Semiclassical coherent-state propagator via path integrals with intermediate states of variable width

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We derive a semiclassical approximation for the coherent state propagator $\langle z''|e^{-iHt/\hbar}|z'\rangle$ using a path integral formulation in which the intermediate coherent states can have arbitrary widths. Our semiclassical formula involves complex trajectories of the smoothed Hamiltonian $\mathcal{H}(q,p,b)=\langle z|\hat{H}|z\rangle$ where b, the width of the coherent state $|z\rangle$, is a free function that can be chosen conveniently. The generality of this formalism enables us to derive a semiclassical approximation which contains, as particular cases, other similar approximations known in the literature, providing a natural link between them. We present numerical results showing that the semiclassical propagation can be very sensitive to the choice of b and we suggest an energy dependent value $b=b_E$ that results in considerable improvement over other choices. This value for the width will be generally different from the widths σ' or σ'' of the initial and final states $|z'\rangle$ and $|z''\rangle$.

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I. INTRODUCTION

Coherent states are a powerful tool in the study of the semiclassical limit of quantum mechanics. They provide a minimum uncertainty overcomplete representation containing explicit information on both position and momentum, leading to a natural phase space picture of quantum mechanics.

The first derivation of the semiclassical coherent state propagator based on path integral techniques was given by Klauder [1–3]. Weissman [4,5] and Heller and collaborators [6,7] also presented a derivation of the semiclassical propagator, based on general semiclassical techniques. Baranger *et al.* [8] have recently given a detailed derivation of the semiclassical coherent state propagator using path integrals.

The overcompleteness of the coherent basis set leads to several possible path integral representations of the evolution operator. These representations, while identical quantum mechanically, lead to different propagators in the semiclassical limit. Klauder and Skagerstam [2] considered this question from the quantum mechanical point of view, presenting two basic constructions for the quantum mechanical path integral. One of these forms is associated with a Hamiltonian H_1 which is a smoothed version of the classical Hamiltonian H. The other involves a different Hamiltonian H_2, which can be thought of as an antismoothed version of the classical H. The semiclassical limits of these basic forms were discussed in detail in [8]. A third construction, which combines the two basic ones, was discussed in [9], and is closely related to the classical Hamiltonian itself. In this paper we shall restrict ourselves to the first type of construction and we shall use the symbol $\mathcal{H}$ for H_1.

In all these previous formulations, the path integrals are constructed using coherent states with the same fixed width, i.e., coherent states of the same harmonic oscillator of mass m and frequency ω. These are given by

$$|z\rangle = e^{-|z|^2/2} e^{z\hat{a}^\dagger}|0\rangle \tag{1}$$

with $|0\rangle$ the harmonic oscillator ground state and

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(\frac{\hat{q}}{b} - i\frac{\hat{p}b}{\hbar}\right), \quad z = \frac{1}{\sqrt{2}}\left(\frac{q}{b} + i\frac{pb}{\hbar}\right). \tag{2}$$

In the above, $\hat{q}$, $\hat{p}$, and $\hat{a}^\dagger$ are operators; q and p are real numbers; z is complex. The parameter

$$b = (\hbar/m\omega)^{1/2} \tag{3}$$

defines the length scale and we call it the *width* of the coherent state.

These states satisfy the identity

$$\mathbb{1} = \int |z\rangle \frac{d^2z}{\pi} \langle z| \tag{4}$$

independent of the width b. In this paper we explore this fact and construct path integrals where the infinitesimal propagations, in which the full evolution operator is broken into, are between coherent states of different widths. In the continuum limit, the width itself becomes a time dependent quantity that can be chosen conveniently to improve the performance of the semiclassical approximation.

Our main result, Eq. (53), is a semiclassical approximation for the propagator $\langle z''|\hat{K}(T)|z'\rangle$ in which the initial and final coherent states have arbitrary widths σ' and σ'', respectively, and $\hat{K}(T)=e^{-i\hat{H}T/\hbar}$ is the evolution operator. This formula involves classical trajectories governed by the Hamiltonian $\mathcal{H}(q,p,b)=\langle z|\hat{H}|z\rangle$ where the "dynamical width" $b=b(t)$ can be chosen appropriately and does not need to coincide with either σ' or σ''.

In order to test our formula in some simple situations, we project the coherent state propagator in the position representation and calculate the semiclassical approximation for the mixed propagator $\langle x|\hat{K}(T)|z'\rangle$. The result, a Gaussian function of x that depends only on the trajectory issuing from $q(0)=q'$, $p(0)=p'$, will be called a Gaussian semiclassical approximation (GSA). The GSA is related to another well

known type of semiclassical approximation called the initial value representation (IVR). IVR's are written as

$$\langle x|\hat{K}(T)|\psi\rangle = \int \frac{dq'dp'}{2\pi\hbar} F(x,z',T)\langle z'|\psi\rangle, \tag{5}$$

where the kernel $F(x,z',T)$ is given solely in terms of classical trajectories starting at q',p'. The GSA described above plays the role of a kernel.

The general idea of initial value representations is to have semiclassical formulas in which only trajectories defined by their initial position and momentum are needed. IVR's avoid the cumbersome calculation of trajectories starting at a certain position and ending at another and have become very popular among chemists [10–18]. Of the three most used IVR kernels, Heller's [10], that of Baranger, de Aguiar, Keck, Korsch, and Schellhaass (BAKKS) [8], and Herman and Kluk's [11,12,19–21], the last seems to be superior in most tested cases (see, however, [22,23]). Our GSA formula is an improvement over the kernels of BAKKS and Heller and might result in a more accurate IVR representation.

This paper is organized as follows. In Sec. II we derive our main formula for the coherent state propagator, Eq. (53), and for the GSA, Eq. (68). Section III is devoted to some analytical and numerical applications of the formalism. Our conclusions are summarized in Sec. IV.

II. FORMALISM

In this section we construct a path integral representation for the coherent state propagator

$$K(z'',z',T) = \langle z''|\hat{\mathcal{T}} e^{-(i/\hbar)\int_0^T \hat{H}(t)dt}|z'\rangle, \tag{6}$$

where $\hat{\mathcal{T}}$ is the time ordering operator. We assume that the quantum Hamiltonian $\hat{H}$ can be written as a power series of the creation and annihilation operators $\hat{a}$ and $\hat{a}^\dagger$ and that the initial and final coherent states have arbitrary widths σ' and σ'', respectively.

We divide the time T into N steps of size τ, so that, in the limit of small τ, the propagator can be written as

$$K(z'',z',T) = \left\langle z_N \left| \prod_{j=0}^{N-1} e^{-(i/\hbar)\hat{H}(t_j)\tau} \right| z_0 \right\rangle, \tag{7}$$

where we have set $z_N = z''$ and $z_0 = z'$ and the time t_j is in the interval $[j\tau,(j+1)\tau]$.

The next step is to insert $(N-1)$ unit operators between each successive exponential. Since σ' and σ'' are arbitrary, there is no *a priori* reason to choose the width of these intermediate states as either one of them. Rather, for each resolution of unit we shall associate a width b_j which, in principle, can take any value. Our main purpose is to obtain a semiclassical approximation for the propagator starting from a path integral formulation where the intermediate states can have arbitrary widths. We shall then verify the sensitivity of the approximation to different choices of intermediate widths $\{b_j\}$.

A. Coherent states of arbitrary widths

A coherent state $|z\rangle$ of the harmonic oscillator is specified by three real parameters q,p, and b, corresponding to the expectation values of the position and momentum operators and the mean square deviation of the position. The parameter b, which is the width of the packet $\psi(x)=\langle x|z\rangle$, is also related to uncertainty in position by $b=\sqrt{2}\Delta q$ and to the frequency of the associated harmonic oscillator by $b=\sqrt{\hbar/m\omega}$.

To make these parameters explicit it is sometimes useful to write $|z\rangle = |q,p,b\rangle$ or $z=z(q,p,b)$, with $(q,p,b)\in \mathbf{R}^2\times\mathbf{R}_+$. In this notation the resolution of unit reads

$$\mathbb{1} = \int\int |q,p,b\rangle \frac{dqdp}{2\pi\hbar}\langle q,p,b| \tag{8}$$

and is independent of b. In order to take advantage of this freedom in the path integral, we shall need to compute the overlap between two coherent states labeled by $z_j = z_j(q_j,p_j,b_j)$ and $z_{j+1}=z_{j+1}(q_{j+1},p_{j+1},b_{j+1})$. A simple calculation gives

$$\langle z_{j+1}|z_j\rangle = \sqrt{\frac{2b_jb_{j+1}}{b_j^2+b_{j+1}^2}} \exp\left\{ -\frac{1}{2}\left(\frac{1}{b_j^2+b_{j+1}^2}\right) \times f(q_j,q_{j+1},p_j,p_{j+1},b_j,b_{j+1}) \right\}, \tag{9}$$

where

$$f(q_j,q_{j+1},p_j,p_{j+1},b_j,b_{j+1}) \equiv f_{j+1,j} = (q_{j+1}-q_j)^2 + \frac{(b_jb_{j+1})^2}{\hbar^2}(p_{j+1}-p_j)^2 - \frac{2i}{\hbar}\left[b_j^2 q_{j+1}p_j - b_{j+1}^2 q_j p_{j+1} + \frac{1}{2}(b_{j+1}^2-b_j^2) \times (q_{j+1}p_{j+1}+q_jp_j) \right]. \tag{10}$$

For $b_j = b_{j+1}$ the overlap between coherent states of the same harmonic oscillator is recovered.

