

Variational truncated Wigner approximation

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In this paper we reconsider the notion of an optimal effective Hamiltonian for the semiclassical propagation of the Wigner distribution in phase space. An explicit expression for the optimal effective Hamiltonian is obtained in the short-time limit by minimizing the Hilbert-Schmidt distance between the semiclassical approximation and the real state of the system. The method is illustrated for the quartic oscillator.

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I. INTRODUCTION

Since the seminal work by Wigner [1], phase-space methods have attracted considerable theoretical attention. The interest in phase-space methods has only increased over the years and it has found important applications in the fields of quantum optics [2–4], atomic physics [5], cold atoms [6], or other bosonic systems [7,8]. Significant theoretical attention has been attracted by the semiclassical (truncated Wigner) approximation of the full quantum phase-space dynamics. The full quantum dynamics can be represented in terms of quantum jumps around the classical (symplectic) phase-space flow. Within the semiclassical truncated Wigner approximation one neglects the quantum jumps. Consequently, the quantum dynamics is approximated by the classical evolution of the system. However, the initial state still carries the signatures of statistics into the time-dependent solution. The justification for this expansion around the classical trajectory is based on the observation that every quantum jump carries an additional factor \hbar^2 [7], which is obvious from the Moyal expansion [9] of the Wigner kernel [10]. The overall goodness of the expansion is however unclear, since each successive term in the Moyal expansion contains higher derivatives of both the distribution and the Hamiltonian.

The modification of the classical mechanics by quantum fluctuations is however precisely the intuitive understanding associated with Feynman's path-integral description [11] of quantum mechanics. By adopting a saddle-point expansion [12] one can, for example, derive the semiclassical Van Vleck–Gutzwiller propagator [13–15]. By construction, the quantum fluctuations around the Euler-Lagrange equations associated with the saddle point are minimal. In that respect it is important to note that the Euler-Lagrange equations for the saddle-point expansion of the Wigner distribution propagator [16] differ from the classical equations of motion, unless the problem is harmonic. Although the classical equation of motion does lie on a saddle point, there are infinitely many others such that it has zero measure in the semiclassical path integral. We therefore expect that there must exist a modified classical phase-space evolution around which the overall quantum fluctuations are smaller.

In the next section we present a method for deriving an effective classical Hamiltonian which generates a classical

phase-space evolution, that is optimal in a well-defined sense. In Sec. III, the method is illustrated by finding this optimal Hamiltonian for the case of a quartic oscillator which starts evolving from a Gaussian Wigner function. The result is shown to compare favorably with the standard truncated Wigner approximation. Finally, some conclusions are drawn in Sec. IV.

II. OPTIMIZING THE CLASSICAL STATE SPACE EVOLUTION

Consider a d -dimensional quantum system, whose initial state at time zero is represented by the density matrix $\hat{\rho}_0$. Under the influence of a time-dependent Hamiltonian $\hat{H}(t)$, the density matrix $\hat{\rho}(t)$ evolves unitarily as $\hat{\rho}(t) = \hat{U}(t)\hat{\rho}_0\hat{U}^\dagger(t)$, with

$$\hat{U}(t) = \hat{T} \exp\left(-\frac{i}{\hbar} \int_0^t \hat{H}(\tau) d\tau\right), \quad (2.1)$$

where \hat{T} denotes the time-ordering operator.

Consider furthermore a set Σ of trial density matrices $\hat{\sigma}(t)$, all generated from the same initial $\hat{\rho}_0$ but by other (approximate) protocols Σ . It would then be interesting to find out how each of those protocols Σ is performing by comparing $\hat{\sigma}(t)$ to $\hat{\rho}(t)$. The goodness of a certain protocol Σ can be assessed by measuring the distance D between the two states underlying $\hat{\sigma}(t)$ and $\hat{\rho}(t)$, a problem that is well established in the field of quantum information theory [17]. The optimal protocol Σ_{opt} is the one that generates the state closest to the real state, implying

$$D(\hat{\sigma}_{\text{opt}}, \hat{\rho}) = \min_{\Sigma \in \Sigma} D(\hat{\sigma}, \hat{\rho}). \quad (2.2)$$

