Classicalization of Quantum Variables

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A systematic procedure to extract classical degrees of freedom in quantum mechanics is formulated based on the stochastic variational method. By using this classicalization, a hybrid model constructed from quantum and classical variables (quantum-classical hybrids) is derived. In this procedure, conservation laws such as energy are maintained, and Eheferst’s theorem is still satisfied with modification. The criterion for the applicability of quantum-classical hybrids is also investigated.

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INTRODUCTION

Classical mechanics (CM) is an effective theory of quantum mechanics (QM) and precisely describes macroscopic physics. In other words, CM and QM are theories belonging to different dynamical hierarchies. Another example of such a hierarchy is observed in dynamics of fluids, where macroscopic behaviors of its constituent particles can be described by a coarse-grained dynamics called hydrodynamics. However, particles which have much larger scales are suspended in a fluid, we need to solve coupled equations of the particles and the fluid [1]. This is an example of the appearance of a hybrid dynamics when quantum and classical degrees of freedom coexist.

In fact, there are several situations where such quantum-classical hybrids (QCH) seem to show up: quantum measurement [2], quantum-to-classical transition in early universe [3], Einstein gravity interacting with quantum objects [4], Berry’s phase [5] and so on. Moreover, QCH has been studied to simplify complex numerical simulations in quantum chemistry [6]. See also Refs. [8, 9] and references therein.

There are already many models of QCH, but still no established theory. The successful theories are constructed so as to combine quantum and classical systems consistently [8,10]. In this paper, we study this problem from a different perspective. We first prepare a quantum system and derive a model of QCH by employing “classicalization”, where quantum degrees of freedom are systematically replaced by classical variables [6].

QUANTIZATION OF TWO-PARTICLE SYSTEM

Our classicalization is based on the fact that quantization can be formulated in the form of the variational principle by using the stochastic variational method (SVM) which was proposed by Yasue [11] so as to reformulate Nelson’s stochastic quantization [12]. As a pedagogical introduction of this approach, see Ref. [13] and also [14,15]. Before discussing QCH, we discuss the SVM quantization.

Let us consider a two particle system with the masses \( m_1 \) and \( m_2 \), and an interaction potential \( V \). Newton’s equation of motion of this system is given by optimizing an action defined by \( T - V \) with \( T \) being a kinetic term. Yasue showed that the Schrödinger equation is derived by employing SVM to this classical action replacing particles trajectories with stochastic variables.

The stochastic trajectories of the two particles \( \mathbf{r}_1(t) \) and \( \mathbf{r}_2(t) \) are characterized by the stochastic differential equations (i=1,2),

\[
d\mathbf{r}_i(t) = u_i(\mathbf{r}_1(t), \mathbf{r}_2(t), t) dt + \sqrt{2\nu_i} d\mathbf{W}_i(t) \quad dt > 0, \tag{1}
\]

where \( dA(t) \equiv A(t+dt) - A(t) \), and \( \mathbf{W}_1(t) \) and \( \mathbf{W}_2(t) \) are independent Wiener processes. The parameter \( \nu_i \) characterizes the noise intensity. Then the stochastic action obtained from the classical action by substituting the stochastic trajectories is given by

\[
L = \sum_{i=1,2} \left\{ \frac{m_i}{2} (\hat{D}\mathbf{r}_i(t))^2 + \frac{1}{2} (\hat{D}\mathbf{r}_i(t))^2 \right\} - V(\mathbf{r}_1(t), \mathbf{r}_2(t)). \tag{2}
\]