B. The path integral

Using Eq. (8) the propagator (7) can be written as

$$K(z'',z',T) = \int \left\{ \prod_{j=1}^{N-1} \frac{d^2 z_j}{\pi} \right\} \prod_{j=0}^{N-1} \{ \langle z_{j+1} | e^{-(i/\hbar)\hat{H}(t_j)\tau} | z_j \rangle \}, \tag{11}$$

where $z_j = z_j(q_j, p_j, b_j)$ and the limits $N \to \infty$, $\tau \to 0$, $N\tau = T$ are implicit. This corresponds to Klauder's *first form* of path integral [2]. Following his steps we write

$$\prod_{j=0}^{N-1} \{ \langle z_{j+1} | e^{-(i/\hbar)\hat{H}(t_j)\tau} | z_j \rangle \} \approx \prod_{j=0}^{N-1} \langle z_{j+1} | z_j \rangle \exp\left\{ \sum_{j=0}^{N-1} -\frac{i\tau}{\hbar} \mathcal{H}_{j+1,j} \right\}, \tag{12}$$

with the notation

$$\mathcal{H}_{j+1,j} \equiv \frac{\langle z_{j+1} | \hat{H}(t_j) | z_j \rangle}{\langle z_{j+1} | z_j \rangle}. \tag{13}$$

From Eqs. (9), (11), and (12), we obtain

$$K(z'',z',T) = \int \left\{ \prod_{j=1}^{N-1} \frac{d^2 z_j}{\pi} \right\} \prod_{j=0}^{N-1} \sqrt{\frac{2 b_j b_{j+1}}{b_j^2 + b_{j+1}^2}} e^{F[q,p,b]}, \tag{14}$$

with

$$F[q,p,b] = \sum_{j=0}^{N-1} \left\{ -\frac{1}{2} \left(\frac{1}{b_j^2 + b_{j+1}^2} \right) f_{j+1,j} - \frac{i\tau}{\hbar} \mathcal{H}_{j+1,j} \right\}. \tag{15}$$

Here we are using the abbreviation $[q,p,b] = (q_0, \ldots, q_N, p_0, \ldots, p_N, b_0, \ldots, b_N)$. We remember that $(q_0, p_0, b_0) = (q', p', \sigma')$ and $(q_N, p_N, b_N) = (q'', p'', \sigma'')$.

In the semiclassical limit $\hbar \to 0$ the integrals in Eq. (14) can be performed in the stationary exponent approximation, which consists of three basic steps.

(1) Calculate the stationary path, i.e., the set of points $(q_1, q_2, \ldots, q_{N-1}, p_1, p_2, \ldots, p_{N-1})$ satisfying

$$\frac{\partial F}{\partial p_k} = \frac{\partial F}{\partial q_k} = 0, \quad k = 1, \ldots, N-1. \tag{16}$$

(2) Expand F to second order around the stationary path and perform the resulting Gaussian integrals.

(3) Simplify the prefactors arising from the Gaussian integrations.

These steps are performed in Secs. II C, II D, and II E, respectively.

C. The stationary trajectory

Equations (16) lead to the equations

$$-\frac{1}{2}\left(\frac{1}{b_k^2 + b_{k+1}^2}\right)\left\{ -\frac{2}{\hbar^2}(b_k b_{k+1})^2 (p_{k+1} - p_k) - \frac{2i}{\hbar}\left[b_k^2 q_{k+1} + \frac{1}{2}(b_{k+1}^2 - b_k^2) q_k \right] \right\} - \frac{1}{2}\left(\frac{1}{b_{k-1}^2 + b_k^2}\right)\left\{ \frac{2}{\hbar^2}(b_{k-1} b_k)^2 (p_k - p_{k-1}) - \frac{2i}{\hbar}\left[-b_k^2 q_{k-1} + \frac{1}{2}(b_k^2 - b_{k-1}^2) q_k \right] \right\} - \frac{i\tau}{\hbar}\left(\frac{\partial \mathcal{H}_{k,k-1}}{\partial p_k} + \frac{\partial \mathcal{H}_{k+1,k}}{\partial p_k} \right) = 0 \tag{17}$$

and

$$-\frac{1}{2}\left(\frac{1}{b_k^2 + b_{k+1}^2}\right)\left\{ -2(q_{k+1} - q_k) - \frac{2i}{\hbar}\left[-b_{k+1}^2 p_{k+1} + \frac{1}{2}(b_{k+1}^2 - b_k^2) p_k \right] \right\} - \frac{1}{2}\left(\frac{1}{b_{k-1}^2 + b_k^2}\right)\left\{ 2(q_k - q_{k-1}) - \frac{2i}{\hbar}\left[b_{k-1}^2 p_{k-1} + \frac{1}{2}(b_k^2 - b_{k-1}^2) p_k \right] \right\} - \frac{i\tau}{\hbar}\left(\frac{\partial \mathcal{H}_{k,k-1}}{\partial q_k} + \frac{\partial \mathcal{H}_{k+1,k}}{\partial q_k} \right) = 0. \tag{18}$$

For $k = 1$ and $k = N-1$, which is equivalent to $t = 0$ and $t = T$, Eqs. (17) and (18) provide the boundary conditions for the classical complex path:

$$\frac{1}{\sqrt{2}}\left(\frac{q(0)}{\sigma'} + i\frac{\sigma' p(0)}{\hbar} \right) = \frac{1}{\sqrt{2}}\left(\frac{q'}{\sigma'} + i\frac{\sigma' p'}{\hbar} \right) = z' \tag{19}$$

and

$$\frac{1}{\sqrt{2}}\left(\frac{q(T)}{\sigma''} - i\frac{\sigma'' p(T)}{\hbar} \right) = \frac{1}{\sqrt{2}}\left(\frac{q''}{\sigma''} - i\frac{\sigma'' p''}{\hbar} \right) = z''^{*}. \tag{20}$$

For intermediate values of k we can expand Eqs. (17) and (18) in terms of the infinitesimal differences $\Delta q_k = q_{k+1}$

$-q_k$, $\Delta p_k = p_{k+1} - p_k$, and $\Delta b_k = b_{k+1} - b_k$. In the limit $\tau \to 0$ only first order terms contribute to the equations. We get

$$\frac{1}{2\hbar^2}(\Delta p_k - \Delta p_{k-1}) + \frac{i}{2\hbar}(\Delta q_k + \Delta q_{k-1}) - \frac{i\tau}{\hbar}\left(\frac{\partial \mathcal{H}_{k,k-1}}{\partial p_k} + \frac{\partial \mathcal{H}_{k+1,k}}{\partial p_k}\right) = 0 \tag{21}$$

and

$$\frac{1}{2b_k^2}(\Delta q_k - \Delta q_{k-1}) - \frac{i}{2\hbar}(\Delta p_k + \Delta p_{k-1}) - \frac{i\tau}{\hbar}\left(\frac{\partial \mathcal{H}_{k,k-1}}{\partial q_k} + \frac{\partial \mathcal{H}_{k+1,k}}{\partial q_k}\right) = 0. \tag{22}$$

As $\tau \to 0$, $\Delta q/\tau \to \dot{q}$, $\Delta p/\tau \to \dot{p}$, and

$$\left(\frac{\partial \mathcal{H}_{k,k-1}}{\partial q_k} + \frac{\partial \mathcal{H}_{k+1,k}}{\partial q_k}\right) \to \frac{\partial \mathcal{H}}{\partial q}, \quad \left(\frac{\partial \mathcal{H}_{k,k-1}}{\partial p_k} + \frac{\partial \mathcal{H}_{k+1,k}}{\partial p_k}\right) \to \frac{\partial \mathcal{H}}{\partial p} \tag{23}$$

(these last relations are demonstrated in Appendix A). Therefore, Eqs. (21) and (22) become simply

$$\dot{q} = \frac{\partial \mathcal{H}}{\partial p} \quad \text{and} \quad \dot{p} = -\frac{\partial \mathcal{H}}{\partial q}. \tag{24}$$

The solutions of Hamilton's equations (24) with boundary conditions (19) and (20) are the extremal paths or trajectories. The Hamiltonian $\mathcal{H}(q,p,b) = \langle z|\hat{H}|z\rangle$, however, contains a nonconstant width $b(t)$ that modifies the dynamics. We recall that $\mathcal{H}$ does not coincide with the Weyl hamiltonian H, which is the most direct classical counterpart of $\hat{H}$. For quantum Hamiltonians of the form $\hat{H} = \frac{1}{2}\hat{p}^2 + \hat{V}$, we obtain $\mathcal{H}(q,p,b) = \frac{1}{2}p^2 + \hbar^2/4b^2 + \mathcal{V}(q,b)$, with $\mathcal{V} \equiv \langle z|\hat{V}|z\rangle$.

