Modification to the pre-factor of the semiclassical propagator

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PACS. 03.65.Sq – .
PACS. 02.70.-c – .
PACS. 31.15.Ar – .

Abstract. – We modify the pre-factor of the semiclassical propagator to improve its efficiency in practical implementations. The new pre-factor represents the smooth portion of an orbit’s contribution, and leads to fast convergence in numerical calculations. As an illustration of the accuracy and efficiency of the resultant propagator, we numerically calculate overlaps between quantum and semiclassical wave functions, as well as low-lying spectrum density in a 10-dimensional system contains unstable classical orbits. This sheds light on applying semiclassical propagator to high dimensional systems.

Semiclassical propagator connects quantum dynamics with classical orbits. It enables one to evaluate quantum quantities from classical orbits. This is in principle applicable to high dimensional quantum systems as an alternative method to do first principle calculations. Since Gutzwiller adds Maslov phase to the Van Vleck semiclassical propagator [1], many tests confirm that the semiclassical propagator has remarkable accuracy [2–5]. Another appealing feature of the semiclassical method is easy to implement parallel computation by requiring each node to handle some orbits. The final result is simply a summation of each orbit’s contribution.

The fundamental approximation of semiclassical method is to treat the Hamiltonian locally as a quadratic function of coordinates and momenta. By expanding the Hamiltonian up to the second order around a phase space point, each orbit is associated to a time dependent quadratic quantum Hamiltonian in semiclassical calculations. In this sense, if numerical performance is not a concern, all kinds of semiclassical formulations are as accurate as the Van Vleck - Gutzwiller (VVG) propagator [1]. The later comes from the stationary phase approximation to the Feynman’s path integral representation of the quantum propagator. In numerical calculations, however, the Herman and Kluk’s (HK) formulation of semiclassical propagator [6] is often a favorite one [7–15].

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Like other formulations, the HK propagator suffers from the sign problem, i.e., fluctuations in nearby orbits’ contributions. An orbit’s contribution is usually a complex number with a phase related to the classical action of the corresponding orbit. The action changes rapidly from orbit to orbit. At the same time, the pre-factor of an orbit’s contribution increases with time rapidly in the HK formulation, this makes the fluctuation increasing drastically with time, and it smears out any useful information sooner or later. The situation is especially worse for systems containing unstable orbits.

A remedy to the sign problem is to use block method to smooth out the fluctuations [16–22]. The basic idea is same as the standard method to do numerical integration of a fluctuating function. Such treatment usually results in an exponential damping term that is equivalent to filter out contribution from unstable orbits. Another consequence of such treatment is that the formulation becomes complicated and the calculation of each orbit’s contribution is numerically more costly.

In this Letter, we present an approach to the sign problem by extracting smooth portion of an orbit’s contribution. The resultant semiclassical propagator converges much faster while maintaining its original accuracy. We achieve this by modifying the pre-factor of the HK formulation with a positive factor. The semiclassical evolution operator with new pre-factor reads

\[ \hat{U}_{sc}(t) = \int \frac{dz}{(2\pi \hbar)^N} R_{z,t} \Delta_{z,t} e^{i(S(z,t))/\hbar} |z_t, \lambda \rangle \langle z, \lambda|. \]  

(1)

Here \( z = (q,p) \) stands for a \( 2 \times N \) dimensional phase space point with \( q \) and \( p \) being the coordinate and momentum respectively. An initial phase space point \( z \) arrives \( z_t = (q_t, p_t) \) at time \( t \) along classical orbit. The action of the orbit is \( S(z,t) = \int_0^t (p \dot{q} - H) dt \) with \( H \) being the Hamiltonian of the system. The states \( |z, \lambda \rangle \) and \( |z_t, \lambda \rangle \) are Gaussian wave packets with \( \lambda \) the squeeze parameter. In coordinate representation, it is

\[ \langle x|z, \lambda \rangle = \left( \frac{\lambda}{\pi \hbar} \right)^{N/4} \exp \left[ -\frac{\lambda}{2\hbar} (x-q)^2 + \frac{i}{\hbar} p(x-q) \right]. \]  