In the above expression, two different time derivatives are introduced, because these trajectories have zig-zag forms and the usual definition of velocity appearing in CM is not applicable [12]. The mean forward derivative \( D \) and the mean backward derivative \( \hat{D} \) are defined by

\[
D\mathbf{r}_i(t) = \lim_{dt \to 0^+} E \left[ \frac{\mathbf{r}_i(t + dt) - \mathbf{r}_i(t)}{dt} | \mathcal{P}_t \right], \tag{3}
\]

\[
\hat{D}\mathbf{r}_i(t) = \lim_{dt \to 0^-} E \left[ \frac{\mathbf{r}_i(t + dt) - \mathbf{r}_i(t)}{dt} | \mathcal{F}_t \right], \tag{4}
\]

respectively. Here \( E[|] \) denotes the expectation value. In particular, the above derivatives are defined as conditional averages, where \( \mathcal{P}_t (\mathcal{F}_t) \) indicates to fix \( \mathbf{r}(t') \) for \( t' \leq t \) (\( t' \geq t \)). Using Eq. (1), the derivatives become

\[
D\mathbf{r}_i(t) = u_i(\mathbf{r}_1(t), \mathbf{r}_2(t), t),
\]

\[
\hat{D}\mathbf{r}_i(t) = u_i(\mathbf{r}_1(t), \mathbf{r}_2(t), t) - 2\nu_i \nabla_i \ln \rho(\mathbf{r}_1(t), \mathbf{r}_2(t), t).
\]
Here the two-particle probability density $\rho(\{x\}, t)$ is given by the solution of the equation of continuity,

$$\partial_t \rho(\{x\}, t) = - \sum_{i=1,2} \nabla_i \cdot \{\rho(\{x\}, t)v_i(\{x\}, t)\},$$

(5)

with $v_i = u_i - \nu_i \nabla_i \ln \rho$ and $\{x\} = (x_1, x_2)$.

The variation of the stochastic trajectories $\hat{r}_i(t)$ leads to the stochastic Euler-Lagrange equation,

$$\left[ D \frac{\partial L}{\partial \dot{\hat{r}}_i(t)} + D \frac{\partial L}{\partial \hat{r}_i(t)} - \frac{\partial L}{\partial \hat{r}_i(t)} \right]_{\hat{r}_i(t) = \hat{r}_i} = 0.$$  

(6)

Note that $\hat{r}_i(t)$ is replaced with a spatial parameter $x_i$ at the last of the calculation. It is because SVM requires that stochastic actions are optimized for any stochastic configuration of $\hat{r}_i(t)$. See [13] for details.

By using Eqs. (5) and (6), we obtain the Schrödinger equation,

$$i\hbar \partial_t \psi(\{x\}, t) = \left[ \sum_{i=1,2} \left\{ - \frac{\hbar^2}{2m_i} \nabla_i^2 + V(\{x\}) \right\} \psi(\{x\}, t) \right],$$

where the wave function is defined by $\psi(\{x\}, t) = \sqrt{\rho(\{x\}, t)} e^{i\theta(\{x\}, t)}$ with the phase defined by

$$m_i v_i(\{x\}, t) = \hbar \nabla_i \theta(\{x\}, t).$$

To obtain this result, we choose

$$\nu_i = \frac{\hbar}{2m_i}. \quad (8)$$

That is, the noise intensity is proportional to the inverse of the particle mass.

The result of optimization depends on the property of $d\hat{r}_i(t)$. If we assume the usual definitions of the classical velocity by taking the vanishing limit of $\nu_i$ in Eqs. (1) (as will be done in Eq. (9) for $i = 1$), Newton’s equation of motion is obtained instead of the Schrödinger equation in SVM. That is, SVM describes QM and CM in a unified way from the point of view of the variational principle.

**QCH OF TWO-PARTICLE SYSTEM**

Let us **classicalize** a part of this two-particle system, assuming $m_1 >> m_2$ and $\hbar/(2m_1) << 1$. From Eq. (8), the effect of the noise for the particle 1 is negligibly small. Then, instead of Eq. (1), we approximately use the following equation,

$$d\hat{r}_1(t) = v_1(\hat{r}_1(t), \hat{r}_2(t), t)dt.$$  

(9)

This immediately affects the calculation of the mean derivatives as $D \hat{r}_1(t) = D \hat{r}_2(t) = v_1(\hat{r}_1(t), \hat{r}_2(t), t)$. On the other hand, the same definition (1) is still employed for $d\hat{r}_2(t)$.

