Equivalence of two approaches for quantum-classical hybrid systems

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We discuss two approaches that are frequently used to describe quantum-classical hybrid system. One is the well-known mean-field theory and the other adopts a set of hybrid brackets which is a mixture of quantum commutators and classical Poisson brackets. We prove that these two approaches are equivalent. © *2008 American Institute of Physics*. [DOI: 10.1063/1.2927348]

Other than systems that are either fully quantum or fully classical, there are many hybrid systems, where a quantum subsystem is coupled to a classical subsystem. These quantum-classical hybrid systems are important and are interesting to researchers from very different backgrounds. Since gravity has not been properly quantized, it has been pondered whether it is ever necessary to quantize gravity.[1,2] If not, then one has to deal with hybrid systems where classical gravity is coupled to other quantized field.[3] Hybrid systems are also encountered in quantum measurement, where the detector, which is coupled to a quantum system, is always classical.[4,5] On a more practical side, hybrid systems are also studied by researchers who are interested in the properties of solids and molecules. Even if these systems are fundamentally quantum, it is adequate to treat the electrons as quantum while treating the heavy ions as classical.[6–10] This is, of course, the well-known Born–Oppenheimer approximation.[11]

Because of the diversity of people, who are interested in hybrid systems, various different approaches have been proposed to these half quantum and half classical systems. These approaches include the mean-field theory,[8,12,13] quasiclassical bracket approach,[14–16] Bohmian method,[17,18] decoherent histories,[19,20] and many others.[21–23] Among these approaches, the most popular ones are the mean-field theory and the quasiclassical brackets. In the mean-field theory, the quantum subsystem evolves according to the Schrödinger equation, while the classical subsystem experiences an energy field which is the expected value of the quantum state. In the quasiclassical bracket approach, brackets that are mixtures of quantum commutators and classical Poisson brackets are introduced and used to derive the equations of motion of the hybrid system.

In this paper, we prove that the mean-field theory and the quasiclassical bracket approach are equivalent. Before we proceed to present our proof, we briefly introduce these two approaches.

The Hamiltonian of a hybrid system, where there is interaction between subsystems, has three parts: The quantum mechanical part $\hat{H}_q$, the classical part H_c, and the interaction part $\hat{H}_i$. Formally, the Hamiltonian can be written as

$$\hat{H} = \hat{H}_q(\hat{\mathbf{p}},\hat{\mathbf{q}}) + H_c(\mathbf{P},\mathbf{Q}) + \hat{H}_i(\hat{\mathbf{q}},\mathbf{Q}), \tag{1}$$

where the dependence of $\hat{H}_i$ only on the coordinates $\mathbf{q}$ and $\mathbf{Q}$ reflects most cases in physical problems.

In the mean-field theory, one uses the following Hamiltonian:

$$H_s = \langle\psi|\hat{H}_q(\hat{\mathbf{p}}_s,\hat{\mathbf{q}}_s) + \hat{H}_i(\hat{\mathbf{q}}_s,\mathbf{Q}_s)|\psi\rangle + H_c(\mathbf{P}_s,\mathbf{Q}_s), \tag{2}$$

where $|\psi\rangle$ is a wave vector describing the quantum subsystem. The subscript s is introduced to distinguish the dynamical variables in the mean-field approach to the same variables in the quasiclassical bracket approach that is to be discussed later. Because the quantum system possesses mathematically the classical Hamiltonian structure,[13,24–26] we introduce the following set of Poisson brackets,

$$\{\psi_j^*,\psi_k\} = i\delta_{jk}/\hbar, \quad \{Q_j,P_k\} = \delta_{jk}, \tag{3}$$

$$\{\psi_j,\psi_k\} = \{Q_j,Q_k\} = \{P_j,P_k\} = 0, \tag{4}$$

where ψ_j is the jth component of the wave vector $|\psi\rangle$ when it is expanded in an orthonormal basis,