D. The stationary exponent and the Gaussian integrals

Once the equations of motion have been obtained, we proceed to expand the exponent $F[q,p,b]$ of Eq. (14) around the extremal paths.

Let us denote the classical trajectory by $(\overline{q_j}, \overline{p_j})$ and the corresponding deviations from it by $Q_j = q_j - \overline{q_j}$ and $P_j = p_j - \overline{p_j}$. We write

$$F = \overline{F} + F_1 + F_2, \tag{25}$$

where $\overline{F}$ is the zeroth order term, corresponding to F evaluated over the classical trajectory. The first order term is of course zero, and the second order term F_2 is a quadratic form in Q and P. It is convenient to define the auxiliary variables

$$u_j = \frac{1}{\sqrt{2}}\left(\frac{q_j}{b_j} + i\frac{b_j p_j}{\hbar}\right), \quad v_j = \frac{1}{\sqrt{2}}\left(\frac{q_j}{b_j} - i\frac{b_j p_j}{\hbar}\right) \tag{26}$$

and the analogous variables U_j and V_j related to Q_j and P_j in the same way. In these variables F_2 can be written as

$$F_2 = -\sum_{j=1}^{N-1} (\alpha_j U_j^2 + \beta_j V_j^2 + \gamma_j U_j V_j + \lambda_j U_j V_{j+1} + \mu_j U_j U_{j+1} + \nu_j V_j V_{j+1} + \vartheta_j U_{j+1} V_j) \tag{27}$$

with coefficients

$$\alpha_j = -\frac{b_{j+1}^2 - b_j^2}{2(b_{j+1}^2 + b_j^2)} + \frac{\tau}{2}\varphi_j, \quad \beta_j = \frac{b_{j+1}^2 - b_j^2}{2(b_{j+1}^2 + b_j^2)} + \frac{\tau}{2}\varrho_j,$$

$$\lambda_j = -\frac{2b_j b_{j+1}}{b_{j+1}^2 + b_j^2} + \tau\kappa_j, \quad \gamma_j = 1, \quad \text{and} \quad \mu_j = \nu_j = \vartheta_j = 0, \tag{28}$$

where

$$\varphi_j = \left(\frac{ib_j^2}{2\hbar}\frac{\partial^2}{\partial q_j^2} - \frac{i\hbar}{2b_j^2}\frac{\partial^2}{\partial p_j^2} + \frac{\partial^2}{\partial q_j \partial p_j}\right)(\mathcal{H}_{j+1,j} + \mathcal{H}_{j,j-1}), \tag{29}$$

$$\varrho_j = \left(\frac{ib_j^2}{2\hbar}\frac{\partial^2}{\partial q_j^2} - \frac{i\hbar}{2b_j^2}\frac{\partial^2}{\partial p_j^2} - \frac{\partial^2}{\partial q_j \partial p_j}\right)(\mathcal{H}_{j+1,j} + \mathcal{H}_{j,j-1}), \tag{30}$$

$$\kappa_j = \frac{1}{2}\left(\frac{ib_j b_{j+1}}{\hbar}\frac{\partial^2 \mathcal{H}_{j+1,j}}{\partial q_j \partial q_{j+1}} - \frac{b_j}{b_{j+1}}\frac{\partial^2 \mathcal{H}_{j+1,j}}{\partial q_j \partial p_{j+1}} + \frac{b_{j+1}}{b_j}\frac{\partial^2 \mathcal{H}_{j+1,j}}{\partial q_{j+1} \partial p_j} + \frac{i\hbar}{b_j b_{j+1}}\frac{\partial^2 \mathcal{H}_{j+1,j}}{\partial p_j \partial p_{j+1}}\right). \tag{31}$$

The coefficients α_j, β_j, and λ_j in Eq. (28) must be handled carefully. Keeping only linear terms in Δb_j we find

$$\alpha_j = \begin{cases} -\Delta b_j/2b_j + \tau\varphi_j/2 & \text{for } j = 1, \ldots, N-2, \\ -\delta''/2 + \tau\varphi_j/2 & \text{for } j = N-1, \end{cases} \tag{32}$$

$$\beta_j = \begin{cases} \Delta b_{j-1}/2b_j + \tau\varrho_j/2 & \text{for } j = 2, \ldots, N-1, \\ \delta'/2 + \tau\varrho_j/2 & \text{for } j = 1, \end{cases} \tag{33}$$

$$\lambda_j = \tau\kappa_j - 1 \quad \text{for } j = 1, \ldots, N-2, \tag{34}$$

where $\delta'' = [\sigma''^2 - b^2(T)]/[\sigma''^2 + b^2(T)]$ and $\delta' = [b^2(0) - \sigma'^2]/[b^2(0) + \sigma'^2]$. Note that α_0, α_N, β_0, β_N, λ_0, λ_{N-1}, and λ_N are never used because U_0, U_N, V_0, and V_N vanish.

Finally, the square root multiplying the exponential in Eq. (14) has only second and higher order terms in Δb_j. Therefore, it contributes only at the extremities of the trajectory, since $b(0)$ does not have to be σ' and $b(T)$ does not have to be σ''. Putting these ingredients together we obtain

$$K(z''^*,z',T)\approx\sqrt{\frac{4\sigma' b(0)\sigma'' b(T)}{[\sigma'^2+b^2(0)][\sigma''^2+b^2(T)]}}e^{\bar{F}}\times\int\left\{\prod_{j=1}^{N-1}\frac{dU_j dV_j}{\pi}\right\}e^{F_2[U,V]}$$
$$=\sqrt{\frac{4\sigma' b(0)\sigma'' b(T)}{[\sigma'^2+b^2(0)][\sigma''^2+b^2(T)]}}\times e^{\bar{F}}[(-1)^{N-1}\det M^{(N-1)}]^{-1/2}, \quad (35)$$

where the symmetric $2(N-1)\times 2(N-1)$ matrix $M^{(N-1)}$ is defined by the relation $2F_2=-\Gamma^T M^{(N-1)}\Gamma$ (see [8]), with $\Gamma^T=(U_{N-1},V_{N-1},\ldots,U_1,V_1)$ and Γ the corresponding column vector.

In order to calculate $\bar{F}$ and $\det M^{(N-1)}$, it is convenient to define the variables

$$\eta(t)=\frac{1}{\sqrt{2}}\left(\frac{q(t)}{\sigma'}+i\frac{\sigma' p(t)}{\hbar}\right),$$
$$\xi(t)=\frac{1}{\sqrt{2}}\left(\frac{q(t)}{\sigma''}-i\frac{\sigma'' p(t)}{\hbar}\right). \quad (36)$$

In these variables the boundary conditions (19) and (20) become simply $\eta(0)\equiv\eta'=z'$ and $\xi(T)\equiv\xi''=z''^*$. The exponent $\bar{F}$ also simplifies to (see Refs. [2,8])

$$\bar{F}=\frac{i}{\hbar}S(\xi'',\eta',T)-\frac{1}{2}(|\eta'|^2+|\xi''|^2)+\frac{(\sigma''^2-\sigma'^2)}{2(\sigma'^2+\sigma''^2)}(\eta'^2-\xi''^2), \quad (37)$$

where $S(\xi'',\eta',T)$ is the complex action,

$$S(\xi'',\eta',T)=\int_0^T\left[\chi\frac{i\hbar}{2}(\xi\dot{\eta}-\eta\dot{\xi})-\mathcal{H}\right]dt-\chi\frac{i\hbar}{2}\times[\eta'\xi(0)+\xi''\eta(T)] \quad (38)$$

and $\chi=2\sigma'\sigma''/(\sigma'^2+\sigma''^2)$.

It can be shown that small variations $\delta\eta'$ and $\delta\xi''$ in S lead to

$$\delta S=-i\hbar\chi[\xi(0)\delta\eta'+\eta(T)\delta\xi'']. \quad (39)$$

Therefore

$$\frac{\partial S}{\partial\eta'}=-i\hbar\chi\xi(0)\equiv-i\hbar\chi\xi',$$
$$\frac{\partial S}{\partial\xi''}=-i\hbar\chi\eta(T)\equiv-i\hbar\chi\eta''. \quad (40)$$

Also

$$-i\hbar\chi\delta\xi'=\frac{\partial^2 S}{\partial\eta'^2}\delta\eta'+\frac{\partial^2 S}{\partial\eta'\partial\xi''}\delta\xi'' \quad (41)$$

and

$$-i\hbar\chi\delta\eta''=\frac{\partial^2 S}{\partial\eta'\partial\xi''}\delta\eta'+\frac{\partial^2 S}{\partial\xi''^2}\delta\xi''. \quad (42)$$

Variation in the propagation time T leads to the usual relation $\partial S/\partial T=-\mathcal{H}$.