This is a unique approximation for our classicalization, but drastically changes the result of the variation. In fact, the stochastic Euler-Lagrange equation now becomes

$$\left[ \tilde{D} \frac{\partial L}{\partial \dot{\tilde{r}}_1(t)} + \frac{\partial L}{\partial \tilde{r}_1(t)} - \frac{\partial L}{\partial \tilde{r}_1(t)} \right]_{\tilde{r}_1(t) = \hat{r}_1} = 0.$$  

(10)

Here, the substitution of $\hat{r}_1(t)$ is changed from $x_1$ to $f_1(x_2, t)$. As mentioned already, SVM requires that the action is optimized for any configuration of stochastic trajectories and thus $\hat{r}_2(t)$ is replaced by the spatial parameter $x_2$. However, as is seen from Eq. (9), $\hat{r}_1(t)$ fluctuates because of the $\hat{r}_2(t)$ dependence in $v_1$. Once $x_2$ is substituted into $\hat{r}_2(t)$, $\hat{r}_1(t)$ does not fluctuate any more and hence cannot be replaced by $x_1$. In this case, the “velocity” on the right hand side of Eq. (9) becomes a function not only of $t$ but also of $x_2$. Therefore we introduce a quantity defined by the solution of the following equation,

$$\partial_t f_1(x_2, t) = v_1(f_1(x_2, t), x_2, t).$$  

(11)

We call $f_1(x_2, t)$ quasi trajectory function, which is substituted into $\hat{r}_1(t)$ in Eq. (10).

The explicit calculation of Eq. (10) leads to

$$\left( \frac{d}{dt} + \frac{\hbar}{m_2} \nabla_2 \text{Im}(\ln \Psi_2(f_1(x_2, t), x_2, t) \cdot \nabla_2) \right) v_1(f_1(x_2, t), x_2, t) = - \frac{1}{m_1} \nabla_1 V(f_1(x_2, t), x_2),$$

(12)

and

$$i\hbar \frac{d}{dt} \Psi_2(f_1(x_2, t), x_2, t) = \dot{\hat{H}}_2(t) \Psi_2(f_1(x_2, t), x_2, t),$$  

(13)

where $\frac{d}{dt} = \partial_t + v_1(f_1(x_2, t), x_2, t) \cdot \nabla_1$, and

$$\dot{\hat{H}}_2(t) = - \frac{m_1}{2} v_1^2(f_1(x_2, t), x_2, t) - \frac{\hbar^2}{2m_2} \nabla_2^2 + V(f_1(x_2, t), x_2).$$

(14)

Here $\Psi_2(f_1(x_2, t), x_2, t)$ is the wave function for the particle 2 and $|\Psi_2|^2 = \rho_2(x_2, t)$ gives the probability density of the particle 2. The phase of $\Psi_2$ is defined in the same way as Eq. (7).

In short, our QCH model consists of Eqs. (11), (12) and (13). Note that Eq. (13) is expressed by the total time derivative $d/dt$, and if we re-express it by $\partial_t$, the sign of the first term in Eq. (14) becomes positive.

If there is no interaction between the particles 1 and 2, $v_1$ is independent of $x_2$, and hence the quasi trajectory function coincides with the classical trajectory $r_1(t)$, because $df_1(t)/dt = dr_1(t)/dt = v_1(r_1(t), t)$. Then Eqs. (12) and (13) are reduced to Newton’s equation of motion and the usual Schrödinger equation with the Hamiltonian operator $-\hbar^2/(2m_2) \nabla_2^2 + V(x_2)$, respectively. The
The expectation values of $\hat{A}$ for the particle 2. Here $\hat{d}$ for the particle 1, and $\langle \hat{A} \rangle$ represents the results of QCH and QM, respectively. For the solid lines, $\alpha = 0.5, 1$ and 2 from the most left line. For comparison, the dot-dashed line represents the trajectory of the particle 1 shown in Fig. 1.

