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Quantum-classical hybrid dynamics – a summary

Hans-Thomas Elze

Dipartimento di Fisica “Enrico Fermi”, Università di Pisa, Largo Pontecorvo 3, I-56127 Pisa, Italia

E-mail: elze@df.unipi.it

Abstract. A summary of a recently proposed description of quantum-classical hybrids is presented, which concerns quantum and classical degrees of freedom of a composite object that interact directly with each other. This is based on notions of classical Hamiltonian mechanics suitably extended to quantum mechanics.

1. Introduction

We briefly review an attempt to construct a theory that describes *quantum-classical hybrids*, consisting of quantum mechanical and classical objects that interact directly with each other [1, 2, 3]. Hybrids might exist as a fundamentally different species of composite objects “out there”, with consequences for the range of applicability of quantum mechanics, or they may serve in an approximate description of certain complex quantum systems.

The concept of quantum-classical hybrids has recently been employed, in order to explore a hypothetical direct coupling of classical time machines to quantum objects [4], while the application of hybrid dynamics to the experiment proposed by Penrose *et al.* [5], which is intended to test the existence of “Schrödinger cat” states of spatially displaced macroscopic objects, and to the manipulation of entanglement among two q-bits is presently under study [6].

2. Quantum-classical hybrids

The direct coupling of quantum mechanical (QM) and classical (CL) degrees of freedom – “*hybrid dynamics*” – departs from quantum mechanics. Details of our approach can be found in Refs. [1, 2, 3], where also additional references and discussion of related works are presented.

Hybrid dynamics has been researched extensively for various reasons. – For example, the Copenhagen interpretation of quantum mechanics entails the measurement problem which, together with the fact that quantum mechanics needs interpretation, in order to be operationally well defined, may indicate that it needs amendments. Such as a theory of the *dynamical* coexistence of QM and CL objects. This should have impact on the measurement problem [7] as well as on the description of the interaction between quantum matter and (possibly) classical spacetime [8].

Furthermore, it is of great practical interest to better understand QM-CL hybrids appearing in QM approximation schemes addressing many-body systems or interacting fields, which are naturally separable into QM and CL subsystems; for example, representing fast and slow degrees of freedom, mean fields and fluctuations, *etc.* (See also the article by Hu and Subasi in this volume for an informative discussion of some related issues [9].)



Concerning the hypothetical emergence of quantum mechanics from some coarse-grained deterministic dynamics (see Refs. [10, 11, 12] with numerous references to related work), the quantum-classical backreaction problem might appear in new form, namely regarding the interplay of fluctuations among underlying deterministic and emergent QM degrees of freedom. Which can be rephrased succinctly as: “*Can quantum mechanics be seeded?*”

2.1. Consistency requirements

Thus, there is ample motivation for the numerous attempts to formulate a satisfactory hybrid dynamics. Generally, however, they are deficient in one or another respect. Which has led to various no-go theorems, in view of the lengthy list of desirable properties or consistency requirements that “*the*” hybrid theory should fulfil, see, for example, Refs. [13, 14]:

- Conservation of energy.
- Conservation and positivity of probability.
- Separability of QM and CL subsystems in the absence of their interaction, recovering the correct QM and CL equations of motion, respectively.
- Consistent definitions of states and observables; existence of a Lie bracket structure on the algebra of observables that suitably generalizes Poisson and commutator brackets.
- Existence of canonical transformations generated by the observables; invariance of the classical sector under canonical transformations performed on the quantum sector only and *vice versa*.
- Existence of generalized Ehrenfest relations (*i.e.* the correspondence limit) which, for bilinearly coupled CL and QM oscillators, are to assume the form of the CL equations of motion (“Peres-Terno benchmark” test [15]).
- ‘Free Will’ [16].
- Locality.
- No-signalling.
- QM / CL symmetries and ensuing separability carry over to hybrids.

These issues have also been discussed for the hybrid ensemble theory of Hall and Reginatto, which does conform with the first six points listed [17, 18] but is in conflict with the last two [1, 19, 20].

We have proposed an alternative theory of hybrid dynamics based on notions of phase space [1]. This extends work by Heslot, demonstrating that quantum mechanics can entirely be rephrased in the language and formalism of classical analytical mechanics [21]. Introducing unified notions of states on phase space, observables, canonical transformations, and a generalized quantum-classical Poisson bracket, this has led to the intrinsically linear hybrid theory to be summarized in the following, which allows to fulfil *all* of the above consistency requirements.