E. The prefactor

The calculation of $\det M^{(N-1)}$ is worked out in Appendix B, and the result is

$$(-1)^{N-1}\det M^{(N-1)}=[\delta v(T)-\delta'\delta u(T)]e^{(2i/\hbar)\mathcal{I}}, \quad (43)$$

where

$$\mathcal{I}=\frac{1}{4}\int_0^T\left[b^2(t)\frac{\partial^2\mathcal{H}}{\partial q^2}+\frac{\hbar^2}{b^2(t)}\frac{\partial^2\mathcal{H}}{\partial p^2}\right]dt \quad (44)$$

and u and v are the continuous versions of the variables defined in Eq. (26):

$$u=\frac{1}{\sqrt{2}}\left(\frac{q}{b}+i\frac{bp}{\hbar}\right),\quad v=\frac{1}{\sqrt{2}}\left(\frac{q}{b}-i\frac{bp}{\hbar}\right). \quad (45)$$

The values $\delta v(T)$ and $\delta u(T)$ appearing in Eq. (43) are obtained by linearizing the above equations around the stationary trajectory and solving them with initial conditions $\delta u(0)=-\delta'$ and $\delta v(0)=1$ (see Appendix B).

Equation (43) assumes a simpler form in terms of the variables η and ξ defined in Eq. (36). Using the conversion relations between $(\delta u,\delta v)$ and $(\delta\eta,\delta\xi)$,

$$\delta u=\frac{\chi}{2}\left[\left(\frac{\sigma''^2+b^2}{\sigma'' b}\right)\delta\eta+\left(\frac{\sigma'^2-b^2}{\sigma' b}\right)\delta\xi\right] \quad (46)$$

and

$$\delta v=\frac{\chi}{2}\left[\left(\frac{\sigma''^2-b^2}{\sigma'' b}\right)\delta\eta+\left(\frac{\sigma'^2+b^2}{\sigma' b}\right)\delta\xi\right], \quad (47)$$

we rewrite Eq. (43) as

$$(-1)^{N-1}\det M^{(N-1)}=\frac{2b(T)\sigma''}{\sigma''^2+b^2(T)}\delta\xi(T)e^{(2i/\hbar)\mathcal{I}}. \quad (48)$$

Evaluating these equations at $t=0$ with $\delta u(0)=-\delta'$ and $\delta v(0)=1$,

$$-\delta'=\frac{\chi}{2}\left[\left(\frac{\sigma''^2+b^2(0)}{\sigma'' b(0)}\right)\delta\eta'+\left(\frac{\sigma'^2-b^2(0)}{\sigma' b(0)}\right)\delta\xi(0)\right], \quad (49)$$

$$1=\frac{\chi}{2}\left[\left(\frac{\sigma''^2-b^2(0)}{\sigma'' b(0)}\right)\delta\eta'+\left(\frac{\sigma'^2+b^2(0)}{\sigma' b(0)}\right)\delta\xi(0)\right], \tag{50}$$

and using Eqs. (41) and (42) we can write $\delta\xi(T)=\delta\xi''$ in terms of the second derivatives of the complex action S. We get $\delta\eta'=0$ and

$$\delta\xi''=-i\hbar\,\frac{2\sigma' b(0)}{\sigma'^2+b^2(0)}\left(\frac{\partial^2 S}{\partial\eta'\partial\xi''}\right)^{-1}. \tag{51}$$

Thus,

$$(-1)^{N-1}\det M^{(N-1)}=-i\hbar\,\frac{4\sigma' b(0)\sigma'' b(T)}{[\sigma'^2+b^2(0)][\sigma''^2+b^2(T)]}\times\left(\frac{\partial^2 S}{\partial\eta'\partial\xi''}\right)^{-1}e^{-(2i/\hbar)\mathcal{I}}. \tag{52}$$

F. The semiclassical propagator

Substituting Eqs. (52) and (37) in Eq. (35), we obtain the final expression for the semiclassical propagator,

$$K(\xi'',\eta',T)=\sqrt{\frac{i}{\hbar}\frac{\partial^2 S}{\partial\eta'\partial\xi''}}e^{(i/\hbar)\mathcal{I}}\exp\left\{\frac{i}{\hbar}S(\xi'',\eta',T)\right\}\times\exp\left\{\frac{1}{2}\left(\frac{\sigma''^2-\sigma'^2}{\sigma''^2+\sigma'^2}\right)(\eta'^2-\xi''^2)-\frac{1}{2}(|\eta'|^2+|\xi''|^2)\right\}, \tag{53}$$

where

$$S(\xi'',\eta',T)=\int_0^T\left[\chi\frac{i\hbar}{2}(\xi\dot{\eta}-\eta\dot{\xi})-\mathcal{H}\right]dt-\chi\frac{i\hbar}{2}[\eta'\xi'+\xi''\eta''], \tag{54}$$

where χ is defined after Eq. (38) and

$$\mathcal{I}=\frac{1}{4}\int_0^T\left[b^2(t)\frac{\partial^2\mathcal{H}}{\partial q^2}+\frac{\hbar^2}{b^2(t)}\frac{\partial^2\mathcal{H}}{\partial p^2}\right]dt. \tag{55}$$

For $\sigma'=\sigma''$ the propagator becomes formally identical to the result in [8], but they do not coincide since in the above formula we are not restricted to $b=\sigma'$ or $b=\sigma''$. The present result is valid for any b, constant or time dependent. We shall explore this arbitrariness latter for a Gaussian semiclassical approximation.

As a test of formula (53) we calculate the semiclassical propagator for the simple harmonic oscillator. The quantum Hamiltonian is given by

$$\hat{H}=\frac{1}{2m}\hat{p}^2+\frac{1}{2}m\omega^2\hat{x}^2, \tag{56}$$

and the corresponding smoothed Hamiltonian reads

$$\mathcal{H}=\frac{1}{2m}p^2+\frac{\hbar^2}{4mb^2}+\frac{1}{2}m\omega^2q^2+\frac{m\omega^2b^2}{4}. \tag{57}$$

The equations of motion can be easily found and written in terms of the variables η and ξ. The solution is given by

$$\eta(t)=\frac{1}{2\sigma' b}[\mathcal{K}(b^2-\sigma'^2)e^{i\omega t}+\mathcal{M}(b^2+\sigma'^2)e^{-i\omega t}] \tag{58}$$

and

$$\xi(t)=\frac{1}{2\sigma'' b}[\mathcal{K}(b^2+\sigma''^2)e^{i\omega t}+\mathcal{M}(b^2-\sigma''^2)e^{-i\omega t}]. \tag{59}$$

The mixed boundary conditions are satisfied for

$$\mathcal{K}=\frac{b[(b^2+\sigma'^2)\sigma''\xi''-(b^2-\sigma''^2)\sigma'\eta' e^{-i\omega T}]}{i(b^4+\sigma'^2\sigma''^2)\sin(\omega T)+b^2(\sigma''^2+\sigma'^2)\cos(\omega T)} \tag{60}$$

and

$$\mathcal{M}=\frac{2b\sigma'}{b^2+\sigma'^2}\eta'-\left(\frac{b^2-\sigma'^2}{b^2+\sigma'^2}\right)\mathcal{K}. \tag{61}$$

The complex action takes the simple form

$$S(\xi'',\eta',T)=-\mathcal{I}-\chi\frac{i\hbar}{2}[\eta'\xi(0)+\xi''\eta(T)]. \tag{62}$$

This expression together with Eqs. (58), (59), (60), and (61) leads to

$$\frac{i}{\hbar}\frac{\partial^2 S}{\partial\eta'\partial\xi''}=\frac{-4\zeta\sigma'\sigma''}{(1-4\zeta^2\sigma'^2\sigma''^2)\sin(\omega T)-2\zeta(\sigma'^2+\sigma''^2)\cos(\omega T)} \tag{63}$$

and

$$\frac{i}{\hbar}(\mathcal{I}+S)+\frac{1}{2}\left(\frac{\sigma''^2-\sigma'^2}{\sigma''^2+\sigma'^2}\right)(\eta'^2-\xi''^2)=\frac{(1/2+2\zeta^2\sigma'^2\sigma''^2)\sin(\omega T)-\zeta(\sigma''^2-\sigma'^2)(\eta'^2-\xi''^2)\cos(\omega T)-4\zeta\sigma'\sigma''\eta'\xi''}{(1-4\zeta^2\sigma'^2\sigma''^2)\sin(\omega T)-2\zeta(\sigma'^2+\sigma''^2)\cos(\omega T)},$$

with $\zeta=i\omega/2\hbar$. The final result is

$$K(\xi'',\eta',T)=2\sqrt{\frac{-\zeta\sigma'\sigma''}{(1-4\zeta^2\sigma'^2\sigma''^2)\sin(\omega T)-2\zeta(\sigma'^2+\sigma''^2)\cos(\omega T)}}e^{-(|\eta'|^2+|\xi''|^2)/2}$$
$$\times\exp\left\{\frac{(1/2+2\zeta^2\sigma'^2\sigma''^2)\sin(\omega T)-\zeta(\sigma''^2-\sigma'^2)(\eta'^2-\xi''^2)\cos(\omega T)-4\zeta\sigma'\sigma''\eta'\xi''}{(1-4\zeta^2\sigma'^2\sigma''^2)\sin(\omega T)-2\zeta(\sigma'^2+\sigma''^2)\cos(\omega T)}\right\}, \tag{64}$$

which coincides with the exact result. Note that this expression is independent of the choice of b. For general potentials this is not expected to occur.

