Hybrid quantum-classical models as constrained quantum systems

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Constrained Hamiltonian description of the classical limit is utilized in order to derive consistent dynamical equations for hybrid quantum-classical systems. Starting with a compound quantum system in the Hamiltonian formulation conditions for classical behavior are imposed on one of its subsystems and the corresponding hybrid dynamical equations are derived. The presented formalism suggests that the hybrid systems have properties that are not exhausted by those of quantum and classical systems.

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A. Introduction

Fundamental assumption of quantum mechanics is that the evolution of an isolated quantum system is given by the linear Schröedinger equation. On the other hand, all macroscopic systems usually obey nonlinear evolution equations of classical mechanics to an excellent approximation. The classical and the quantum theory have developed different formalism to successfully describe interactions between systems belonging to their respective domains. Correlations between quantum objects are mathematically captured by the direct product structure of the Hilbert spaces. On the other hand compound classical systems are described on the Cartesian product of the component’s phase spaces. Attempts to formulate a consistent dynamical theory of interacting quantum-classical, commonly called hybrid, systems are numerous as is illustrated by the following rather partial list of references [1-8]. Current technologies are sufficiently developed to enable experimental studies of the interaction between typically quantum and typically classical objects [9, 10], but such experiments require detailed preliminary theoretical models.

In this work the framework of the theory of Hamiltonian dynamical systems is used to treat the hybrid quantum-classical systems and to develop a description of the interactions within such systems which is consistent with the main physically justified requirements. In fact, it is well known [6,11-17] that quantum mechanics can be formalized as a Hamiltonian dynamical system with the corresponding phase space and with the quantum observables described by functions which are quadratic forms of the canonical variables. More general functions on the quantum phase space do not have any physical interpretation. This formalism is used in [8] to develop a description of the hybrid classical-quantum systems by treating both, quantum and classical, formally as Hamiltonian systems described in the Hamiltonian language. The coupling between the systems is introduced somewhat ad hoc as if both systems were classical, just because they are both described in the framework of the Hamiltonian dynamical systems. This assumption about the treatment of compound systems is not trivially obvious. For example, such treatment of coupling between two quantum systems, both separately described in the Hamiltonian framework, would be incorrect. In this paper we start with the total compound quantum system in the geometric Hamiltonian framework. The next step is to consider a classical limit of one of the component systems. To this purpose we utilize our recently developed theory of general quantum constraints within the Hamiltonian approach [13], and the corresponding description of the classical limit [16, 17]. The classical behavior of one of the components is accomplished by constraining the Hamiltonian evolution so that the quantum fluctuations of the would be classical degrees of freedom remain minimal for all times. This in effect constrains the evolution onto a manifold which is the Cartesian product of the quantum phase space of the quantum subsystem and the manifold corresponding to the coherent states of the would be classical one. The evolution equations for the interacting hybrid systems are obtained in the macro limit applied on the coarse-grained subsystem and the constrained Hamiltonian equations. The Hamiltonian form of the derived evolution equations of the hybrid system turns out to be the same as the one postulated in Ref. [8] and therefore satisfies a list of standard requirements collected and tested in [8]. We also provide a discussion of a puzzling fact, pointed out also in [8], regarding the physical interpretation of functions of both the classical and the quantum degrees of freedom.

B. Selective Coarse-graining and hybrid dynamics

The framework of constrained Hamiltonian description for the treatment of quantum systems with nonlinear constraints and its application on the problem of classical limit was developed and discussed in [16, 17] and shall not be repeated here. Here we apply the general theory in order to derive consistent dynamical equations for the hybrid systems. Consider a quantum system composed of two quantum subsystems, for convenience fancifully called the first and the second. The Hilbert space of the composite is \( H = H_1 \otimes H_2 \) and the quantum phase space of the composite is denoted \( \mathcal{M} \). An arbitrary vector from \( \mathcal{H} \) is denoted \( |\psi\rangle \) and the corresponding point from \( \mathcal{M} \)
has complex canonical coordinates \((\psi(x), \psi^*(x))\) which are expansion coefficients in a basis \(\{\langle x|\}\) of \(|\psi\rangle\) and its dual vector. The Poisson bracket of a two functions on \(M\) is given by

\[
\{f_1, f_2\}_M = \frac{1}{i\hbar} \int dx \left( \frac{\delta f_1}{\delta \psi(x)} \frac{\delta f_2}{\delta \psi^*(x)} - \frac{\delta f_2}{\delta \psi(x)} \frac{\delta f_1}{\delta \psi^*(x)} \right).
\]