(2)

The pre-factor \( R_{z,t} \) is the square root of a determinant of the complex stability matrix,

\[ R_{z,t} = \sqrt{\det \left[ \frac{1}{2} \left( M_{qq} + M_{pp} - i\lambda M_{qp} + \frac{i}{\lambda} M_{pq} \right) \right]}, \]  

(3)

where the \( N \times N \) matrices \( M_{qq} = \partial_q \dot{q}(q,p), M_{pp} = \partial_p \dot{p}(q,p), M_{qp} = \partial_q \dot{p}(q,p), \) and \( M_{pq} = \partial_p \dot{q}(q,p) \) constitute the stability matrix \( M = \partial_z z(z) \) of the orbit.

Without the modification factor \( \Delta_{z,t} \), Eq. (1) is just the HK propagator. Note that the role of squeeze parameter \( \lambda \) is equivalent to a scale transformation [19], i.e., one obtains the same result by applying the canonical transformation \( q \rightarrow \sqrt{\lambda} q, p \rightarrow p/\sqrt{\lambda} \) to the underlying classical dynamics while keeping \( \lambda = 1 \) in [14] to [15]. In the following discussions, we set \( \lambda = 1 \). With this setting, the modification factor has a simple form,

\[ \Delta_{z,t} = (2\beta + 1)^N [\det(2\beta M^T M + 1)]^{-1/2}, \]  

(4)

where \( \beta \) is a large positive number, and the superscript \( T \) stands for matrix transpose. Since the determinant of the symplectic stability matrix \( M \) is unit, \( \det M = 1 \), and the inverse of \( M \) is already known, we use \( \Delta_{z,t} = (2\beta + 1)^N [\det(2\beta M^T M^{-1})]^{-1/2} \) for practical calculations. Computation cost of the determinant of a \( 2N \times 2N \) real positive matrix is about the same as that of a \( N \times N \) complex matrix, thus calculation of the modification factor needs about
the same computer operations as that of the original pre-factor. This ensures the efficiency to implement the semiclassical evolution operator.\[11\]

The modification factor \[11\] represents the smooth portion of an orbit’s contribution. We obtain it from a kind of block treatment to the HK propagator. The starting point is similar to that in Refs. [16–20]. It is also referred as Filinov transformation to the HK propagator. The basic idea of this block approach is to replace one orbit’s contribution with a weighted average of nearby orbits’ contribution. For weight function in Gaussian form, the summation of the nearby orbits’ contribution has analytic result. Here, the Hamiltonian within each block is approximated as a time dependent quadratic function of coordinates and momenta associated with a representing orbit. This is equivalent to treat the nearby orbits within a block via linearized dynamics associated with the representing orbit. It is apparent that the form of the weight function determines the performance of the resultant propagator.

We perform the weighted average in coherent state (Gaussian wave packet) representation of HK propagator, \((z',\lambda'|\hat{U}_{sc}^{HK}(t)|z_0,\lambda\rangle\). Here \(\hat{U}_{sc}^{HK}(t)\) is the semiclassical evolution operator \[11\] without the modification term \(\Delta_{z,t}\). In principle, any representation should give the same result, provided that one chooses proper weight function. The coherent state representation is over complete, it suffices to consider the case that the initial Gaussian is the same as the final one, \(z'_0 = z_0\). The squeeze parameter \(\lambda'\) can be chosen arbitrary. We set \(\lambda' = 1\), i.e., equal to \(\lambda\) in Eq. 3. Under this specification, we choose a weight function in the following Gaussian form:

\[
W_\beta(z - z') = A_W \exp[-\frac{\beta}{2\hbar} (z_t - z'_t)^2 + i\epsilon(z_t - z'_t)].
\] (5)

Here \(A_W\) is the normalization constant. The phase points \(z\) and \(z'\) move to \(z_t\) and \(z'_t\) along classical orbits at time \(t\), respectively. The width parameter \(\beta > 0\) is a large number to ensure that the weight function is effectively distributed near its center point. The imaginary part of the exponent is a small adjusted phase to cancel fluctuation in the average procedure. We choose \(\epsilon\) to make the orbit starting from \(z\) being a stationary phase orbit.