Recently Burić and collaborators have shown that the dynamical aspects of our proposal can indeed be derived for an all-quantum mechanical composite system by imposing constraints on fluctuations in one subsystem, followed by suitable coarse-graining [22, 23, 24].

3. A representation of quantum mechanics in classical terms

We recall that evolution of a *classical* object can be described in relation to its $2n$ -dimensional phase space, its *state space*. A real-valued regular function on this space defines an *observable*, *i.e.*, a differentiable function on this smooth manifold.

There always exist (local) systems of *canonical coordinates*, commonly denoted by (x_k, p_k) , $k = 1, \dots, n$, such that the *Poisson bracket* of any pair of observables f, g assumes the standard form (Darboux's theorem):

$$\{f, g\} = \sum_k \left(\frac{\partial f}{\partial x_k} \frac{\partial g}{\partial p_k} - \frac{\partial f}{\partial p_k} \frac{\partial g}{\partial x_k} \right) . \quad (1)$$

This is consistent with $\{x_k, p_l\} = \delta_{kl}$, $\{x_k, x_l\} = \{p_k, p_l\} = 0$, $k, l = 1, \dots, n$, and has the properties defining a Lie bracket operation, mapping a pair of observables to an observable.

General transformations \mathcal{G} of the state space are restricted by compatibility with the Poisson bracket structure to so-called *canonical transformations*, which do not change physical properties of an object. They form a Lie group and it is sufficient to consider infinitesimal transformations. An *infinitesimal transformation* \mathcal{G} is *canonical*, if and only if for any observable f the map $f \rightarrow \mathcal{G}(f)$ is given by $f \rightarrow f' = f + \{f, g\}\delta\alpha$, with some observable g , the so-called *generator* of \mathcal{G} , and $\delta\alpha$ an infinitesimal real parameter. – Thus, for example, the canonical coordinates transform as follows:

$$x_k \rightarrow x'_k = x_k + \frac{\partial g}{\partial p_k} \delta\alpha , \quad p_k \rightarrow p'_k = p_k - \frac{\partial g}{\partial x_k} \delta\alpha . \quad (2)$$

This illustrates the fundamental relation between observables and generators of infinitesimal canonical transformations in classical Hamiltonian mechanics.

Following Heslot's work, we learn that the previous analysis can be generalized and applied to quantum mechanics; this concerns the dynamical aspects as well as the notions of states, canonical transformations, observables, and measurements [21].

The following derives from the fact that the *Schrödinger equation* and its adjoint are *Hamiltonian equations* following from an action principle [1]. We must add the *normalization condition*, $\mathcal{C} := \langle \Psi(t) | \Psi(t) \rangle \stackrel{!}{=} 1$, for all state vectors $|\Psi\rangle$, which is essential for the probability interpretation of amplitudes; state vectors that differ by an unphysical constant phase are to be identified. Thus, the *QM state space* is formed by the rays of the underlying Hilbert space.

3.1. Oscillator representation

A unitary transformation describes QM evolution, $|\Psi(t)\rangle = \hat{U}(t - t_0)|\Psi(t_0)\rangle$, with $U(t - t_0) = \exp[-i\hat{H}(t - t_0)/\hbar]$, solving the Schrödinger equation. Thus, a stationary state, characterized by $\hat{H}|\phi_i\rangle = E_i|\phi_i\rangle$, with real energy eigenvalue E_i , performs a harmonic motion, *i.e.*, $|\psi_i(t)\rangle = \exp[-iE_i(t - t_0)/\hbar]|\psi_i(t_0)\rangle \equiv \exp[-iE_i(t - t_0)/\hbar]|\phi_i\rangle$. We assume a denumerable set of such states. Following these observations, it is quite natural to introduce what we may call the *oscillator representation*.