However, in quantum information theory the protocols are usually noisy approximate implementations of the ideal evolution \hat{U} , from which one tries to find the optimal implementation. Here we are concerned with a different type of approach. In quantum dynamics, the time evolution $\hat{U}(t)$ is usually analytically and/or numerically inaccessible. But soluble trial Hamiltonians provide approximation schemes Σ which allow one to calculate $\hat{\sigma}(t)$. The distance then provides a measure for the quality of each approximation. For this purpose, we propose the Hilbert-Schmidt distance measure, i.e.,

$$D_2(\hat{\rho}, \hat{\sigma}) = \sqrt{\text{Tr}[(\hat{\rho} - \hat{\sigma})^\dagger(\hat{\rho} - \hat{\sigma})]}, \quad (2.3)$$

since it is analytically better tractable than the more important trace distance. So far this is still completely general and one

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can put every possibly conceivable approximation in Σ . We now specifically turn to the problem of finding the optimal classical evolution of the Wigner distribution in phase space.

The Wigner distribution is a joint quasiprobability distribution of canonical conjugate variables, denoted by $(\mathbf{x}, \mathbf{p}) = (\{x_i\}, \{p_i\})$. Although the Wigner function has the correct marginal probability distributions, it is a quasidistribution as it can attain negative values. These negative values are the reason why one must use a quantum measure for the distance between states, rather than the classical Kullback-Leibler distance between the Wigner distributions. Denoting the Wigner functions $f_\rho(\mathbf{x}, \mathbf{p}, t)$ and $f_\sigma(\mathbf{x}, \mathbf{p}, t)$ associated with the states underlying $\hat{\rho}(t)$ and $\hat{\sigma}(t)$, respectively, the Hilbert-Schmidt distance between the two states becomes

$$\frac{D_2^2(\hat{\rho}, \hat{\sigma}, t)}{2\pi\hbar} = \iint d\mathbf{x} d\mathbf{p} [f_\rho(\mathbf{x}, \mathbf{p}, t) - f_\sigma(\mathbf{x}, \mathbf{p}, t)]^2. \quad (2.4)$$

Initially this distance is zero, because then both compared states are equal. In order to assess the goodness of the classical approximation f_σ one should investigate the increase of D_2 over time. The time evolution of the exact Wigner function f_ρ associated with the unitary evolution $\hat{U}(t)$ is given by

$$\frac{\partial f_\rho(\mathbf{x}, \mathbf{p}, t)}{\partial t} - \{H(\mathbf{x}, \mathbf{p}, t), f_\rho(\mathbf{x}, \mathbf{p}, t)\}_M = 0, \quad (2.5)$$

where $\{\cdot, \cdot\}_M$ denotes the Moyal bracket [9], and where $H(\mathbf{x}, \mathbf{p}, t)$ is the Weyl representation [7,18] of the Hamiltonian $\hat{H}(t)$. The Moyal bracket has the interesting property that

$$\{\cdot, \cdot\}_M = \{\cdot, \cdot\} + O(\hbar^2), \quad (2.6)$$

where $\{\cdot, \cdot\}$ is the Poisson bracket. This expansion forms the basis of the semiclassical truncated Wigner approximation [7]. By neglecting the quantum fluctuations of $O(\hbar^2)$, the problem of propagating the initial Wigner distribution in time becomes classical. The corrections around the Poisson bracket are however higher powers of the Poisson bracket. Therefore, the overall quality of the approximation will depend on the smoothness of the distributions on which it acts. It is easy to show that the Moyal bracket and the Poisson bracket of any quadratic function with any arbitrary distribution equal each other. As a consequence, the time evolution of any state under a quadratic Hamiltonian is identical to its classical time evolution in phase space.

Instead of approximating the time evolution of the system by its classical time evolution, consider a classical Hamiltonian H_σ , which differs from the original one. The corresponding state evolves according to

$$\frac{\partial f_\sigma}{\partial t} - \{H_\sigma, f_\sigma\} = 0. \quad (2.7)$$

Although the full problem (2.5) is not supposed to be soluble, we can expand f_ρ around the approximate solution f_σ . In fact, if f_σ is the optimal approximation of f_ρ there is no better way to estimate the real solution. Up to lowest order, hence in the short-time limit, we find that the distance between the two solutions grows with time according to

$$\frac{D_2^2(\hat{\rho}, \hat{\sigma}, t)}{2\pi\hbar} = \iint d\mathbf{x} d\mathbf{p} \left[\int_0^t d\tau \begin{pmatrix} \{H, f_\sigma\}_M \\ -\{H_\sigma, f_\sigma\} \end{pmatrix} \right]^2.$$