After the weighted average, an orbit’s contribution to the propagator gains an extra factor

\[
\Delta_{z,t} = \left(\frac{2\beta + 1}{\pi}\right)^N \int dz' e^{-[2\beta(\delta z_t)^2 + (\delta z)^2 + 2(z - z_0)\delta z]/4\hbar},
\] (6)

where \(\delta z = z' - z\), \(\delta z_t = z'_t - z_t\), and \(z\) is the initial phase space point of the orbit. We obtain the above result by applying linearized dynamics to the actions of the nearby orbits. Details of the procedure is similar to that in Refs. [16–20]. Another approximation is that the terms \((\delta z_t)^2 + 2(z - z_0)\delta z_t\), as well as a small normalization term are dropped from the exponent of the integrand. These terms are small compared to the first term of the exponent.

Note that the right hand side of (6) is real and positive definite, i.e. the integrand’s phase vanishes. This comes from two facts: (1) Since we set \(\lambda' = \lambda = 1\), the second order terms of an nearby orbit’s action cancel with the second order terms of the phase of the Gaussian wave packets; (2) The first order terms of the action plus the first order terms of the phase of the Gaussian wave packet are \((p_t - p_0)\delta q_t - (q_t - q_0)\delta p_t - (p - p_0)\delta q + (q - q_0)\delta p\). Under linearized dynamics, \((p - p_0)\delta q - (q - q_0)\delta p\) is symplectic, i.e., it is equal to \((p_t - p_0)\delta q_t - (q_t - q_0)\delta p_t\), where \(z_0 = (q_0, p_0)\) moves to \(z_t = (q_t, p_t)\) along classical orbit at time \(t\). Thus the first order terms of the integrand’s phase are linearly dependent on \(\delta z_t = (\delta q_t, \delta p_t)\). By proper choice of the adjust parameter \(\epsilon\) in the weight function, the integrand’s phase vanishes.

The integral in (6) represents an overlap of two classical density distributions at time \(t\). One of them is initially \(\rho_1(0) = \exp\{-[(\delta z)^2 + 2(z - z_0)\delta z]/4\hbar\}\). After evolution for a period of time \(t\) according to classical dynamics, its overlap with the density distribution

\[
\rho_2 = \exp\{-\beta(\delta z_t)^2/2\hbar\}
\] gives the integral in (6).
From consideration of classical dynamics, we argue that the second term in the exponent of $\rho_1$ is negligible. At initial time $t = 0$, the second density distribution $\rho_2$ is highly localized in comparison with $\rho_1$. Within the effective distributed area of $\rho_2$, $\rho_1$ is virtually a constant. Thus $\rho_2$ dominates the integral and $\rho_1$ can be replaced by a constant at initial time. As time $t$ increases, phase space points stretch out in some directions, and folding up in others. Such stretching and folding of phase space make the distribution $\rho_1$ distorted in phase space. The quadratic term of $\rho_1$, i.e., $\rho_{11} = \exp[-(\delta z)^2/4\hbar]$ has only finite effective distribution area that is distorted during evolution. The distorted area overlaps only partially with $\rho_2$ at time $t$. On the other hand, the second term of $\rho_1$, i.e., $\rho_{12} = \exp[-(z-z_0)\delta z/2\hbar]$, however, behaves in a quite different way. This term is unbounded, and it is smoother than the quadratic term. Thus the distortion of phase space does not affect its overlap with the distribution $\rho_2$. Similar to the initial time $t = 0$, within the effective distribution area of $\rho_2$, $\rho_{12}$ is effectively a constant, and can be dropped from the integral.