$$|\psi\rangle = \sum_j \psi_j|j\rangle. \tag{5}$$

With these Poisson brackets, one can derive a set of equations of motion from the mean-field Hamiltonian in Eq. (2)

$$|\dot{\psi}\rangle = \frac{1}{i\hbar}[\hat{H}_{qs} + \hat{H}_{is}]|\psi\rangle, \tag{6}$$

$$\dot{\mathbf{Q}}_s = \frac{\partial H_s}{\partial \mathbf{P}_s} = \frac{\partial H_{cs}}{\partial \mathbf{P}_s}, \tag{7}$$

$$\dot{\mathbf{P}}_s = -\frac{\partial H_s}{\partial \mathbf{Q}_s} = -\frac{\partial}{\partial \mathbf{Q}_s}[\langle\psi|\hat{H}_{is}|\psi\rangle + H_{cs}]. \tag{8}$$

where $\hat{H}_{qs}$ is a shorthand notation for $\hat{H}_q(\hat{\mathbf{p}}_s,\hat{\mathbf{q}}_s)$ and similarly for $\hat{H}_{is}$ and H_{cs}. The mean-field force in Eq. (8)

$$\mathbf{F}_s = -\frac{\partial}{\partial \mathbf{Q}_s}[\langle\psi|\hat{H}_{is}|\psi\rangle], \tag{9}$$

is just the Hellman–Feynman force that has been widely used in molecular dynamic simulations.[27]

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Note that the equations of motion in Eqs. (6)–(8) are usually directly written down.[8–10,19,28,29] To derive them in a coherent theoretical framework as we have presented was first done in Ref. 13.

The quasiclassical bracket approach explores the similarity between classical Poisson brackets and quantum commutators. In this approach, one tries to find the equations of motion for hybrid systems by introducing a new set of brackets which are mixtures of classical Poisson brackets and quantum commutators. We call these new brackets quasiclassical brackets, a name used by Anderson.[3] There are several different kinds of quasiclassical brackets.[3,7,14,30–32] One of these quasiclassical brackets is[3]

$$[A,B]_{qc} = [A,B] + i\hbar\{A,B\}. \tag{10}$$

The difference between these different quasiclassical brackets is subtle.[33,34] However, this subtle difference disappears for most of the interesting systems in physics, whose Hamiltonian contains no terms that are multiples of noncommutative operators. For example, there are no terms such as $\hat{\mathbf{q}}\cdot\hat{\mathbf{p}}$ in the Hamiltonians for almost all systems in nature. In this paper, we consider only this class of systems and use the bracket in Eq. (10) to avoid controversy or confusion.

In this quasiclassical bracket approach, the Hamiltonian is different from the one in the mean-field theory; we write it as

$$\hat{H}_h = \hat{H}_q(\hat{\mathbf{p}}_h,\hat{\mathbf{q}}_h) + \hat{H}_i(\hat{\mathbf{q}}_h,\mathbf{Q}_h) + H_c(\mathbf{P}_h,\mathbf{Q}_h), \tag{11}$$

where the subscript h is the counterpart of the subscript s in the mean-field theory. With the quasiclassical brackets in Eq. (10), we can obtain a set of Heisenberg-like equations of motion

$$\hat{\mathbf{q}}_h(t) = \frac{1}{i\hbar}[\hat{\mathbf{q}}_h(t),\hat{H}_{qh}(t) + \hat{H}_{ih}(t)]_{qc}, \tag{12}$$

$$\hat{\mathbf{p}}_h(t) = \frac{1}{i\hbar}[\hat{\mathbf{p}}_h(t),\hat{H}_{qh}(t) + \hat{H}_{ih}(t)]_{qc}, \tag{13}$$

$$\dot{\mathbf{Q}}_h(t) = \frac{\partial H_{ch}}{\partial \mathbf{P}_h}, \tag{14}$$