The notation for the basis \(\{|x]\}\) and the integral in (1) should be understood symbolically and could denote a denumerable or finite basis and summation respectively. The Schrödinger i.e. the Hamiltonian evolution is generated by the function \(H(\psi, \psi^*) = \langle \psi|H_1 + H_2 + H_{12}|\psi\rangle\), where the meaning of the notation is obvious.

For the sake of simpler presentation we shall consider the system such that the first of the subsystems is in a coherent state and there is no entanglement always in a coherent state and there is no entanglement.

\[
F(X_\psi) = \sum_{i=1}^k (\Delta \tilde{q}_i)^2 + (\Delta \tilde{p}_i)^2 - \min = 0,
\]

is preserved minimal during the evolution. This condition represents a nonlinear constraint on the admissible states of the total system. The evolution of the fully quantum composite system must be modified in such a way that the constraint is respected, and to this end we use the method developed in [15, 16]. The manifold \(\tilde{\Gamma}\) of the constraint (2) is a nonlinear symplectic submanifold of \(\tilde{\Gamma}\) locally isomorphic with the Cartesian product \(\Gamma_1 \times \Gamma_2\), where \(\Gamma_1\) is the manifold of the standard Heisenberg algebra minimal uncertainty coherent states (MUCS) of the first subsystem, denoted by \(|\alpha\rangle\) or \(|q,p\rangle\), and \(\Gamma_2 \sim H_2\) is the quantum phase space of the second subsystem. Therefore, at each point \(|C\rangle\) of \(\Gamma_1 \times \Gamma_2\) given by

\[
|\langle C|\rangle = |\alpha\rangle|\omega_2\rangle \equiv |q,p\rangle|\omega_2\rangle,
\]

there are local symplectic coordinates \((q, p, \omega_2(x_2), \omega_2^*(x_2))\) expressed in terms of \(|\langle C|\rangle\) as \(q = \langle \langle C|\langle q|\rangle\rangle\), \(p = \langle \langle C|\langle p|\rangle\rangle\) and \(\omega_2(x_2) = \langle \langle x_2|\langle q,p|\rangle\rangle\). The vectors \(\{|x_2\rangle\}\) symbolize a basis in \(H_2\) not necessarily the generalized eigen-basis of some multiplication operator as the notation might suggest. Notice that the requirement of minimal quantum fluctuations set only on the first subsystem automatically implies that the first subsystem is always in a coherent state and there is no entanglement between the two subsystems. Also, there can be no entanglement between the degrees of freedom of the first subsystem. No restriction on the type of the second subsystem is set by the constraint (2), so the quantum subsystem can be in an entangled state.

The fundamental assumption concerning the dynamics of the putative hybrid system is that the nonlinear constraint (2) is preserved during such evolution. This ensures that the first subsystem is minimally quantum (as closest as possible to classical) while the second subsystem is quantum in nature. Thus, our proposal for the dynamical equations of these coupled subsystems are the Hamiltonian equations given by the original Hamiltonian plus the additional terms that guarantee the preservation of the constraint (2). The resulting equations will by construction preserve the minimally quantum nature of the first subsystem.