The minimization of this distance results in the following requirement for the effective Hamiltonian H_{eff} of the optimal classical evolution:

$$\int_0^t d\tau \{H_{\text{eff}}, f_\sigma\} = \int_0^t d\tau \{H, f_\sigma\}_M.$$

We would of course like to have the optimal solution for all final times t . Moreover, we would like the Hamiltonian to depend locally on time, such that the approximate evolution (2.7) stays Markovian. Consequently, we have to equate the previous expression time by time which yields the following Euler-Lagrange equation for the optimal Hamiltonian:

$$\{H_{\text{eff}}, f_\sigma\} = \{H, f_\sigma\}_M. \quad (2.8)$$

Since the approximate evolution has to satisfy Eq. (2.7), this equation can also be written as

$$\left\{ \frac{\partial f_\sigma}{\partial t} - \{H_{\text{eff}}, f_\sigma\}_M, f_\sigma \right\} = 0.$$

This implies that the equation of motion (2.7) for f_σ differs from the equation of motion (2.5) of the true quantum system by an effective quantum jump distribution:

$$\frac{\partial f_\sigma}{\partial t} - \{H, f_\sigma\}_M = \left(\frac{\partial f_\sigma}{\partial t} \right)_{\text{jump}}, \quad (2.9)$$

with $\left(\frac{\partial f_\sigma}{\partial t} \right)_{\text{jump}} = \{H_{\text{eff}}, f_\sigma\} - \{H, f_\sigma\}_M$. (2.10)

If $\{(\partial_t f_\sigma)_{\text{jump}}, f_\sigma\} = 0$ and if H_{eff} is a solution of Eq. (2.8), the optimal trial distribution f_σ evolves classically. Possible implications of this condition that the jump distribution and the trial distribution are in mutual involution are under current investigation.

It is clear that Eq. (2.8) cannot be solved in general. A possible way to simplify the problem is to parametrize the model Hamiltonian in order to include specific additional physics. In this way the minimization of the distance will not result in a differential equation for the Hamiltonian but it will give a set of algebraic equations for the undetermined parameters in the model Hamiltonian. In [19] we contributed to this possibility in the context of quantum transport. In that work we minimized the distance (2.4) under the ansatz that the effective Hamiltonian,

$$H_{\text{eff}}(x, p) = \frac{p^2}{2m} + V_{\text{eff}}(x),$$

is parametrized by a scalar potential $V_{\text{eff}}(x)$.

Another option is to look for a solution of Eq. (2.8) for specific simple Wigner functions. Below we illustrate this approach for the quartic oscillator. Although of limited practical interest, this example provides the required background for treating the contact potential in field theory.

III. GAUSSIAN INITIAL STATE FOR A QUARTIC OSCILLATOR

As an example, consider a one-dimensional quartic oscillator

$$H = \frac{p^2}{2} + \frac{x^2}{2} + \frac{gx^4}{4}, \quad (3.1)$$

expressed in natural units of the harmonic oscillator, i.e., $\hbar = m = \omega = 1$. In this case the Moyal expansion has a finite number of terms and becomes

$$\{H, f\}_M = \{H, f\} - \frac{gx}{4} \frac{\partial^3 f}{\partial p^3}, \quad (3.2)$$

with
$$\{H, f\} = (x + gx^3) \frac{\partial f}{\partial p} - p \frac{\partial f}{\partial x}, \quad (3.3)$$

Since the Moyal bracket is expanded in the Poisson bracket plus a correction, it is natural to expand the trial Hamiltonian as

$$H_{\text{eff}} = H + H_c, \quad (3.4)$$

in which H_c accounts for the correction and satisfies the following partial differential equation:

$$\{\{H_c, f_\sigma\}, f_\sigma\} = -\frac{g}{4} \left\{ x \frac{\partial^3 f_\sigma}{\partial p^3}, f_\sigma \right\}. \quad (3.5)$$