$$\dot{\mathbf{P}}_h(t) = -\langle t_0|\frac{\partial}{\partial \mathbf{Q}_h}\hat{H}_{ih}(t)|t_0\rangle - \frac{\partial}{\partial \mathbf{Q}_h}H_{ch}, \tag{15}$$

where we have used shorthand notations $\hat{H}_{qh}=\hat{H}_q(\hat{\mathbf{q}}_h,\mathbf{Q}_h)$, $\hat{H}_{ih}=\hat{H}_i(\hat{\mathbf{q}}_h,\mathbf{Q}_h)$, and $H_{ch}=H_c(\mathbf{P}_h,\mathbf{Q}_h)$. The wave vector $|t_0\rangle$ is the initial wave vector of the quantum subsystem. One of the many problems for the quasiclassical brackets is that one may have to deal with equations whose left-hand side is a c-number while whose right-hand side is an operator.[35] To overcome this, we have taken the expectation value of the right-hand side over the initial wave vector in Eq. (15) as in Ref. 31.

We now set to prove that the mean-field theory and the quasiclassical approach to hybrid systems are equivalent, that is, the dynamics described by the set of equations [Eqs. (6)–(8)] is the same as the one by Eqs. (12)–(15).

If we hold the classical variables fixed, the hybrid system is reduced to a fully quantum mechanical system. In this case, the mean field theory is just the Schrödinger picture and the quasiclassical bracket approach becomes the Heisenberg picture. Their equivalence has been proven a long time ago by Dirac.[36] It is not clear whether this is still true when the classical variables are allowed to evolve under the influence of the quantum backreaction in a hybrid system.

We know that the quantum dynamics described by Eq. (6) is the same as the one described by Eqs. (12) and (13) if we have

$$\mathbf{Q}_s(t) = \mathbf{Q}_h(t), \quad \mathbf{P}_s(t) = \mathbf{P}_h(t). \tag{16}$$

Consequently, the whole proof comes down to show that the above equalities hold. We compare Eqs. (7) and (8) and Eqs. (14) and (15). The only difference is the quantum backreaction force. One is given by Eq. (9) and the other by

$$\mathbf{F}_h = -\frac{\partial}{\partial \mathbf{Q}_h}[\langle t_0|\hat{H}_{ih}(t)|t_0\rangle]. \tag{17}$$

Whether these two forces are the same depends on whether

$$E_s(t) = \langle\psi|\hat{H}_{is}|\psi\rangle \tag{18}$$

and

$$E_h(t) = \langle t_0|\hat{H}_{ih}(t)|t_0\rangle \tag{19}$$

are identical. As we shall show, we indeed have $E_s(t) = E_h(t)$.

We notice that $\mathbf{Q}$, $\mathbf{P}$, and E are mutually dependent. That is, $\mathbf{Q},\mathbf{P}$ depend on E and at the same time E depends on $\mathbf{Q},\mathbf{P}$. This mutual dependence means that the equalities in Eq. (16) are equivalent to a more complete set of equalities

$$\mathbf{Q}_s(t) = \mathbf{Q}_h(t), \quad \mathbf{P}_s(t) = \mathbf{P}_h(t), \quad E_s(t) = E_h(t). \tag{20}$$

Once these equalities are proven, the proof is done. The time evolutions of E_s and E_h are very similar. For E_s, we have

$$\begin{aligned}\frac{dE_s(t)}{dt} &= \left(\frac{d}{dt}\langle\psi|\right)\hat{H}_{is}|\psi\rangle + \langle\psi|\hat{H}_{is}\left(\frac{d}{dt}|\psi\rangle\right)\\ &= \frac{1}{i\hbar}\langle\psi|[\hat{H}_{is},\hat{H}_{qs} + \hat{H}_{is}]|\psi\rangle\\ &= \frac{1}{i\hbar}\langle\psi|[\hat{H}_{is},\hat{H}_{qs}]|\psi\rangle.\end{aligned} \tag{21}$$