The constrained manifold \(\tilde{\Gamma}\) is symplectic and in this case, as was explained in detail in [16], the constrained system is Hamiltonian with the Hamilton’s function given by the original Hamilton’s function \(\langle \psi|\hat{H}|\psi\rangle\) evaluated on the constrained manifold. Therefore, the dynamics is generated by the Poisson bracket on \(M\) and the Hamiltonian

\[
\hat{H}_t = \langle C|\langle \hat{H}_{\alpha}|\rangle\langle \hat{H}_{\alpha}\rangle|C\rangle = \langle \psi|\hat{H}_{\alpha}|\psi\rangle\langle q,p|\hat{H}_{\alpha}|q,p\rangle|\psi\rangle = \langle \psi|\hat{H}_{\alpha}|q,p\rangle|\psi\rangle,
\]

where \(\hat{H}_{\alpha}(q,p) = |q,p\rangle\langle q,p| \otimes \langle q,p|\hat{H}|q,p\rangle\). In fact the constrained evolution of an arbitrary function-observable \(A(\psi) = \langle \langle \hat{A}|\psi\rangle\rangle\) on the constrained manifold is obtained by reducing the following equation

\[
\hat{A}(\psi) = \{ A(\psi), H_1 \}_M = \frac{1}{i\hbar} \int dx \left( \frac{\delta A(\psi)}{\delta \psi(x)} \frac{\delta H}{\delta \psi^*(x)} - \frac{\delta H}{\delta \psi(x)} \frac{\delta A(\psi)}{\delta \psi^*(x)} \right)
\]

on the constrained manifold \(\tilde{\Gamma}\).

For example, before reduction on \(\tilde{\Gamma}\) the dynamical equation for \(q = \langle \langle \tilde{q}|\rangle\rangle\) and \(p = \langle \langle \tilde{p}|\rangle\rangle\) are given, by

\[
\dot{q} = \frac{1}{i\hbar} \langle \langle \hat{q}|\hat{\Gamma}_1|\psi\rangle\rangle + \frac{\partial H_{\alpha}}{\partial p}, \quad \dot{p} = \frac{1}{i\hbar} \langle \langle \hat{p}|\hat{\Gamma}_1|\psi\rangle\rangle - \frac{\partial H_{\alpha}}{\partial q}.
\]

Short computation shows that the first terms in these equations are in fact equal to zero on the constrained manifold \(\tilde{\Gamma}\). In fact, for an arbitrary operator \(\hat{A}\) acting only in \(H_1\) one has \(\langle \langle \hat{A}|\hat{\Gamma}_1|\psi\rangle\rangle|_F = 0\). Therefore, the dynamical equations for the first system’s coordinates and momenta are

\[
\dot{q} = \frac{\partial H_{\alpha}}{\partial p} \quad \dot{p} = -\frac{\partial H_{\alpha}}{\partial q}.
\]

Let us now compute the dynamical equations for the functions of the form

\[
\omega_2(x_2) = \langle \langle x_2|\omega_2(\psi)\rangle\rangle = \langle \langle x_2|\langle q,p|\psi\rangle\rangle\.
\]

Starting again with the equation

\[
\dot{\omega}_2(x_2) = \frac{1}{i\hbar} \int dx \left( \frac{\delta \omega_2}{\delta \psi(x)} \frac{\delta H_{\alpha}}{\delta \psi^*(x)} - \frac{\delta H_{\alpha}}{\delta \psi(x)} \frac{\delta \omega_2}{\delta \psi^*(x)} \right)
\]
and after somewhat lengthy calculation one obtains before the reduction on $\Gamma$

$$\begin{align*}
\hbar \omega_2(x_2) &= \langle x_2 | \langle \hat{q}, \hat{p} \rangle \hat{H} | q, p \rangle | \omega_2 \rangle \\
&+ \left( \frac{q \partial H_1}{2 \partial q} + \frac{p \partial H_1}{2 \partial p} \right) \omega_2(x_2) \\
&+ \frac{i}{\hbar} \langle x_2 | \langle \hat{q}, \hat{p} \rangle (\hat{p} - p/2) \rangle | \psi \rangle \langle \psi | \hat{H}_a | \psi \rangle \\
&- \frac{i}{\hbar} \langle x_2 | \langle \hat{q}, \hat{p} \rangle (\hat{q} - q/2) \rangle | \psi \rangle \langle \psi | \hat{H}_a | \psi \rangle \rangle. \quad (10)
\end{align*}$$