G. Gaussian semiclassical Approximation

In order to study the role of the width in our semiclassical formula, we shall derive a simpler Gaussian semiclassical approximation of the propagator. This will allow us to avoid the complications introduced by complex trajectories and focus only on the implications of using different widths.

We consider the ''mixed propagator''

$$\langle x|\hat{K}(T)|z'\rangle=\int\frac{d^2z''}{\pi}\langle x|z''\rangle\langle z''|\hat{K}(T)|z'\rangle, \tag{65}$$

with $\langle z''|\hat{K}(T)|z'\rangle$ given by Eq. (53), and $\sigma'=\sigma''=\sigma$ for simplicity. The mixed propagator is a possible (but not the only) kernel $F(x,z',t)$ in Eq. (5), since for any quantum state $|\psi\rangle$

$$\langle x|\psi(T)\rangle=\int\frac{d^2z'}{\pi}\langle x|\hat{K}(T)|z'\rangle\langle z'|\psi(0)\rangle. \tag{66}$$

The GSA is obtained from Eq. (65) by Taylor expanding the complex action around the *real* trajectory starting at (q',p'). If we denote the final point of this trajectory by (q_r,p_r) or equivalently by (η_r,ξ_r), then the action can be expanded as

$$\frac{i}{\hbar}S(\xi'',\eta',T)\approx\frac{i}{\hbar}S(\xi_r,\eta',T)+\eta_r(\xi''-\xi_r)+\frac{1}{2}\gamma(\xi''-\xi_r)^2, \tag{67}$$

where we have used Eq. (40) to express the first order term, and defined $\gamma\equiv i/\hbar(\partial^2S/\partial\xi''^2)|_r$. This procedure is supported by the assumption that the contribution to the propagator falls in a Gaussian-like way as the complex trajectories get farther away from the real trajectory. With the above expansion, Eq. (65) becomes a simple Gaussian integral in the variables q'' and p''. A detailed calculation of this integral and the many simplifications that follow were presented in [8] for the case of fixed widths. In the present case the steps of the calculation are very similar, and we write down the final result directly:

$$\langle x|\hat{K}(T)|z'\rangle=\frac{\pi^{-1/4}\sigma^{-1/2}}{\sqrt{1+\gamma}}\sqrt{\frac{i}{\hbar}\frac{\partial^2S}{\partial\eta'\partial\xi''}}\Bigg|_r$$
$$\times\exp\left\{-\frac{1}{2}\frac{1-\gamma}{1+\gamma}\left(\frac{x-q_r}{\sigma}\right)^2\right\}$$
$$\times\exp\left\{\frac{i}{\hbar}\left[p_r(x-q_r)+\frac{1}{2}q'p'+S_H+\mathcal{I}_r\right]\right\}. \tag{68}$$

The quantities with the subscript r are evaluated over the real trajectory, and S_H is Hamilton's action

$$S_H=\int_i^f(pdq-\mathcal{H}dt). \tag{69}$$

The approximate wave function given by Eq. (68) is always Gaussian, which justifies the name GSA. The corresponding IVR formula is Eq. (66) with the GSA as the kernel, which is integrated over all q' and p', resulting in a non-Gaussian propagated wave function. We emphasize that formula (68) is valid for any choice of b, time dependent or not.

III. APPLICATIONS

A. Special limits

Expression (68) is a very flexible GSA. It contains as particular cases the Gaussian semiclassical approximation presented in [8], which we call the BAKKS GSA (simply by setting $b=\sigma$), and the Heller thawed GSA in the more subtle limit $b\to0$. The first case follows directly from Eq. (68), by inspection. Let us demonstrate the assertion on the Heller GSA.

From the definition of the smoothed potential we have

$$\mathcal{V}(q,b)=\frac{1}{\sqrt{\pi}b}\int V(x)e^{-(x-q)^2/b^2}dx$$
$$=\int\delta^{(b)}(x-q)V(x)dx, \tag{70}$$

where

$$\delta^{(b)}(x-q)\equiv\frac{1}{\sqrt{\pi}b}e^{-(x-q)^2/b^2} \tag{71}$$

is a representation of the Dirac delta function, in the sense that

$$\lim_{b\to 0}\left\{\int \delta^{(b)}(x-q)V(x)dx\right\}=V(q), \tag{72}$$

if $V(x)$ is a continuous function. Thus, as $b\to 0$,

$$\mathcal{H}\to\frac{1}{2}p^2+\frac{\hbar^2}{4b^2}+V(q)=H+\frac{\hbar^2}{4b^2}. \tag{73}$$

The action S_H and the phase factor $\mathcal{I}_r$ become, in this limit,

$$S_H=\int_i^f\left\{pdq-\left(H+\frac{\hbar^2}{4b^2}\right)dt\right\},\quad \mathcal{I}_r=\int_i^f\frac{\hbar^2}{4b^2}dt, \tag{74}$$

so that

$$S_H+\mathcal{I}_r=\int_i^f(pdq-Hdt)\equiv S_c. \tag{75}$$

The divergent factor $\hbar^2/4b^2$ cancels out exactly and the result is the usual action for the dynamics governed by the classical H. Since the action (38) appears in (68) only through its derivatives, the diverging term does not contribute. Therefore,

$$\begin{aligned}\langle x''|\hat{K}(T)|z'\rangle_{b\to 0}=&\frac{\pi^{-1/4}\sigma^{-1/2}}{\sqrt{1+\gamma}}\sqrt{\frac{i}{\hbar}\frac{\partial^2 S}{\partial\eta'\partial\xi''}}\Bigg|_r\\ &\times\exp\left\{-\frac{1}{2}\frac{1-\gamma}{1+\gamma}\left(\frac{x''-q_r}{\sigma}\right)^2\right\}\\ &\times\exp\left\{\frac{i}{\hbar}\left[p_r(x''-q_r)+\frac{1}{2}q'p'+S_c\right]\right\}\\ &=\langle x''|\hat{K}(T)|z'\rangle_{Heller},\end{aligned} \tag{76}$$

where all the quantities are calculated with the classical Hamiltonian H. As shown in [8], the expression (76) is precisely Heller's propagator.

B. Propagation in a harmonic potential

Now let us consider the propagation of a coherent state of width σ in a harmonic potential of frequency ω where $b_h\equiv\sqrt{\hbar/m\omega}\neq\sigma$.

The quantum Hamiltonian is given by Eq. (56) and the corresponding smoothed Hamiltonian by Eq. (57). The equations of motion can be readily solved and all quantities entering the GSA formula can easily be computed. The final result is

$$\begin{aligned}\langle x|\hat{K}(T)|z'\rangle=&\sqrt{\frac{\pi^{-1/2}\sigma}{\sigma^2\cos(\omega T)+ib_h^2\sin(\omega T)}}\\ &\times\exp\left\{-\frac{\sigma^2(x-q_r)^2}{2[b_h^4\sin^2(\omega T)+\sigma^4\cos^2(\omega T)]}\right\}\\ &\times\exp\left\{\frac{i(b_h^4-\sigma^4)\sin(\omega T)\cos(\omega T)}{2b_h^2[b_h^4\sin^2(\omega T)+\sigma^4\cos^2(\omega T)]}\right.\\ &\left.\times(x-q_r)^2+\frac{i}{\hbar}p_r(x-q_r/2)\right\},\end{aligned} \tag{77}$$

which coincides with the exact result and is completely independent of the choice of b.

C. Propagation in generic potentials

The GSA (68) has a limited capacity to describe the exact quantum propagation due to its Gaussian nature. However, its simplicity enables us to verify the influence of the choice of different widths in the semiclassical propagation in a simple way.

When the potential is not harmonic, the semiclassical results may be quite sensitive to the choice of b. For anharmonic potentials a completely analytical treatment is not possible, and the following results refer to numerical calculations. In this section we compare the semiclassical propagation using many distinct but constant b's. We have demonstrated that the BAKKS GSA ($b=\sigma$) and the Heller GSA ($b\to 0$) belong to this category, and have seen that all GSA's derived from Eq. (68) give the exact result for the harmonic oscillator. If the potential is not harmonic, its characteristic frequency depends on the energy of the trajectory: $\omega=\omega(E)$. Therefore, a natural choice for the width is

$$b=\sqrt{\frac{\hbar}{m\omega(E)}}\equiv b_E, \tag{78}$$

where $E=H(q',p')$.