We expand state vectors with respect to a complete orthonormal basis, $\{|\Phi_i\rangle\}$:

$$|\Psi\rangle = \sum_i |\Phi_i\rangle (X_i + iP_i)/\sqrt{2\hbar} , \quad (3)$$

where the time dependent coefficients are separated into real and imaginary parts, X_i, P_i . This expansion allows to evaluate the *Hamiltonian function* defined by $\mathcal{H} := \langle \Psi | \hat{H} | \Psi \rangle$:

$$\mathcal{H} = \frac{1}{2\hbar} \sum_{i,j} \langle \Phi_i | \hat{H} | \Phi_j \rangle (X_i - iP_i)(X_j + iP_j) =: \mathcal{H}(X_i, P_i) . \quad (4)$$

Choosing the set of energy eigenstates, $\{|\phi_i\rangle\}$, as basis of the expansion, we obtain:

$$\mathcal{H}(X_i, P_i) = \sum_i \frac{E_i}{2\hbar} (P_i^2 + X_i^2) , \quad (5)$$

hence the name *oscillator representation*. – Evaluating $|\dot{\Psi}\rangle = \sum_i |\Phi_i\rangle (\dot{X}_i + i\dot{P}_i)/\sqrt{2\hbar}$ according to Hamilton's equations with \mathcal{H} of Eq. (4) or (5), gives back the Schrödinger equation. – Furthermore, the *normalization condition* becomes:

$$\mathcal{C}(X_i, P_i) = \frac{1}{2\hbar} \sum_i (X_i^2 + P_i^2) \stackrel{!}{=} 1 . \quad (6)$$

Thus, the vector with components given by (X_i, P_i) , $i = 1, \dots, N$, is confined to the surface of a $2N$ -dimensional sphere with radius $\sqrt{2\hbar}$, which presents a major difference to CL Hamiltonian mechanics.

The (X_i, P_i) may be considered as *canonical coordinates* for the state space of a QM object. Correspondingly, we introduce a *Poisson bracket*, cf. Eq.(1), for any two *observables* on the *spherically compactified state space*, i.e. real-valued regular functions F, G of the coordinates (X_i, P_i) :

$$\{F, G\} = \sum_i \left(\frac{\partial F}{\partial X_i} \frac{\partial G}{\partial P_i} - \frac{\partial F}{\partial P_i} \frac{\partial G}{\partial X_i} \right) . \quad (7)$$

As usual, time evolution of an observable O is generated by the Hamiltonian: $dO/dt = \partial_t O + \{O, \mathcal{H}\}$. In particular, we find that the constraint of Eq. (6) is conserved: $d\mathcal{C}/dt = \{\mathcal{C}, \mathcal{H}\} = 0$.

3.2. Canonical transformations and quantum observables

In the following, we recall briefly the compatibility of the notion of observable introduced in passing above – as in classical mechanics – with the usual QM one. This can be demonstrated rigourously by the implementation of canonical transformations and analysis of the role of observables as their generators. For details, see Refs. [1, 2, 3, 21].

The Hamiltonian function has been defined as observable in Eq. (4), which relates it directly to the corresponding QM observable, namely the expectation of the self-adjoint Hamilton operator. This is indicative of the general structure with the following most important features.

3.2.1. Compatibility of unitary transformations and Poisson structure. – Classical canonical transformations are automorphisms of the state space which are compatible with the Poisson bracket. Automorphisms of the QM Hilbert space are implemented by unitary transformations. This implies a transformation of the canonical coordinates (X_i, P_i) here. From this, one derives the invariance of the Poisson bracket defined in Eq. (7) under unitary transformations. Consequently, the *unitary transformations on Hilbert space are canonical transformations on the (X, P) state space*.

3.2.2. Self-adjoint operators as observables. – Any infinitesimal unitary transformation \hat{U} can be generated by a self-adjoint operator \hat{G} , such that: $\hat{U} = 1 - (i/\hbar)\hat{G}\delta\alpha$, which leads to the QM relation between an observable and a self-adjoint operator. By a simple calculation, one obtains:

$$X_i \rightarrow X'_i = X_i + \frac{\partial\langle\Psi|\hat{G}|\Psi\rangle}{\partial P_i}\delta\alpha , \quad P_i \rightarrow P'_i = P_i - \frac{\partial\langle\Psi|\hat{G}|\Psi\rangle}{\partial X_i}\delta\alpha . \quad (8)$$

From these equations, the relation between an observable G , defined in analogy to classical mechanics (as above), and a self-adjoint operator \hat{G} can be inferred:

$$G(X_i, P_i) = \langle\Psi|\hat{G}|\Psi\rangle , \quad (9)$$

i.e., by comparison with the classical result. Hence, a *real-valued regular function* G of the state is an observable, if and only if there exists a self-adjoint operator \hat{G} such that Eq. (9) holds. This implies that all QM observables are quadratic forms in the X_i 's and P_i 's, which are essentially fewer than in the corresponding CL case. Interacting QM-CL hybrids require additional discussion, cf. below.