FIG. 2: The time evolution of $(x_2)$. The solid and dashed lines represent the results of QCH and QM, respectively. For the solid lines, $\alpha = 0.5, 1$ and 2 from the most left line. For comparison, the dot-dashed line represents the trajectory of the particle 1 shown in Fig. 1.

The energy, for example, obtained from Eq. (2) is given by

$$E = \left\langle \sum_{i=1}^{2} \frac{m_i}{2} v_i^2(x_i, t) + V(f_1(x_2, t), x_2) \right\rangle + \frac{\hbar^2}{8m_2} \left( \nabla_2 \ln |\Psi_2(f_1(x_2, t), x_2, t)|^2 \right)^2_2,$$

where $\langle A \rangle_2 = \int d^3x_2 |\Psi_2(f_1(x_2, t), x_2, t)A\Psi_2(f_1(x_2, t), x_2, t)|$ for an arbitrary function $A$. One can confirm that this quantity is conserved by substituting our equations.

EHERENFEST’S THEOREM

Eherenfest’s theorem is satisfied for our QCH model, but in a modified way. The expectation values of $\hat{r}_1(t)$, $x_1$, $x_2$ and $v_2$ of our model are given by

$$\frac{d}{dt} \langle x_1(t) \rangle_1 = \langle \hat{v}_1(x_1, t) \hat{x}_1(t) \rangle_1,$$

$$\frac{d}{dt} \langle x_2(t) \rangle_2 = -\frac{1}{m_1} \langle \nabla_1 V(f_1(x_2, t), x_2) \rangle_2,$$

for the particle 1, and

$$\frac{d}{dt} \langle x_2(t) \rangle_2 = \frac{1}{m_2} \langle \hat{p}_2 \rangle_2,$$

$$\frac{d}{dt} \langle \hat{p}_2 \rangle_2 = -\langle \nabla_2 V(f_1(x_2, t), x_2) \rangle_2,$$

for the particle 2. Here $\hat{p}_2 = -i\hbar \nabla_2$ and we have used $[d, \hat{p}_2] = [\partial_t + v_1 \cdot \nabla_1, \hat{p}_2] = i\hbar \sum_{j=1}^{3} (\nabla_2 v_1^j) \nabla_1^j$. Note that Eq. (19) is obtained from Eq. (2), and this corresponds to the (mean) trajectory of the particle 1.

One can see that the above four equations correspond to Ehrenfest’s theorem in QM when $f_1(x_2, t)$ coincides with the particle trajectory $\hat{r}_1(t)$. To study this difference, let us consider a harmonic potential $V(x_1, x_2) = K(x_1 - x_2)^2/2$ where the dynamics is linear and the behaviors of the expectation values $\langle x_1 \rangle$ and $\langle \hat{p}_1 \rangle$ in QM exactly agree with Newton’s equations of motion. Then the evolutions are independent of the detailed form of the wave function by fixing the initial values of $\langle x_1 \rangle$ and $\langle \hat{p}_1 \rangle$. However, the behaviors in our QCH depend on the behaviors of the wave function around $\langle x_1 \rangle$ and $\langle \hat{p}_1 \rangle$.

We consider a one-dimensional system with $m_1 = 5m_2$ and $K = \hbar^2/(2m_2\lambda^2)$ with $\lambda$ being a parameter with a spatial dimension. Positions are divided by $\lambda$ and become adimensional and $T = \hbar/(2m_2\lambda^2)$. The initial conditions are given by $\hat{r}_1(0) = f_1(x_2, 0) = 0.5$, $\frac{2m_2}{\hbar^2} v_1(f_1(x_2, 0), x_2, 0) = -1$ and

$$\Psi_2(f_1(x_2, 0), x_2, 0) = (2\alpha/\pi)^{1/4} e^{-\alpha x_2^2}.$$
approximately replaced by a point-like particle for the particle 1. This approximation is justified as the distance between the two particles 1 and 2 enlarges. Increases the value of \( \alpha \), decreases the overlap between the two particles. This is effectively equivalent to separate off the two particles. This is why the deviations become smaller as \( \alpha \) increases.