As an example, we consider the Gaussian propagation in the quartic potential

$$V(x)=\frac{1}{2}\omega_0^2x^2+\frac{1}{8}\ell x^4, \tag{79}$$

whose corresponding smoothed Hamiltonian is

$$\begin{aligned}\mathcal{H}=&\frac{1}{2}p^2+\frac{\hbar^2}{4b^2}+\frac{1}{2}\omega_0^2q^2+\frac{\omega_0^2b^2}{4}\\ &+\frac{1}{8}\ell(q^4+3b^2q^2+3b^4/4).\end{aligned} \tag{80}$$

In what follows we shall set $\hbar=0.05$, $\omega_0=1/2$, $\ell=1/16$, and $m=1$. As a first illustration we compare the exact and semiclassical propagations using $b=\sigma$, $b=0.0$, and $b=b_E$. Figure 1 shows the square modulus of the wave functions at $T=0.0$, $T=2.0$ and $T=16.0$. The initial packet is given by

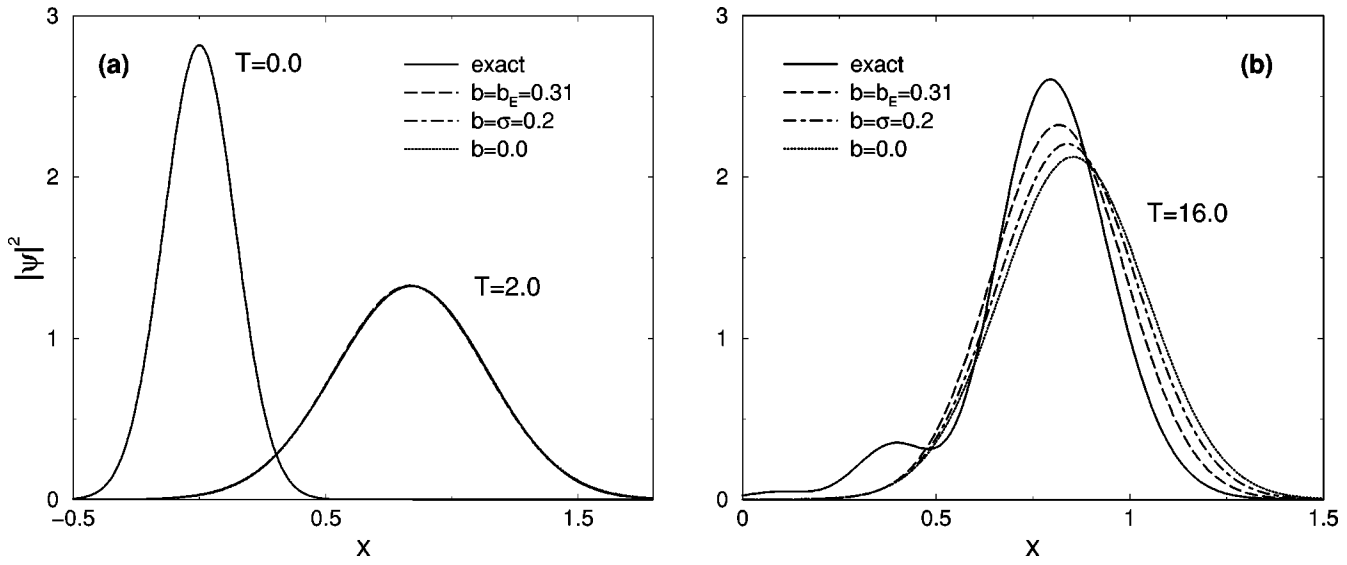

FIG. 1. Square modulus of the exact and semiclassical wave functions as a function of the position (in arbitrary units) for (a) $T=0$ and $T=2$; and (b) $T=16$.

$q'=0.0$, $p'=0.5$, and $\sigma=0.2$. For this system and initial state $E=1/8$ and $b_E\approx 0.31$. As can be seen from Fig. 1(a), at short times ($T=2.0$) all the propagators are equivalent. For longer times, however, the differences become clear, as shown in Fig. 1(b) for $T=16.0$.

Snapshots of the probability density are a very illustrative procedure, but it restricts the analysis to a small set of times and says nothing about phases. A more reliable procedure is to follow the overlap $\langle \psi_E | \psi_{SC} \rangle$ of the exact and semiclassical results as a function of time. Figure 2 shows the modulus of this overlap for a time interval of approximately three classical periods. Four initial configurations with the same total energy are displayed: (a) $q'=0.0$, $p'=0.5$; (b) $q'=0.97$, $p'=0.0$; (c) $q'=0.6$, $p'=0.4$; and (d) $q'=0.6$, $p'=-0.4$. In all situations σ is fixed at 0.2 ($\sigma<b_E$) and five distinct values of the width b are used in the semiclassical approximation: $b=\sigma$, $b=0$, $b=b_E$, and $b=b_E\pm 0.1$. It is clear from this figure that the best results are achieved for $b=b_E$ or $b=b_E+0.1$. The same conclusions hold for $\sigma=0.5>b_E$, i.e., the result is better for $b=b_E$ or $b=b_E+0.1$, depending on the initial configuration.

The quality of the approximation with $b=b_E$ seems to be consistently better than any other choices of b. We have performed extensive tests in many distinct situations, including propagation in other bounded potentials, with stronger anharmonicity and with or without asymmetry. In all cases the propagation with $b=b_E$ (or in some cases b slightly larger than b_E) is better than any other choice. In general, for $b>\mathcal{D}$, where $\mathcal{D}$ is the size of the classically allowed region, the accuracy of the GSA becomes very poor.

IV. CONCLUDING REMARKS

We derived a semiclassical approximation for the coherent state propagator

$$K(z''^*,z',T)=\langle z''|\hat{\mathcal{T}}e^{-(i/\hbar)\int_0^T \hat{H}(t)dt}|z'\rangle, \tag{81}$$

using intermediate states of arbitrary widths. The resulting expression, Eq. (53), is written in terms of classical trajectories governed by the smoothed Hamiltonian $\mathcal{H}(q,p,b)=\langle z|\hat{H}|z\rangle$. The "dynamical width" b appearing in $\mathcal{H}$ is not necessarily equal to the widths σ' or σ'' of the initial state and final states $|z'\rangle$ and $|z''\rangle$, respectively. We have also derived a Gaussian semiclassical approximation, Eq. (68), by projecting $K(z''^*,z',T)$ into the coordinate representation. We have shown that both the Heller and BAKKS GSA's can be obtained as particular cases of this formula. This unified view enables us to discuss more clearly the efficiency of the GSA's. Our analysis shows that, in general, neither Heller's GSA nor the BAKKS GSA are the best semiclassical formulas. The simple choice $b\simeq b_E=\sqrt{\hbar/m\omega(E)}$ presents a considerable improvement over the Heller and BAKKS results for a variety of potentials. We emphasize, however, that b_E is not the *optimal* constant value for b, as demonstrated by Figs. 2(a) and 2(d). It only provides a simple and systematic way to improve the propagation of wave packets. Better choices of b can certainly be found for specific potentials. In particular, for very nonlinear potentials, like x^8, our numerical calculations show that the optimal b seems to be about $2b_E$.

As mentioned in [8], for very small values of $\hbar$ Heller's GSA is expected to become very efficient. This is in agreement with condition (78), since when $\hbar\to 0$ we have $b_E=\sqrt{\hbar/m\omega}\to 0$. In other words, the GSA with $b=b_E$ becomes the Heller GSA in the classical limit.

It is also interesting to consider the total time derivative of $\mathcal{H}$. Assuming that the original Hamiltonian H is time independent, we have

$$\frac{d\mathcal{H}}{dt}=\dot{q}\frac{\partial\mathcal{H}}{\partial q}+\dot{p}\frac{\partial\mathcal{H}}{\partial p}+\dot{b}\frac{\partial\mathcal{H}}{\partial b}=\dot{b}\frac{\partial\mathcal{H}}{\partial b}. \tag{82}$$

If we want the smoothed $\mathcal{H}$ to be conserved, like its original counterpart H, there are only two choices: either b is constant