For E_h, we get

$$\frac{dE_h(t)}{dt} = \langle t_0|\frac{d}{dt}\hat{H}_{ih}(t)|t_0\rangle = \frac{1}{i\hbar}\langle t_0|[\hat{H}_{ih}(t),\hat{H}_{qh}(t)]|t_0\rangle. \tag{22}$$

We are ready for the final step of our proof. At the initial moment t_0, we have

$$\dot{\mathbf{Q}}_s(t_0) = \dot{\mathbf{Q}}_h(t_0), \quad \dot{\mathbf{P}}_s(t_0) = \dot{\mathbf{P}}_h(t_0), \tag{23}$$

and

$$E_s(t_0) = E_h(t_0), \qquad \left.\frac{dE_s(t)}{dt}\right|_{t_0} = \left.\frac{dE_h(t)}{dt}\right|_{t_0}. \tag{24}$$

These equalities imply that, at the next moment $t_1 = t_0 + dt$, we have

$$\mathbf{Q}_s(t_1) = \mathbf{Q}_s(t_0) + \dot{\mathbf{Q}}_s(t_0)dt = \mathbf{Q}_h(t_0) + \dot{\mathbf{Q}}_h(t_0)dt = \mathbf{Q}_h(t_1), \tag{25}$$

$$\mathbf{P}_s(t_1) = \mathbf{P}_s(t_0) + \dot{\mathbf{P}}_s(t_0)dt = \mathbf{P}_h(t_0) + \dot{\mathbf{P}}_h(t_0)dt = \mathbf{P}_h(t_1), \tag{26}$$

and

$$E_s(t_1) = E_s(t_0) + \left.\frac{dE_s(t)}{dt}\right|_{t_0} dt = E_h(t_0) + \left.\frac{dE_h(t)}{dt}\right|_{t_0} dt = E_h(t_1). \tag{27}$$

For the following moments, $t_2 = t_1 + dt$, $t_3 = t_2 + dt, \ldots$, $t_n = t_{n-1} + dt, \ldots$, we can similarly show that the equalities in Eq. (20) hold. This completes our proof that the mean-field theory and the quasiclassical approach are equivalent.

There is an alternative to the above proof. We outline it here. One should first notice that both sets of equations [Eqs. (6)–(8) and Eqs. (12)–(15)] have unique solutions once the initial conditions are specified. Then, the equivalence is proved when one shows that the solution of one set of equations also satisfies the other set.

We consider an example, where a classical magnetic particle is coupled to a $1/2$ quantum spin fixed in space through dipole interaction. For simplicity, we restrict the motion of the classical particle in a plane. This example was used in Ref. 13; we follow the notations there. The Hamiltonian operator describing the interaction between the spin and the classical magnetic particle is

$$\hat{H}_i = -\mu \begin{pmatrix} B_z & B_x - iB_y \\ B_x + iB_y & -B_z \end{pmatrix}, \tag{28}$$

where $\mu = |\boldsymbol{\mu}|$ is the magnetic moment of the classical particle and $\boldsymbol{B}$ is the dipolar field generated at the location of spin by the particle. Assuming the wave function in mean-field approach is $|\psi\rangle = (\psi_1, \psi_2)^T$, we have the total Hamiltonian for the mean-field approach as,

$$H_s = \langle\psi|\hat{H}_i|\psi\rangle + \mathbf{P}^2/2m = (|\psi_2|^2 - |\psi_1|^2)\mu B + \mathbf{P}^2/2m, \tag{29}$$

where $B = \sqrt{B_x^2 + B_y^2 + B_z^2}$ and $\mathbf{P}$ is the momentum of the classical particle. This Hamiltonian leads to the following set of equations of motions:

$$\dot{\psi}_1 = \frac{i\mu}{\hbar}(B_z\psi_1 + B_x\psi_2 - iB_y\psi_2), \tag{30}$$

$$\dot{\psi}_2 = \frac{i\mu}{\hbar}(B_x\psi_1 + iB_y\psi_1 - B_z\psi_2), \tag{31}$$