Upon reduction on the constrained manifold $\Gamma$ the last two terms are annulled and the relevant dynamical equations can be written in the form

$$\begin{align*}
\hbar \omega_2(x_2) &= \langle x_2 | \langle \alpha | \hat{H} | \alpha \rangle | \omega_2 \rangle + \left( \frac{q \partial H_1}{2 \partial q} + \frac{p \partial H_1}{2 \partial p} \right) \omega_2(x_2). \\
& \quad \text{(11)}
\end{align*}$$

The last term of this equation implies pure phase change and can be gauged away resulting with

$$\begin{align*}
\hbar \omega_2(x_2; \psi) &= \langle x_2 | \langle \alpha | \hat{H} | \alpha \rangle | \omega_2(\psi) \rangle. \quad (12)
\end{align*}$$

The equation (12) has the form of a Schrödinger equation for the state vector $\omega_2(x_2; \psi) = \langle x_2 | \langle \psi | q, p \rangle \rangle \in \mathcal{H}_2$, with the Hamiltonian operator $\langle \alpha | \hat{H} | \alpha \rangle$ acting on $\mathcal{H}_2$ and depending on $q = \langle \psi | q \rangle$ and $p = \langle \psi | p \rangle$.

The dynamical equations (7) and (12) can be written as Hamiltonian dynamical equations in local coordinates on the constrained manifold $\Gamma$ by introducing the Poisson bracket on $\Gamma$ for arbitrary functions on $\Gamma$ represented in the local coordinates $(q, p, \omega_2, \omega_2^*)$ as

$$\begin{align*}
\{f_1, f_2 \}_\Gamma &= \sum_{i=1}^{k} \left( \frac{\partial f_1}{\partial q_i} \frac{\partial f_2}{\partial p_i} - \frac{\partial f_1}{\partial p_i} \frac{\partial f_2}{\partial q_i} \right), \\
+ \frac{1}{\hbar} \int dx_2 \left( \frac{\partial f_1}{\partial \omega_2(x_2)} \frac{\delta f_2}{\delta \omega_2^*(x_2)} - \frac{\delta f_2}{\delta \omega_2(x_2)} \frac{\partial f_1}{\partial \omega_2^*(x_2)} \right). \quad (13)
\end{align*}$$


Thus, the Hamiltonian form of the hybrid system on the constrained manifold $\Gamma$ as the phase space reeds

$$\begin{align*}
\dot{q} &= \{ q, H_1 \}_\Gamma, \quad \dot{p} = \{ p, H_1 \}_\Gamma, \\
\dot{\omega}_2 &= \{ \omega_2, H_1 \}_\Gamma, \quad \dot{\omega}_2^* = \{ \omega_2^*, H_1 \}_\Gamma,
\end{align*}$$

where the Hamilton’s function $H_1(q, p, \omega_2(x_2), \omega_2^*(x_2))$ in local coordinates on $\Gamma$ is given by (4).

At this point we may briefly discuss the case of general i.e. mixed quantum states. Such a state is given by a positive normalized function on $\mathcal{M}$ which has quadratic dependence on the canonical coordinates $(\psi, \psi^*)$. Restriction of such a function on the nonlinear submanifold $\Gamma$ results with a function $\rho(q, p, \omega_2(x_2), \omega_2^*(x_2))$ which depends quadratic on $(\omega_2(x_2), \omega_2^*(x_2))$. On the other hand, $\rho(q, p, \omega_2(x_2), \omega_2^*(x_2))$ for fixed $(\omega_2(x_2), \omega_2^*(x_2))$ can be an arbitrary positive function of $(q, p)$ with a unit integral over $\Gamma$, since $(q, p)$ are not a subset of the canonical coordinates on $\mathcal{M}$, but are physical observables $q = \langle \langle \psi | q | \psi \rangle \rangle$, $p = \langle \langle \psi | p | \psi \rangle \rangle$. In fact they are a subset of the canonical coordinates on the nonlinear submanifold $\Gamma$. In terms of the Poisson bracket on $\Gamma$ the dynamics of $\rho(q, p, \omega_2(x_2), \omega_2^*(x_2))$ is given by the corresponding Liouville equation

$$\begin{align*}
\dot{\rho}(q, p, \omega_2, \omega_2^*) &= \{ H_1(q, p, \omega_2, \omega_2^*), \rho(q, p, \omega_2, \omega_2^*) \}_\Gamma. \quad (16)
\end{align*}$$

The constrained dynamics which preserves minimal value of the quantum fluctuations of one of the subsystems is only the first step. The second step is the relevant macro-limit so that the minimal quantum fluctuations still present in the corresponding coherent states can be neglected when compared with actual values of the dynamical variables. Therefore the macro-limit should be applied on the equations (14) relevant for the first subsystem. This is illustrated in the following example.