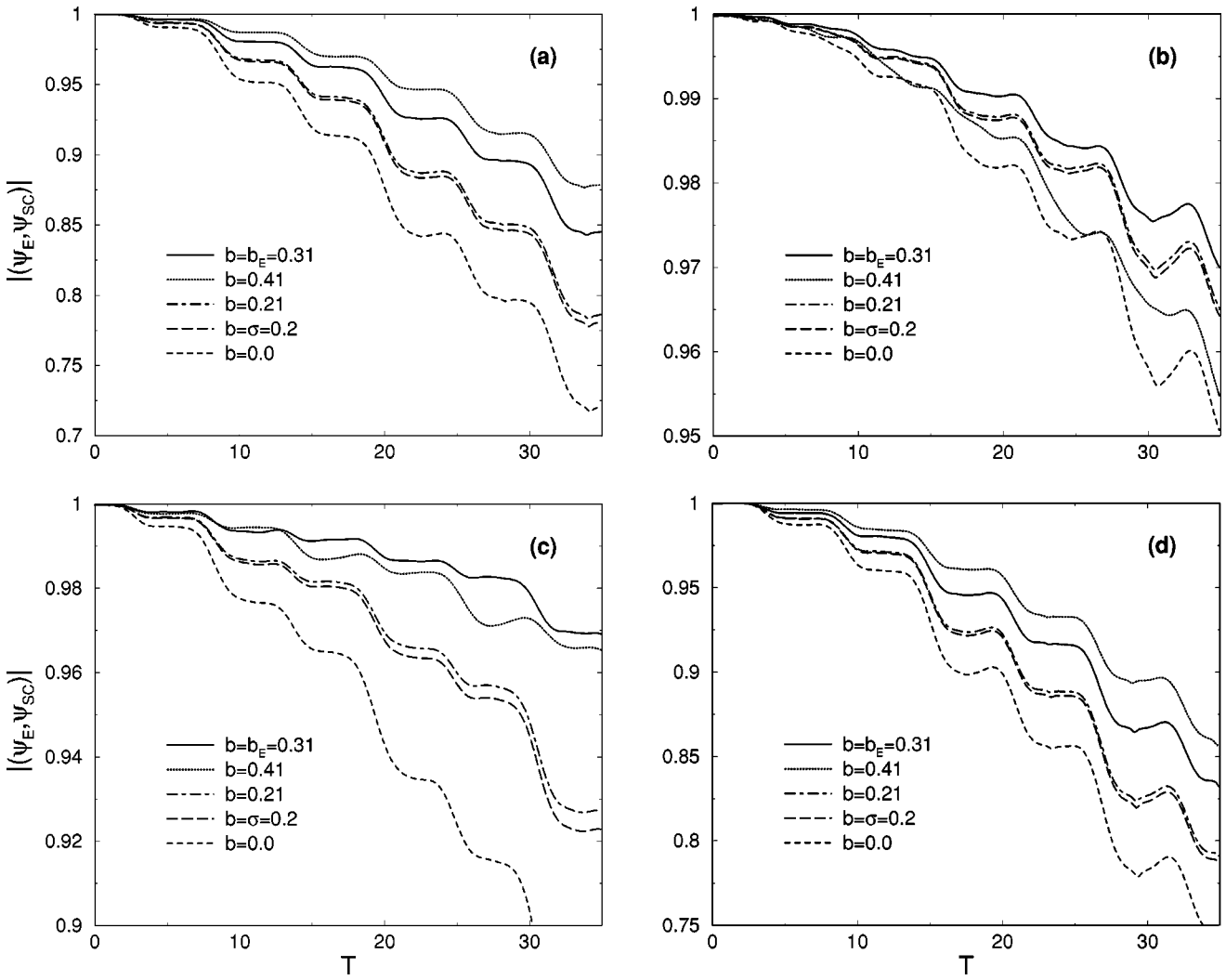

FIG. 2. Overlap between the exact and semiclassical propagations as a function of the time (in arbitrary units) for different b's. The initial conditions are (a) $q'=0.0$, $p'=0.5$; (b) $q'=0.97$, $p'=0.0$; (c) $q'=0.6$, $p'=0.4$; and (d) $q'=0.6$, $p'=-0.4$. The time interval corresponds to approximately three vibrational periods.

or $\partial\mathcal{H}/\partial b=0$. Solving this last equation gives $b=b(q,p)$ as another prescription for the width. We have not shown results with nonconstant b's in this paper, but our preliminary calculations show that this prescription does not improve the calculation very much with respect to b_E for the quartic potential Eq. (79).

Finally, we remark that an important application of the present results is the use of our GSA as an improved kernel to the IVR, Eq. (5). This point is currently under investigation and the results will be published in the near future.

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APPENDIX A: PROOF OF EQS. (23)

For quantum Hamiltonians $\hat{H}$ which can be written as a power series of creation and annihilation operators,

$$\hat{H}=\sum_{n,m} A_{n,m}(\hat{a}^\dagger)^n\hat{a}^m, \tag{A1}$$

the smoothed Hamiltonian is simply

$$\mathcal{H}=\sum_{n,m} A_{n,m}(z^*)^n z^m. \tag{A2}$$

In this form, it is easy to calculate the derivatives of $\mathcal{H}$. For example

$$\frac{\partial\mathcal{H}}{\partial q}=\sum_{n,m}\frac{A_{n,m}}{\sqrt{2}b}[m(z^*)^n z^{m-1}+n(z^*)^{n-1}z^m]. \tag{A3}$$

Let $\hat{a}_j$ and $\hat{a}_j^\dagger$ be the creation and annihilation operators of the harmonic oscillator with coherent state $|z_j\rangle=|q_j,p_j,b_j\rangle$. Let $\hat{H}$ be written in terms of these operators as

$$\hat{H}=\sum_{n,m}\mathcal{A}_{n,m}(\hat{a}_j^\dagger)^n\hat{a}_j^m. \tag{A4}$$

In order to calculate $\mathcal{H}_{j+1,j}$, we need to express $\hat{H}$ in terms of $\hat{a}_{j+1}^\dagger$ and $\hat{a}_j$ in normal ordering. From the definition of $\hat{q}$ and $\hat{p}$ in terms of creation and annihilation operators we find $b_j(\hat{a}_j+\hat{a}_j^\dagger)=b_{j+1}(\hat{a}_{j+1}+\hat{a}_{j+1}^\dagger)$ and $b_{j+1}(\hat{a}_j-\hat{a}_j^\dagger)=b_j(\hat{a}_{j+1}-\hat{a}_{j+1}^\dagger)$. Eliminating $\hat{a}_{j+1}^\dagger$ we obtain

$$\hat{a}_j^\dagger=\left(\frac{2b_jb_{j+1}}{b_{j+1}^2+b_j^2}\right)\hat{a}_{j+1}^\dagger+\left(\frac{b_{j+1}^2-b_j^2}{b_{j+1}^2+b_j^2}\right)\hat{a}_j. \tag{A5}$$

In the limit $\tau\to 0$, $\Delta b=b_{j+1}-b_j$ becomes small and we can write $\hat{a}_j^\dagger=\hat{a}_{j+1}^\dagger+O(\Delta b_j)$ and $[\hat{a}_j,\hat{a}_{j+1}^\dagger]=1+O(\Delta b_j)$, so that

$$\hat{H}=\sum_{n,m}\mathcal{A}_{n,m}(\hat{a}_{j+1}^\dagger)^n\hat{a}_j^m+O(\Delta b_j) \tag{A6}$$

and

$$\mathcal{H}_{j+1,j}=\sum_{n,m}\mathcal{A}_{n,m}(z_{j+1}^*)^nz_j^m+O(\Delta b_j). \tag{A7}$$

Therefore,

$$\frac{\partial\mathcal{H}_{j+1,j}}{\partial q_j}=\sum_{n,m}\frac{\mathcal{A}_{n,m}}{\sqrt{2}b_j}m(z_{j+1}^*)^nz_j^{m-1}\xrightarrow{\tau\to 0}\sum_{n,m}\frac{A_{n,m}}{\sqrt{2}b}m(z^*)^nz^{m-1}. \tag{A8}$$

This is the first term in expansion (A3). A similar procedure for the derivatives of $\mathcal{H}_{j,j-1}$ yields the other term, which proves the first equation (23). A completely analogous calculation proves the second equation.

APPENDIX B: THE DETERMINANT OF $M^{(N-1)}$

In this appendix we will calculate the determinant of $M^{(N-1)}$, which is a $2(N-1)\times 2(N-1)$ symmetric matrix given by

$$M^{(N-1)}\equiv\begin{pmatrix}
-\delta''+\tau\varphi_{N-1} & 1 & 0 & 0 & \cdots & 0 & 0\\
1 & \overline{\Delta}_{N-1}+\tau\varrho_{N-1} & \tau\kappa_{N-1}-1 & 0 & \cdots & 0 & 0\\
0 & \tau\kappa_{N-1}-1 & -\Delta_{N-2}+\tau\varphi_{N-2} & 1 & \cdots & 0 & 0\\
\vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots\\
0 & 0 & 0 & \cdots & \overline{\Delta}_2+\tau\varrho_2 & \tau\kappa_2-1 & 0\\
0 & 0 & 0 & \cdots & \tau\kappa_2-1 & -\Delta_1+\tau\varphi_1 & 1\\
0 & 0 & 0 & \cdots & 0 & 1 & \delta'+\tau\varrho_1
\end{pmatrix}, \tag{B1}$$

where $\overline{\Delta}_j=\Delta b_{j-1}/b_j$ and $\Delta_j=\Delta b_j/b_j$. Expanding the determinant with respect to the first line we obtain

$$\det M^{(N-1)}=(-\delta''+\tau\varphi_{N-1})\det F^{(N-1)}-\det G^{(N-1)}, \tag{B2}$$

where

$$F^{(N-1)}=\begin{pmatrix}
\overline{\Delta}_{N-1}+\tau\varrho_{N-1} & \tau\kappa_{N-1}-1 & 0 & 0 & \cdots\\
\tau\kappa_{N-1}-1 & -\Delta_{N-2}+\tau\varphi_{N-2} & 1 & 0 & \cdots\\
0 & 1 & \overline{\Delta}_{N-2}+\tau\varrho_{N-2} & \tau\kappa_{N-1}-1 & \cdots\\
0 & 0 & \tau\kappa_{N-2}-1 & -\Delta_{N-3}+\tau\varphi_{N-3} & \cdots\\
\vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix} \tag{B3}$$

and

$$G^{(N-1)}=\begin{pmatrix}
1 & \tau\kappa_{N-1}-1 & 0 & 0 & \cdots\\
0 & -\Delta_{N-2}+\tau\varphi_{N-2} & 1 & 0 & \cdots\\
0 & 1 & \overline{\Delta}_{N-2}+\tau\varrho_{N-2} & \tau\kappa_{N-1}-1 & \cdots\\
0 & 0 & \tau\kappa_{N-2}-1 & -\Delta_{N-3}+\tau\varphi_{N-3} & \cdots\\
\vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}. \tag{B4}$$