$$\dot{x} = P_x/m, \quad \dot{y} = P_y/m, \tag{32}$$

$$P_x = \mu\left[2\frac{\partial B_x}{\partial x}\,\mathrm{Re}(\psi_1^*\psi_2) + 2\frac{\partial B_y}{\partial x}\,\mathrm{Im}(\psi_1^*\psi_2) + \frac{\partial B_z}{\partial x}(|\psi_1|^2 - |\psi_2|^2)\right], \tag{33}$$

$$P_y = \mu\left[2\frac{\partial B_x}{\partial y}\,\mathrm{Re}(\psi_1^*\psi_2) + 2\frac{\partial B_y}{\partial y}\,\mathrm{Im}(\psi_1^*\psi_2) + \frac{\partial B_z}{\partial y}(|\psi_1|^2 - |\psi_2|^2)\right]. \tag{34}$$

For the approach of quasiclassical bracket, the total Hamiltonian is

$$\hat{H}_h = \hat{H}_i + \mathbf{P}^2/2m. \tag{35}$$

With the brackets in Eq. (10), the equations of motion are

$$\dot{\sigma}_x = \frac{2\mu}{\hbar}(\sigma_y B_z + i\sigma_x\sigma_y B_y), \tag{36}$$

$$\dot{\sigma}_y = -\frac{2\mu}{\hbar}(i\sigma_x\sigma_y B_x + \sigma_x B_z), \tag{37}$$

$$\dot{x} = P_x/m, \quad \dot{y} = P_y/m, \tag{38}$$

$$\dot{P}_x = \mu\left(\langle t_0|\sigma_x|t_0\rangle\frac{\partial B_x}{\partial x} + \langle t_0|\sigma_y|t_0\rangle\frac{\partial B_y}{\partial x} - i\langle t_0|\sigma_x\sigma_y|t_0\rangle\frac{\partial B_z}{\partial x}\right), \tag{39}$$

$$\dot{P}_y = \mu\left(\langle t_0|\sigma_x|t_0\rangle\frac{\partial B_x}{\partial y} + \langle t_0|\sigma_y|t_0\rangle\frac{\partial B_y}{\partial y} - i\langle t_0|\sigma_x\sigma_y|t_0\rangle\frac{\partial B_z}{\partial y}\right). \tag{40}$$

We have numerically solved the above two sets of equations of motion for various different initial conditions. Our results show that they are identical to each other within numerical errors, offering a supplementary support for our analytical proof. Our experience is that the numerical computation with the mean-field theory is much less time consuming than the other approach.

Although quantum mechanics and classical mechanics are very different physically, they share at least two common mathematical features. One is that the Schrödinger equation has also a classical Hamiltonian structure,[24,25] which is utilized by the mean-field theory of a hybrid system. The other is that the Poisson brackets in the classical mechanics and the quantum commutators share a similar algebraic structure. The common feature is explored by the quasiclassical bracket approach. Interestingly, these seemingly quite different methods lead to the same dynamics as we have shown. However, there is a difference between these two approaches that is worth mentioning.

The mean-field theory is mathematically rigorous. One can derive the equations of motion [Eqs. (6)–(8)] from the Hamiltonian in Eq. (2) by rigorously following the classical Hamiltonian theory. However, this is not so for the quasiclassical approach. First, there are several different ways to setting up the quasiclassical brackets as we have mentioned;

second, Eq. (15) is written with some arbitrariness. There can be other alternatives. For example, one obvious alternative is to replace $\langle t_0|\hat{H}_{ih}|t_0\rangle$ with

$$H_i(\mathbf{Q}_h,\langle t_0|\hat{q}_h|t_0\rangle). \tag{41}$$

There seem no *a priori* principles that favor one over another. One can only make a choice based on the consequence of each choice.

In conclusion, we have proved the equivalence of two popular but different methods for quantum-classical hybrid systems. This conclusion suggests that many approaches that have been proposed for hybrid systems may also be equivalent to one another.

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