This qualitative nature can be seen even from the behavior of the quasi trajectory defined by \( \langle f_1(x_2, t) \rangle \). Its differential equation is given by

\[
\frac{df_1(x_2, t)}{dt} = \langle v_1(f_1(x_2, t), x_2, t) \rangle + \frac{i}{\hbar} \langle H_2(t), f_1(x_2, t) \rangle.
\] (20)

Comparing to Eq. (16), the quasi trajectory can be identified with the trajectory \( E[\hat{r}_1(t)] \) itself, if the contribution from the second term on the right hand side is sufficiently small. In Fig. 3, the difference of the trajectories, \( E[\hat{r}_1(t)] - \langle f_1(x_2, t) \rangle \), is shown. The difference starts to grow up around \( T \sim 0.4 \) where the two particles intersect. As \( \alpha \) increases, that is, the overlap between the two particles becomes smaller, the difference between the two trajectories decreases. All these observations confirm our argument of the limited applicability. Note that this difference can be used to characterize the applicability of the QCH approach.

In the above simulations, we fixed the mass ratio by \( m_1/m_2 = 5 \). We confirmed numerically that the deviation from QM decreases even by increasing this ratio. This is consistent with our approximation (9).

**QCH of \( N_c + N_q \)-Particle System**

Our result is extended to a many particle system which consists of \( N_c \) classical \( \{ \hat{r} \} \) and \( N_q \) quantum \( \{ \hat{q} \} \) variables. When the interaction potential is given by \( V = V(\{ \hat{r} \}, \{ \hat{q} \}) \), the stochastic variations lead to

\[
\frac{d}{dt} + \sum_{\beta=1}^{N_q} \frac{\hbar}{m_\beta} \nabla_\beta \text{Im}(\Psi_q) \cdot \nabla_\beta \right) v_a = -\frac{1}{m_a} \nabla_a V, \quad (21)
\]

where \( d/dt = \partial_t + \sum_{a=1}^{N_a} v_a \cdot \nabla_a \), and

\[
\partial_t \hat{f}_a(\{ x \}, t) = v_a(\{ f \}, \{ x \}, t),
\]

\[
\hat{H}_q(t) = -\sum_{a=1}^{N_a} \frac{m_a}{2} v_a^2 - \sum_{a=1}^{N_a} \frac{\hbar^2}{2m_a} \nabla_a^2 + V. \quad (24)
\]

**Concluding Remarks**

In this paper, we formulated classicization of quantum variables based on SVM and derived a QCH model. This model conserves any quantity associated with the invariant transforms of the action and satisfies the extended Eherenfest theorem. This model is applicable to the case where the mass difference between classical and quantum particles is large and there is no significant overlap between classical and quantum states. This will be an appropriate approximation for systems with repulsive interactions. The failure of QCH can be estimated by calculating the difference between the trajectory and quasi trajectory. This quantity may play a role of an order parameter of the quantum-to-classical transition.

There are already many proposals for QCH, but most of the models cannot preserve important laws of physics and/or consistency requirements such as the energy conservation, the positivity of probability and so on [9]. So far there are three models which are considered to be reliable [8, 10]. See also Ref. [18]. In such models, there is no concept of the quasi trajectory and thus ours is different from these models. We do not find any inconsistency in our model, but the relation to these models should be investigated carefully. For example, a hybrid state is characterized by the combination of the Hilbert space of QM and the phase space of CM in such models, while it is not clear how the phase space is introduced in our model. The advantage of our approach is that conserved quantities are defined from the stochastic Noether theorem straightforwardly.

SVM is applicable to the field quantization [17] and thus a QCH model of a field system will be constructed. This is left as a future task.

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