Expanding the determinants one more time we get

$$\det F^{(N-1)} = (\overline{\Delta}_{N-1} + \tau\varrho_{N-1})\det L^{(N-2)} - (\tau\kappa_{N-1} - 1)\det R^{(N-2)},$$
$$\det G^{(N-1)} = \det L^{(N-2)}, \tag{B5}$$

where the matrices $L^{(N-2)}$ and $R^{(N-2)}$ are given by

$$L^{(N-2)} = \begin{pmatrix} -\Delta_{N-2} + \tau\varphi_{N-2} & 1 & 0 & 0 & \cdots \\ 1 & \overline{\Delta}_{N-2} + \tau\varrho_{N-2} & \tau\kappa_{N-2} - 1 & 0 & \cdots \\ 0 & \tau\kappa_{N-2} - 1 & -\Delta_{N-3} + \tau\varphi_{N-3} & 1 & \cdots \\ 0 & 0 & 1 & \overline{\Delta}_{N-3} + \tau\varrho_{N-3} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{B6}$$

and

$$R^{(N-2)} = \begin{pmatrix} \tau\kappa_{N-1} - 1 & 1 & 0 & 0 & \cdots \\ 0 & \overline{\Delta}_{N-2} + \tau\varrho_{N-2} & \tau\kappa_{N-2} - 1 & 0 & \cdots \\ 0 & \tau\kappa_{N-2} - 1 & -\Delta_{N-3} + \tau\varphi_{N-3} & 1 & \cdots \\ 0 & 0 & 1 & \overline{\Delta}_{N-3} + \tau\varrho_{N-3} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{B7}$$

Finally, we close the cycle with the equations

$$\det L^{(N-2)} = (-\Delta_{N-2} + \tau\varphi_{N-2})\det F^{(N-2)} - \det G^{(N-2)},$$
$$\det R^{(N-2)} = (\tau\kappa_{N-1} - 1)\det F^{(N-2)}. \tag{B8}$$

Substituting Eqs. (B8) in (B5) and keeping only first order terms in τ and Δb we get two coupled difference equations

$$\det F^{(N-1)} = -(\overline{\Delta}_{N-1} + \tau\varrho_{N-1})\det G^{(N-2)} - (1 - 2\tau\kappa_{N-1})\det F^{(N-2)},$$
$$\det G^{(N-1)} = (-\Delta_{N-2} + \tau\varphi_{N-2})\det F^{(N-2)} - \det G^{(N-2)}. \tag{B9}$$

Defining $F_{N-1} = (-1)^{N-1}\det F^{(N-1)}$ and $G_{N-1} = (-1)^{N-1}\det G^{(N-1)}$, these equations become

$$F_{N-1} - F_{N-2} = (\overline{\Delta}_{N-1} + \tau\varrho_{N-1})G_{N-2} - 2\tau\kappa_{N-1}F_{N-2},$$
$$G_{N-1} - G_{N-2} = -(-\Delta_{N-2} + \tau\varphi_{N-2})F_{N-2}. \tag{B10}$$

Taking the limit $\tau \to 0$ we obtain the differential equations

$$\dot{F} = \left(\frac{\dot{b}}{b} + \varrho\right)G - 2\kappa F \quad \text{and} \quad \dot{G} = -\left(-\frac{\dot{b}}{b} + \varphi\right)F, \tag{B11}$$

where

$$\varphi = \frac{1}{2}\left(\frac{ib^2}{\hbar}\frac{\partial^2\mathcal{H}}{\partial q^2} - \frac{i\hbar}{b^2}\frac{\partial^2\mathcal{H}}{\partial p^2}\right) + \frac{\partial^2\mathcal{H}}{\partial q\,\partial p}, \tag{B12}$$

$$\varrho = \frac{1}{2}\left(\frac{ib^2}{\hbar}\frac{\partial^2\mathcal{H}}{\partial q^2} - \frac{i\hbar}{b^2}\frac{\partial^2\mathcal{H}}{\partial p^2}\right) - \frac{\partial^2\mathcal{H}}{\partial q\,\partial p}, \tag{B13}$$

and

$$\kappa = \frac{1}{2}\left(\frac{ib^2}{\hbar}\frac{\partial^2\mathcal{H}}{\partial q^2} + \frac{i\hbar}{b^2}\frac{\partial^2\mathcal{H}}{\partial p^2}\right). \tag{B14}$$

The second derivatives of $\mathcal{H}_{j+1,j}$ have been calculated with the same procedure presented in Appendix A for the first derivatives. In order to put Eqs. (B11) in a more symmetric form we make the transformation

$$F = \mathcal{F}e^{-\int_0^T \kappa(t)dt} \equiv \mathcal{F}e^{(2i/\hbar)\mathcal{I}}, \qquad G = \mathcal{G}e^{-\int_0^T \kappa(t)dt} \equiv \mathcal{G}e^{(2i/\hbar)\mathcal{I}}. \tag{B15}$$

We get

$$\dot{\mathcal{F}} = -\kappa\mathcal{F} + (\dot{b}/b + \varrho)\mathcal{G} \quad \text{and} \quad \dot{\mathcal{G}} = (\dot{b}/b - \varphi)\mathcal{F} + \kappa\mathcal{G}. \tag{B16}$$

We now compare these equations with the linearized Hamilton's equations in terms of the variables u and v, defined by Eq. (45). We get

$$\dot{u} = \frac{1}{\sqrt{2}}\left(\frac{\dot{q}}{b} + \frac{ib}{\hbar}\dot{p}\right) - \frac{\dot{b}}{b}v \Rightarrow \delta\dot{u} = \frac{1}{\sqrt{2}}\left(\frac{\delta\dot{q}}{b} + \frac{ib}{\hbar}\delta\dot{p}\right) - \frac{\dot{b}}{b}\delta v \tag{B17}$$

and

$$\dot{v}=\frac{1}{\sqrt{2}}\left(\frac{\dot{q}}{b}-\frac{ib}{\hbar}\dot{p}\right)-\frac{\dot{b}}{b}u\Rightarrow\delta\dot{v}=\frac{1}{\sqrt{2}}\left(\frac{\delta\dot{q}}{b}-\frac{ib}{\hbar}\delta\dot{p}\right)-\frac{\dot{b}}{b}\delta u. \tag{B18}$$

Using

$$\dot{q}=\frac{\partial\mathcal{H}}{\partial p}\Rightarrow\delta\dot{q}=\frac{\partial^2\mathcal{H}}{\partial q\partial p}\delta q+\frac{\partial^2\mathcal{H}}{\partial p^2}\delta p, \tag{B19}$$

$$\dot{p}=-\frac{\partial\mathcal{H}}{\partial q}\Rightarrow\delta\dot{p}=-\frac{\partial^2\mathcal{H}}{\partial q^2}\delta q-\frac{\partial^2\mathcal{H}}{\partial q\partial p}\delta p, \tag{B20}$$

and expressing these relations in terms of δu and δv we obtain

$$\delta\dot{u}=-\kappa\delta u-(\dot{b}/b+\varrho)\delta v,\quad \delta\dot{v}=-(\dot{b}/b-\varphi)\delta u+\kappa\delta v. \tag{B21}$$

Comparing with Eqs. (B16) we find that $\mathcal{F}=\delta u$ and $\mathcal{G}=-\delta v$. The initial conditions are determined by the matrices $F^{(N-1)}$ and $G^{(N-1)}$ for $N=2$. We have

$$F^{(1)}=\begin{pmatrix}0&-1&0\\-1&0&1\\0&1&\delta'\end{pmatrix}\quad\text{and}\quad G^{(1)}=\begin{pmatrix}1&-1&0\\0&0&1\\0&1&\delta'\end{pmatrix}. \tag{B22}$$

Thus,

$$\det F^{(1)}=-\delta'\quad\Rightarrow\quad F_1=\mathcal{F}(0)=\delta u(0)=-\delta',$$
$$\det G^{(1)}=-1\quad\Rightarrow\quad G_1=\mathcal{G}(0)=-1\Rightarrow\delta v(0)=1. \tag{B23}$$

Therefore, the solutions of Eqs. (B11) are

$$F(t)=\delta u(t)e^{(2i/\hbar)\mathcal{I}}\quad\text{and}\quad G(t)=-\delta v(t)e^{(2i/\hbar)\mathcal{I}}, \tag{B24}$$

subjected to the conditions (B23). Substituting in (B2) we get

$$(-1)^{N-1}\det M^{(N-1)}=[\delta v(T)-\delta'\delta u(T)]e^{(2i/\hbar)\mathcal{I}}, \tag{B25}$$

which is the final result.

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