**I. AN EXAMPLE: TWO 1/2-SPINS AND A CLASSICAL NONLINEAR OSCILLATOR**

Consider a system of interacting equal qubits each coupled to the same nonlinear oscillator. The quantum Hamiltonian of the total system is

$$\hat{H} = \varepsilon \hat{\sigma}_1^z + \varepsilon \hat{\sigma}_2^z + \mu \hat{\sigma}_1^x \hat{\sigma}_2^x + \frac{\mu^2}{2m} + V(\hat{q}) + \hat{q} \left( \lambda_1 \hat{\sigma}_1^z + \lambda_2 \hat{\sigma}_2^z \right),$$

where $V(\hat{q})$ is a polynomial expression in terms of $\hat{q}$ such that $d^2V(q)/dq^2 |_{\hat{q}=0} = m\Omega^2$. The constraining and the macro-limit will be applied on the nonlinear oscillator subsystem.

The total Hamilton function of the constrained system is $H_t = \langle \mathcal{C}(\psi) | \hat{H} | \mathcal{C}(\psi) \rangle$, where $\langle \mathcal{C}(\psi) \rangle = \langle q, p | \omega \rangle$. The complex coefficients of an arbitrary $\omega = c_1 + c_2 \hat{\sigma}_1 + c_3 \hat{\sigma}_2 + c_4 \hat{\sigma}_1 \hat{\sigma}_2$ are real and imaginary components are the canonical coordinates given by $(x_i, y_i) = \sqrt{2}(\text{Re}(c_i), \text{Im}(c_i))$, $i = 1, 2, 3, 4$. The expectation of the spin part of the Hamiltonian (17) in the vector $|\mathcal{C}\rangle$ is

$$H_s = \varepsilon(\hat{x}_1^2 + \hat{x}_2^2 - \hat{y}_1^2 - \hat{y}_2^2) + \mu(\hat{y}_2 \hat{x}_4 + \hat{y}_4 \hat{x}_2 + \hat{x}_2 \hat{x}_4 + \hat{x}_1 \hat{x}_3),$$

the expectation in a vector $|\mathcal{C}\rangle$ of the interaction part is

$$H_{int} = \lambda_1 \hat{q}(\hat{y}_1^2 + \hat{y}_2^2 - \hat{y}_3^2 - \hat{y}_4^2 + \hat{x}_1^2 + \hat{x}_2^2 - \hat{x}_3^2 - \hat{x}_4^2)/2 + \lambda_2(\hat{y}_1^2 - \hat{y}_2^2 + \hat{y}_3^2 - \hat{y}_4^2 + \hat{x}_1^2 - \hat{x}_2^2 + \hat{x}_3^2 - \hat{x}_4^2)/2, \quad (19)$$

where $q = \langle q, p | q, p \rangle$ is the coherent state expectation of the oscillator’s coordinate. Finally, the $|\mathcal{C}\rangle$ expectation of the oscillator’s Hamiltonian is

$$H_{osc} = \frac{p^2}{2m} + V(q) + \sum_{k=1}^{\infty} \frac{1}{2k!} \frac{\hbar^k V^{(2k)}(q)}{(2m\Omega)^k}, \quad (20)$$

where we used the explicit expression of $(q, p| V(\hat{q}) | q, p)$ derived in [16]. In the macro-limit the term containing $h \to 0$ is zero, leading to the Hamiltonian of the classical nonlinear oscillator.

The total Hamiltonian generating the dynamics of the five degrees of freedom $(q, p)$ and $(x_i, y_i)$, $i = 1, 2, 3, 4$.
via the Hamiltonian dynamical equations (14) and (15) is the sum of the three functions (18), (19) and (20).