As in any problem of quantum dynamics, the initial state has to be given, and can by no means be calculated. Because of the Heisenberg uncertainty principle, a reasonable example of an initial distribution function is a Gaussian wave packet in position and momentum. Although many other trial time evolutions can be imagined, we here illustrate the optimization method for a displaced version in time of this initial wave packet:

$$f_\sigma(x, p, t) = \frac{1}{2\pi\sigma_x\sigma_p} e^{-\frac{(x-x_0(t))^2}{2\sigma_x^2} - \frac{(p-p_0(t))^2}{2\sigma_p^2}}$$

with
$$2\sigma_x\sigma_p \geq 1. \quad (3.6)$$

The condition $2\sigma_x\sigma_p \geq 1$ accounts for the uncertainty relation. With this trial distribution function, the equation (3.5) becomes a inhomogeneous second-order partial differential equation in x and p , with the solution

$$H_c = \frac{x^2 g}{48\sigma_p^2} \left(18 - x \frac{3x - 4x_0}{\sigma_x^2} - 6 \frac{(p - p_0)^2}{\sigma_p^2} \right) + u \left(\frac{(x - x_0)^2}{2\sigma_x^2} + \frac{(p - p_0)^2}{2\sigma_p^2} \right),$$

where u is an arbitrary function. The Poisson bracket of f_σ with this function u always vanishes. Therefore, one can set $u = 0$, because it does not contribute to the dynamics. The optimal effective Hamiltonian (3.4) along these lines thus becomes

$$H_{\text{eff}} = \frac{p^2}{2} + \left(1 + \frac{3g}{4\sigma_p^2} \right) \frac{x^2}{2} + \left(1 - \frac{1}{(2\sigma_x\sigma_p)^2} \right) \frac{gx^4}{4} + \frac{g}{(2\sigma_x\sigma_p)^2} \frac{x_0 x^3}{3} - \frac{g}{4\sigma_p^4} \frac{x^2(p - p_0)^2}{2}.$$

From this effective Hamiltonian one can calculate the effective jump distribution (2.10), which turns out to vanish, i.e., $(\partial_t f_\sigma)_{\text{jump}} = 0$. Consequently, the equation of motion (2.10) of the trial f_σ is identical to the equation of motion (2.5) of the true state f_ρ . The nonlinearity of the equations of motion will however distort the Gaussian such that the ansatz state starts to deviate from the real state.

The characteristics of Eq. (2.7) satisfy

$$\frac{dx}{dt} = p - \frac{g}{4} \frac{x^2(p - p_0)}{\sigma_p^4},$$

$$\frac{dp}{dt} = -x + \frac{g}{4} \left(\frac{x(p - p_0)^2}{\sigma_p^4} - \frac{3x}{\sigma_p^2} + x^2 \frac{x - x_0}{\sigma_x^2 \sigma_p^2} - 4x^3 \right).$$

Clearly the equations of motion for the average phase-space position of the state become

$$\frac{dx_0}{dt} = p_0,$$

$$\frac{dp_0}{dt} = -x_0 \left(1 + \frac{3}{4} \frac{g}{\sigma_p^2} \right) - gx_0^3,$$

which, for $\sigma_p \rightarrow \infty$ (i.e., $\sigma_x \rightarrow 0$), reduce to the equations of motion of the real Hamiltonian (3.1). The latter equations, including the σ_p -dependent term, express Ehrenfest's theorem [20].

The restoration of Ehrenfest's theorem is indicative of the gain made by propagating the classical trial system with the effective Hamiltonian rather than the real Hamiltonian. It should moreover be noted that, at least for the present example, the initial behavior of the distance is drastically different in both situations. Within the truncated Wigner approximation the initial distance will always increase linear in time. The slope is simply determined by the initial value of the $O(\hbar^2)$ correction to the Poisson bracket in order to obtain the Moyal bracket. So although the correction is of $O(\hbar^2)$, it does cause a discrepancy between the exact and the truncated distribution which increases linearly in time. The variational result however has vanishing corrections within first order, which implies that the initial increase in the distance is quadratic. The result is thus correct up to second order, i.e., up to the deviation from Gaussianity due to the nonlinearity of the equations of motion. The curvature cannot be estimated within the present approach but can be found by doing perturbation theory in terms of quantum jumps [7] around the variational state.

Finally, note that the present effective Hamiltonian can be used as an ansatz effective Hamiltonian for the optimization of states that are not Gaussian. The efficiency of course greatly depends on the shape of the state but, if properly parametrized, the initial time evolution can never be worse than the truncated Wigner result.

IV. CONCLUSION

In conclusion, we have presented a method to extract the optimal Hamiltonian for the classical time evolution of the Wigner distribution associated with the unitary evolution of an arbitrary initial state. In general, this effective classical Hamiltonian is different from the Hamiltonian which generates the quantum dynamics. The effective classical Hamiltonian was explicitly calculated for an initial Gaussian trial state in a quartic oscillator. Unlike in the truncated Wigner approximation, the equation of motion was shown to be in agreement with Ehrenfest's theorem and the quantum corrections around the result are of second order.

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