contained in the expectation values of all these observables by the probability density $P(x,q,t)$. So $P(x,q,t)$ is itself an observable.

We assume a set of possible histories labeled by an index α, each history with probability p_α. At $t = t_0$ all hybrid states are separable with a common quantum state $\psi(q)$, and classical state described by a pair $[P_\alpha(x),S_\alpha(x)]$. For simplicity we assume a time-independent potential $V(x,q)$ for $t > t_0$. The expectation value of the observables of the type described above, taken over the set of histories, depends on the probability density

$$P(x,q,t) = \sum_\alpha p_\alpha P_\alpha(x,q,t), \tag{4.29}$$

where $P_\alpha(x,q,t)$ is the probability density of the history α, as obtained by the hybrid evolution of the SECS approach.

Statistical consistency requires that $P(x,q,t)$ should depend only on the initial classical probability density function $\rho(x,k)$ and not on its decomposition into histories [Eq. (4.28)]. We call *statistical invariants* the quantities which are independent of the concrete decomposition. Hence, $\rho(x,k)$, as well as $\psi(q)$ and $V(x,q)$, are invariants and all other invariants, including $P(x,q,t)$, derive from them. It is useful to classify the nontrivial invariants [i.e., not involving $\psi(q)$ and $V(x,q)$] by the number of derivatives they carry. These invariants are

$$\begin{aligned} I_{n_1,n_2}(x) &= \nabla^{n_1}\int dk\,k^{n_2}\rho(x,k) \\ &= \sum_\alpha p_\alpha \nabla^{n_1}[P_\alpha(\nabla S_\alpha)^{n_2}], \quad n_1,n_2 = 0,1,2,\ldots \end{aligned} \tag{4.30}$$

Now, the function $P(x,q,t)$ can be computed as a Taylor series in $t - t_0$. Inspection of the evolution equations (4.10) indicates that each finite order term in the Taylor expansion will contain a finite number of derivatives with respect to x and q of the initial data and the potential. If statistical consistency holds, the combinations of derivatives allowed cannot be arbitrary; on the contrary, they should involve the invariants in Eq. (4.30). Subsequently, we show that this is not the case. The breakdown occurs for the first time at order $(t - t_0)^4$. The length of the Taylor coefficients increases rapidly with the order. For this reason, instead of presenting the proof using generic functions, we take a concrete case which is sufficient to prove the breakdown of statistical consistency.

Specifically, let the system evolve in $1 + 1$ dimensions, and

$$\begin{aligned} t_0 = 0, \quad P_\alpha(x,q,t_0) = e^{l_\alpha(x)+\kappa q}, \\ S_\alpha(x,q,t_0) = 0, \quad V(x,q) = vxq. \end{aligned} \tag{4.31}$$

Here $l_\alpha(x)$ are generic functions and κ,v are two real constants. [The wave function $\psi(q)$ is not normalizable as given. This is inessential. The proof can be carried out for generic functions, or we can add a Gaussian factor. Alternatively, the equations are local, and the form assumed in Eq. (4.31) is used only locally.]

[12]Pure classical states (x_α,k_α) could be used to make a standard decomposition of $\rho(x,k)$, since they can be cast in the (P,S) form, for example, with $P_\alpha(x) = \delta(x - x_\alpha)$ and $S_\alpha(x) = k_\alpha x$. The problem [apart from $P_\alpha(x)$ being too singular for using it in the hybrid dynamics Eq. (4.10)] is that, for generic interactions, the form of $S_\alpha(x)$ is not preserved by the classical evolution, so one should be prepared to prove that the evolution does not depend on the concrete of choice of $S_\alpha(x)$. Besides, the lack of statistical consistency in the quantum sense remains.

The evolution equations (4.10) can be conveniently written in terms of the variable $L(x,q,t) = \ln[P(x,q,t)]$,

$$L_t = -\frac{1}{M}(L_x S_x + S_{xx}) - \frac{1}{m}(L_q S_q + S_{qq}),$$
$$S_t = -\frac{1}{2M}S_x^2 - \frac{1}{2m}S_q^2 + \frac{\hbar^2}{8m}\left(L_q^2 + 2L_{qq}\right) - V. \tag{4.32}$$