3.2.3. Commutators as Poisson brackets. – From the relation (9) between observables and self-adjoint operators and the Poisson bracket (7) one derives:

$$\{F, G\} = \langle \Psi | \frac{1}{i\hbar} [\hat{F}, \hat{G}] | \Psi \rangle , \quad (10)$$

with both sides of the equality considered as functions of the variables X_i, P_i and with the commutator defined as usual. Hence, the QM commutator is a Poisson bracket with respect to the (X, P) state space and relates the algebra of its observables to the algebra of self-adjoint operators.

In conclusion, quantum mechanics shares with classical mechanics an even dimensional state space, a Poisson structure, and a related algebra of observables. It differs essentially by a restricted set of observables and the requirements of phase invariance and normalization, which compactify the underlying Hilbert space to the complex projective space formed by its rays.

4. Quantum-classical Poisson bracket, hybrid states and their evolution

The far-reaching parallel of classical and quantum mechanics, as we have seen, suggests to introduce a *generalized Poisson bracket* for QM-CL hybrids:

$$\{A, B\}_\times := \{A, B\}_{\text{CL}} + \{A, B\}_{\text{QM}} \quad (11)$$

$$:= \sum_k \left(\frac{\partial A}{\partial x_k} \frac{\partial B}{\partial p_k} - \frac{\partial A}{\partial p_k} \frac{\partial B}{\partial x_k} \right) + \sum_i \left(\frac{\partial A}{\partial X_i} \frac{\partial B}{\partial P_i} - \frac{\partial A}{\partial P_i} \frac{\partial B}{\partial X_i} \right) , \quad (12)$$

of any two observables A, B defined on the Cartesian product of CL and QM state spaces. It shares the usual properties of a Poisson bracket. – Note that due to the convention introduced by Heslot [21], to which we adhered in Sect. 3, the QM variables X_i, P_i have dimensions of (action)^{1/2} and, consequently, no \hbar appears in Eqs. (11)–(12). At the expense of introducing appropriate rescalings, these variables could be made to have their usual dimensions and \hbar to appear explicitly here. – For the remainder of this article, instead, we choose units such that $\hbar \equiv 1$.

Let an observable “belong” to the CL (QM) sector, if it is constant with respect to the canonical coordinates of the QM (CL) sector. Then, the $\{ , \}_\times$ -bracket has the important properties:

- It reduces to the Poisson brackets introduced in Eqs. (1) and (7), respectively, for pairs of observables that belong *either* to the CL *or* the QM sector.
- It reduces to the appropriate one of the former brackets, if one of the observables belongs only to either one of the two sectors.
- It reflects the *separability* of CL and QM sectors, since $\{A, B\}_\times = 0$, if A and B belong to different sectors.

Hence, if a canonical transformation is performed on the QM (CL) sector only, then observables that belong to the CL (QM) sector remain invariant.

4.1. The hybrid phase space density

The hybrid density ρ for a self-adjoint density operator $\hat{\rho}$ in a given state $|\Psi\rangle$ is defined by [1] :

$$\rho(x_k, p_k; X_i, P_i) := \langle \Psi | \hat{\rho}(x_k, p_k) | \Psi \rangle = \frac{1}{2} \sum_{i,j} \rho_{ij}(x_k, p_k) (X_i - iP_i)(X_j + iP_j) \quad , \quad (13)$$

using Eq. (3) and $\rho_{ij}(x_k, p_k) := \langle \Phi_i | \hat{\rho}(x_k, p_k) | \Phi_j \rangle = \rho_{ji}^*(x_k, p_k)$. It describes a *QM-CL hybrid ensemble* by a real-valued, positive semi-definite, normalized, and possibly time dependent regular function on the Cartesian product state space canonically coordinated by $2(n + N)$ -tuples $(x_k, p_k; X_i, P_i)$; the variables x_k, p_k , $k = 1, \dots, n$ and X_i, P_i , $i = 1, \dots, N$ are reserved for CL and QM sectors, respectively.