The dynamics of the two qubits in the form of the Schrödinger equation (12) is given by the Hamilton operator on \( \mathcal{H}_2 = \mathbb{C}^4 \) which depends also on the oscillator coordinate \( q = \langle q, p | \hat{q} q, p \rangle \)

\[
\langle q, p | \hat{H} | q, p \rangle = \varepsilon q^2 + \varepsilon \sigma_z^2 + \mu \sigma_x^2 + \lambda_1 q \sigma_z + \lambda_2 q \sigma_z. \tag{21}
\]

II. DISCUSSION AND SUMMARY

In summary, we have derived from the first principles the Hamiltonian dynamical model corresponding to the hybrid quantum-classical systems that has been postulated in \( \mathcal{M} \). In the derivation we have started from a quantum system composed of two quantum subsystems and then we have assumed that one of the subsystems has and preserves the classical properties during the interaction with the quantum subsystem. This is implemented by the corresponding constrained Hamiltonian dynamics. In this way the approach adopted in \( \mathcal{M} \) is justified from the first principles, which is our main result.

The main properties of the hybrid dynamical equations in their Hamiltonian form (14) and (15) have been studied in detail in \( \mathcal{M} \) and therefore need not to be repeated here. However, we would like to comment on the following peculiar property of the hybrid Hamiltonian dynamical system already analyzed in \( \mathcal{M} \). Consider the Liouville equation (16) in the case that the hybrid Hamiltonian \( H_1(q, p, \omega_2, \omega_2^\dagger) \) and the density \( \rho(q, p, \omega_2, \omega_2^\dagger) \) both depend on the same canonical pair of the classical subsystem. If the density \( \rho(q, p, \omega_2, \omega_2^\dagger) \) generates a mixed state on the quantum subsystem then it must be a quadratic function of the canonical coordinates \( (\omega_2(x_2), \omega_2^\dagger(x_2)) \) corresponding to the quantum subsystem. The Hamiltonian is also a quadratic function of the canonical coordinates of the quantum subsystem. However, the set of such quadratic functions of the quantum canonical coordinates which also depend on the classical coordinates is not closed under the Poisson bracket (13) on \( \Gamma \). This is in sharp contrast with the purely quantum case. Therefore, the Hamiltonian dynamical model that corresponds to the hybrid system must include functions of the quantum canonical variables which do not have the physical interpretation of quantum observables. In fact, the hybrid Hamiltonian dynamical system does not preserve the metrical properties of the hybrid phase space \( \Gamma \). This is akin to the purely classical case where the corresponding dynamics preserves the symplectic structure, i.e. the system is Hamiltonian, but does not preserve the metrical properties, which are therefore not considered as a part of the classical system’s structure. Analogously, hybrid mixed states, i.e. probability densities on \( \Gamma \), must be assumed to be of a more general form than in the purely quantum case. Quantum mechanical average of an observable \( \hat{F} \) in the state \( \hat{\rho} : \hat{F} = \text{Tr}[\hat{\rho} \hat{F}] \) is reproduced with \( \tilde{F} = \int_\mathcal{M} F(X) \mu(X) dX \) using any of the probability densities \( \mu(X) \) with the same first moment that is fixed by the requirement that the quantum expectation is equal to \( \tilde{F} \). The fact that the quantum mixed state \( \hat{\rho} \) determines only an equivalence class of densities \( \mu(X) \), those with the appropriate first moment, is equivalent to the non-uniqueness of the expansion of the mixed state in terms of convex combinations of pure states and is crucially quantum property of the Hamiltonian system on \( \mathcal{M} \). We see that in the hybrid systems even if the initial state \( \rho(q, p, \omega_2, \omega_2^\dagger) \) generates a quantum mixed state on the quantum subsystem, i.e. is quadratic in terms of the canonical variables of the quantum subsystem, such a state will evolve into a probability density of a more general form. This fact suggest that the truly hybrid systems, if existent, must be considered as conceptually independent class and not as such whose properties are exhausted by the properties of quantum and of classical systems.

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