As usual, we treat the overlap between $\rho_{11}$ and $\rho_2$ at time $t$ via linearized dynamics. The result is $\langle 1 \rangle$. Since this modification factor is independent of the wave packet $|z_0, \lambda', \eta\rangle$, we obtain the evolution operator in the form of Eq. $\langle 1 \rangle$. This concludes our theoretical derivation.

We test the performance of the semiclassical evolution operator $\langle 1 \rangle$ via Hénon-Heiles (HH) Hamiltonian [23]. This system contains unstable classical orbits, and the original HK propagator converges only in a rather short time scale. Properties of the HH system is widely investigated classically, quantum mechanically, as well as semi-classically, including improvement to the semiclassical propagator by block treatments [17–19].

We first compare semiclassical wave function with exact quantum result via overlap between semiclassical and quantum wave functions. Solid lines in Fig. $\langle 1 \rangle$ are the result of a particle of unit mass in the 2-dimensional Hénon-Heiles potential $V(x, y) = \frac{1}{2}(\omega_x^2 x^2 + \omega_y^2 y^2) + \lambda y(x^2 + \eta y^2)$, where $\omega_x = 1.3$, $\omega_y = 0.7$, $\lambda = -0.1$, $\eta = 0.1$, and the Planck constant is set to 1. The wave function of the particle is initially a Gaussian with center position at $(1, 1)$ and center momentum vanished. The semiclassical wave function is normalized to unit before doing overlap. These parameters are the same as that of Ref. [18], in which there is a similar calculation in a time scale between 0 to 100, and it shows that the original HK propagator converges only for time less than 50. We see that, within a normalization constant, the semiclassical wave function possesses remarkable accuracy. As comparison, we show by dashed lines the corresponding result using formulation of Ref. [18], which is more suitable for calculation of wave function than other existing formulations. It is evident that for time $t > 100$, Eq. $\langle 1 \rangle$ is more stable and converges faster.

As is shown in Fig. $\langle 1 \rangle$, the accuracy of the semiclassical wave function is rather insensitive to the value of $\beta$, provided that $\beta$ is large enough, or the effective distribution area of the weight function is sufficiently localized. Small value of $\beta$, or wider distributed weight function, leads to faster convergence, i.e., one needs less orbits. However, if $\beta$ is improperly small, the linearized dynamics treatment to the modification factor is invalid beyond certain time. When this happens, we find that the normalization constant of the wave function becomes vanishing small after certain time. We use this property to check the validness of the width parameter $\beta$.

Next, we test the semiclassical propagator’s performance in finding energy spectrum of quantum systems. In fact, calculation of energy spectrum in high dimensional systems is fundamental important, and is still a challenge in many systems. Similar to Ref. [19], we make numerical test in a high dimensional Hénon-Heiles system, i.e., a particle of unit mass moving in a $N$-dimensional HH potential, $V(x) = \frac{1}{2}\sum_{i=1}^{N} x_i^2 + \lambda \sum_{i=1}^{N-1} (x_i^2 x_{i+1} + \eta x_i^3)$, where $\lambda = 0.1$, and $\eta = -0.3$. The initial wave function is a Gaussian wave packet whose central position is $q_i = 2$ and central momentum vanishes, $p_i = 0$. Classical orbit in such region is
more unstable than that of Fig. 1. One can obtain energy spectrum from auto-correlation function by Fourier transformation, or more advanced filter diagonalization [24]. In Fig. 2(a), we show the auto-correlation function versus time in a 2-dimensional case, and in Fig. 2(b) we show the real part of its Fourier transformation, namely, the spectrum density. Here the thick solid line is the exact quantum result, and the dashed line is semiclassical result from Eq. (1). The thin solid line is the semiclassical result using formulation of Ref. [19], an improved version of Walton’s formulation [17]. We see that in a remarkable time scale, the semiclassical auto-correlation function is very close to the quantum result. Such time scale is enough to resolve the spectrum, and the semiclassical spectrum density is able to reproduce quantum result very well. This is especially the case for the peaks of the spectrum density, whose positions correspond to the energy spectrum. The behavior of the auto-correlation function is about the same as that of the wave function as shown in Fig. 1. Our test shows that the spectrum density converges faster than the wave function, and the peaks of the spectrum density are not sensitive to the width parameter $\beta$. In calculations of Fig. 2(a), we use $10^4$ orbits by setting the width parameter to 1,000. However the spectrum density of Fig. 2(b) is resultant of 2,000 orbits with the width parameter of 100. In fact, auto-correlation function in shorter time is more important to determine the position of the peaks of the spectrum density, and shorter time wave function converges faster than that of longer time, and is more insensitive to the width parameter. This explains the fast convergence rate of the spectrum density. Note that, although Eq. (1) gives more accurate correlation function in longer times than that of Ref. [19], the two semiclassical results in Fig. 2 yield almost the same spectrum density. This property of the spectrum density sheds light on applying semiclassical propagator to find energy spectrum in high dimensional systems.