Note that the relation between an observable in (X, P) -space and a self-adjoint operator, Eq. (9), can be written as: $G(X_i, P_i) = \text{Tr}(|\Psi\rangle\langle\Psi|\hat{G})$, with the QM pure state acting as one-dimensional projector here. Concerning the hybrid density ρ , we may use the representation of $\hat{\rho}$ in terms of its eigenstates, $\hat{\rho} = \sum_j w_j |j\rangle\langle j|$, to obtain:

$$\rho(x_k, p_k; X_i, P_i) = \sum_j w_j(x_k, p_k) \text{Tr}(|\Psi\rangle\langle\Psi|j\rangle\langle j|) = \sum_j w_j(x_k, p_k) |\langle j | \Psi \rangle|^2 \quad , \quad (14)$$

with $0 \leq w_j \leq 1$ and $\sum_j \int \Pi_l(dx_l dp_l) w_j(x_k, p_k) = 1$. – This shows that $\rho(x_k, p_k; X_i, P_i)$ is the *probability density to find in the hybrid ensemble the QM pure state $|\Psi\rangle$* , parametrized by X_i, P_i through Eq. (3), *together with the CL state* given by a point in phase space, specified by coordinates x_k, p_k .

Further remarks about superposition, pure/mixed, or separable/entangled QM states that may enter the hybrid density can be found in Ref. [2, 23]. Generally, the simplest observable-like form of ρ – a bilinear function of QM “phase space” variables X_i, P_i , as above – has to be replaced for interacting hybrids, allowing for the form of an *almost-classical observable*; see Sect. 5.4 in [1] and a more detailed study discussing measurements in [3].

In particular, the density ρ evolves according to the hybrid Liouville equation (see the following subsection). This will lead to a solution $\rho(x_k, p_k; X_i, P_i; t)$ that is not necessarily bilinear in the QM variables X_i, P_i . However, we can (re)construct the self-adjoint density operator for the QM subsystem of the hybrid by:

$$\hat{\rho}(x_k, p_k; t) = \Gamma_N^{-1} \int_{\delta S_{2N}(\sqrt{2})} \Pi_i(dX_i dP_i) \rho(x_k, p_k; X_i, P_i; t) |\Psi(X_i, P_i)\rangle \langle \Psi(X_i, P_i)| \quad , \quad (15)$$

i.e., conditioned on the state of the CL subsystem parametrized by (x_k, p_k) and consistent with Eq. (13); the measure of integration here has been evaluated in detail in Ref. [1].

4.2. Phase space evolution

The *Liouville equation* for the evolution of hybrid ensembles [1] must be based on the generalized Poisson bracket defined in Eqs. (11)–(12) and Liouville’s theorem. This leads us to:

$$-\partial_t \rho = \{\rho, \mathcal{H}_\Sigma\}_\times \quad , \quad (16)$$

with $\mathcal{H}_\Sigma \equiv \mathcal{H}_\Sigma(x_k, p_k; X_i, P_i)$ and:

$$\mathcal{H}_\Sigma := \mathcal{H}_{\text{CL}}(x_k, p_k) + \mathcal{H}_{\text{QM}}(X_i, P_i) + \mathcal{I}(x_k, p_k; X_i, P_i) \quad , \quad (17)$$

defining the relevant Hamiltonian function, including a hybrid interaction; \mathcal{H}_Σ is required to be an *observable*, in order to have a meaningful notion of energy. – Note that *energy conservation* follows from $\{\mathcal{H}_\Sigma, \mathcal{H}_\Sigma\}_\times = 0$.

Finally, the Liouville equation describes a Hamiltonian flow, which implies that:

- The normalization and positivity of the probability density ρ are conserved in presence of a hybrid interaction; hence, its interpretation remains valid under hybrid evolution.

5. Conclusion

Besides constructing the QM-CL hybrid formalism, as outlined here, and showing how it conforms with the strong consistency requirements presented in Sec. 2.1, we earlier discussed the possibility to have classical-environment induced decoherence, quantum-classical backreaction, a deviation from the Hall-Reginatto proposal [17, 18] in presence of translation symmetry, and closure of the algebra of hybrid observables [1, 3, 22]. Questions of locality, symmetry vs. separability, incorporation of superposition, separable, and entangled QM states, and ‘Free Will’ were considered in Ref. [2, 16, 23], while an exotic application to (a class of) time machines coupled to quantum mechanical degrees of freedom has been shown in Ref. [4] and further studies of the Penrose *et al.* experiment, designed to study reduction (or not) of macroscopic Schrödinger cat states [5], and of entanglement control are underway [6].

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