When S vanishes at $t = 0$ and V is an even function of t, it follows [from inspection of Eq. (4.32)] that S is an odd function of t and P or L is even. [Equivalently, Eq. (4.26) admits a solution with $\psi(x,q,t) = \psi^*(x,q,-t)$.] These conditions hold in our case, so $L_\alpha(x,q,t)$ contains only even powers of t and $S_\alpha(x,q,t)$ contains only odd powers. Straightforward solution of the equations yields

$$L_\alpha = l_\alpha + \kappa q + \left(\frac{v}{M}l'_\alpha q + \frac{v\kappa}{m}x\right)\frac{t^2}{2} + \left(-\frac{\hbar^2\kappa v}{4mM^2}(l'_\alpha l''_\alpha + l'''_\alpha) + O(\hbar^0)\right)\frac{t^4}{4!} + O(t^6),$$
$$S_\alpha = \left(\frac{\hbar^2\kappa^2}{8m} - vxq\right)t + \left(\frac{\hbar^2\kappa v}{4mM}l'_\alpha - \frac{v^2}{M}q^2 - \frac{v^2}{m}x^2\right)\frac{t^3}{3!} + O(t^5). \tag{4.33}$$

In the term of order t^4 we have omitted contributions without $\hbar$. For the probability density [using $P_\alpha = e^{L_\alpha}$ in Eq. (4.29)] this implies

$$\left.\frac{\partial^4 P(x,q,t)}{\partial t^4}\right|_{t=0} = -\frac{\hbar^2\kappa v}{4mM^2}e^{\kappa q}\sum_\alpha p_\alpha e^{l_\alpha}(l'_\alpha l''_\alpha + l'''_\alpha) + O(\hbar^0). \tag{4.34}$$

The sum over α in this expression is not a statistical invariant. From Eq. (4.30), the invariant with $n_1 = 3$ and $n_2 = 0$ is found to be

$$I_{3,0}(x) = \sum_\alpha p_\alpha e^{l_\alpha}[(l'_\alpha)^3 + 3l'_\alpha l''_\alpha + l'''_\alpha]. \tag{4.35}$$

Therefore, classical statistical consistency is violated at order t^4. It can be verified that there is no violation in the purely classical case; that is, the terms without $\hbar$ involve statistical invariants only, and this is true also for generic initial data.

V. CONCLUSIONS

We have discussed the conditions for a perfect quantum-classical hybrid dynamics and have presented a short and general proof implying that such perfect hybridization is not viable. This result relies on the assumption that (i) hybrid observables can be obtained by tensor product and that, also in the hybrid case, there is a bracket which is (ii) antisymmetric, (iii) a derivation, and (iv) reduces to the standard brackets in each subsector.

We have then introduced a consistency requirement for quantum-classical hybrids based on rearrangement invariance of statistical mixtures; that is, the observable properties of the state should depend on the mixture itself and not on how it was obtained. Such invariance is automatically fulfilled by classical and quantum dynamics, but it is a nontrivial requirement for quantum-classical hybrids of nonlinear type. In particular, an autonomous consistent evolution equation for the density matrix cannot be written for the mean-field approach and so statistical consistency is violated by this scheme.

The SECS is analyzed in some detail. This approach is rather complicated technically since it is highly nonlinear. We point out several problematic features of this scheme. First, no systematic construction of hybrid observables by tensor product is provided. This avoids the immediate application of the no-go theorem,[13] but it implies an enormous proliferation of hybrid functionals, the large majority of which cannot possibly correspond to observables. As a consequence of this ambiguity it is not known whether the set of observables is closed under the operation of taking the dynamical bracket. Certainly one could start by taking the bracket between classical and quantum observables and then recursively with the new functionals so generated close the minimal subalgebra containing quantum and classical observables [66]. However, the bracket of a generic classical observable with a generic quantum one is already so complicated that our own conjecture is that such minimal subalgebra is essentially the whole (or a very large) set of functionals, most of which are certainly not observables. Second, the bracket of a generic classical observable with a generic quantum observable is not zero. This leads to ghost interaction between the two sectors when they are entangled, even after the coupling is no longer present. In particular, the kinetic energy of one sector responds to physical actions on the other sector, which seems odd. The scheme is designed to treat position-momentum variables, and so it is of limited applicability in the presence of internal degrees of freedom, including conservation of spin angular momentum, internal symmetries, and relativistic invariance for particles with spin, such as electrons or photons. Statistical consistency of the SECS has been studied too. We find that, as for the mean-field case, the requirement is not fulfilled, a consequence of the lack of linearity of the hybrid dynamics. Specifically, it was shown that identical classical statistical mixtures obtained from different rearrangements evolved differently after switching on the interaction.

The above analysis tends to reinforce the view that truly classical systems do not exist in nature and quantum-classical dynamics are to be regarded as approximations of fully quantum mechanical systems.

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[13] More importantly, the proof of the theorem also assumes a vanishing bracket between different sectors, and this assumption does not hold in the SECS approach.

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