Our numerical calculation for high dimensional HH system confirms the above properties in the lowlying energy. The lowlying spectrum density converges much faster than the higher ones, and the accuracy is quite insensitive to the width parameter $\beta$. In calculations for different width parameters $\beta$. Figure 3 is semiclassical spectrum density versus energy in a 10-dimensional HH system. To confirm the convergence, we make calculations for different width parameters $\beta$. The thick solid, dashed, and dotted lines are for width parameter $\beta = 100, 200$, and 50 respectively. From Fig. 3 it is evident that the spectrum density for energy less than 30 is well converged. Small $\beta$ leads to fast convergence without sacrificing the accuracy of lowlying spectrum. We use 20,000, 60,000, and 10,000 orbits to produce the solid, dashed, and dotted lines, respectively. In fact, for $\beta = 50, 2,000$ orbits is almost enough to obtain the lowlying spectrum, i.e., the peak positions of the spectrum density. Again, the thin solid line is the result using formulation of Ref. [19]. Although it gives almost the same spectrum, result from Eq. (1) has better resolution, which demonstrates better accuracy in longer times.

In summary, we have introduced a modification to the pre-factor of the semiclassical propagator in the HK formulation. It represents the smooth portion of an orbit’s contribution to the semiclassical propagator. Unlike other formulations, this modification factor is just an overlap between two classical density distributions. Our treatment to this classical overlap yields a concise expression of the modification factor which is positive definite. The resultant semiclassical propagator converges much faster while maintaining its original accuracy. This improvement to the convergence is prominent in the calculation of lowlying spectrum density for high dimensional systems. This result sheds light on the efforts towards applying semiclassical propagator as a practical tool of first principle computation.

This work is supported in part by the National Natural Science Foundation (Grant No. 10375042), the Research Fund of the State Education Ministry of China, and the Research Fund of the Wuhan University. BL is partly supported by Faculty Research Grant of National
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Fig. 1 – Overlap between normalized semiclassical wave function and exact quantum wave function versus time. Solid and dashed lines are results of Eq. (1) and Herman’s formulation [18], respectively. $\beta$ is the width parameter, and $n$ is the number of orbits used in semiclassical calculations.
Fig. 2 – (a) Real part of the auto-correlation function $C(t)$ versus time. (b) Real part of the spectrum density versus energy. Thick solid, dashed and thin solid lines are exact quantum result and semiclassical result from Eq. (1), as well as semiclassical result using formulation of Ref. [19], respectively.
Fig. 3 – Spectrum density versus energy in 10-dimensional HH system. The number of orbits $n$ and the width parameter $\beta$ in semiclassical calculations are indicated accordingly. The thin solid line is the semiclassical result of Ref. [19] with $\beta = 100$ and $n = 10000$. 