Uniform Approximation for the Coherent-State Propagator Using a Conjugate Application of the Bargmann Representation

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We propose a conjugate application of the Bargmann representation of quantum mechanics. Applying the Maslov method to the semiclassical connection formula between the two representations, we derive a uniform semiclassical approximation for the coherent-state propagator which is finite at phase space caustics.

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Semiclassical approximations have been widely used in many areas of physics. They are fundamental to the conceptual understanding of the quantum-classical connection and are also very important in practical situations where quantum calculations are difficult, as in systems with many degrees of freedom or with complicated potential functions. However, semiclassical formulas are often not globally valid; i.e., they are not appropriate to describe the corresponding quantum function in all regions of the space of parameters. The WKB formula for the eigenfunctions of a particle in a one-dimensional potential well provides a simple example [1]: on the classically allowed side of the well the wave function is oscillatory, whereas on the classically forbidden side it is given by a single decreasing exponential. At the boundary between the two regions, the turning point, the WKB formula becomes singular. The formula actually fails in a whole neighborhood of the singularity, whose size goes to zero as $\hbar$ goes to zero. For nonstationary wave functions the singularities occur at focal points or caustics. After a focal point, but sufficiently away from it, the semiclassical formulas for wave functions or propagators still provide good approximations, provided the proper Morse phases are added [2].

This general problem of semiclassical expressions, which leads to divergences and discontinuities in the semiclassical results, can usually be eliminated by properly connecting the semiclassical expressions on the different regions of validity and eliminating spurious contributions. The most direct way to do that is to solve the Schrödinger equation in the vicinity of the singularity and extend the solution towards the two regions. For the WKB problem this amounts to linearizing the potential about the turning point, leading to the well known solution involving the Airy function [1]. For nonstationary wave functions, however, this approach is not usually possible and the Maslov method has to be used [2–4]. It consists basically of changing to a dual representation, where the singularity does not exist. For a singularity in coordinates, one uses the momentum representation and vice versa. The trick is that, when transforming back to the original representation, one should go beyond the quadratic approximation, otherwise the singularity reappears. Usually, a stationary phase approximation with the exponent expanded up to cubic terms is enough, giving rise once again to corrections involving Airy functions.

In this Letter, we study the singularities of the semiclassical propagator in the coherent-state representation. These singularities, called phase space caustics (PSC), have been first identified in [5] and later studied in [6–8]. All these previous works were concerned with ways to identify the singularities and prune the branches of spurious contributions arising from them. Here we tackle the problem of how to improve the semiclassical formula in order to avoid its divergence at the caustics. This is a very peculiar situation, since the phase space representation provided by the coherent states makes use of both coordinate and momentum, leaving no room for a natural dual representation. In this Letter we define an application that works as the canonical conjugate of the Bargmann representation [9] and we use it to derive a uniform semiclassical formula for the coherent-state propagator valid in the vicinity of the phase space caustics. For the sake of clarity, we restrict ourselves to systems with 1 degree of freedom. Results for multidimensional systems, which can be treated along the same lines, and detailed numerical applications, will be published elsewhere.

The non-normalized coherent state $|z_0\rangle$ is defined as

$$|z_0\rangle = e^{z_0\hat{a}^\dagger}|0\rangle, \tag{1}$$

where

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(\frac{\hat{q}}{b} - i\frac{\hat{p}}{c}\right), \qquad z_0 = \frac{1}{\sqrt{2}}\left(\frac{q_0}{b} + i\frac{p_0}{c}\right). \tag{2}$$

Here $|0\rangle$ is the ground state of a harmonic oscillator of frequency $\omega = \hbar/mb^2$, $\hat{a}^\dagger$ is the creation operator, and q_0, p_0 are the mean values of the position $\hat{q}$ and momentum $\hat{p}$ operators, respectively. The widths in position b and momentum c satisfy $bc = \hbar$ and z_0 is complex. The semiclassical approximation for the coherent-state propagator $K(z_f^*, z_0, T) \equiv \langle z_f|e^{-i\hat{H}T/\hbar}|z_0\rangle$ is given by [10–12]

$$K(z_f^*, z_0, T) \approx \sum_{\text{traj.}} \sqrt{\frac{1}{|M_{vv}|}} \exp\left\{\frac{i}{\hbar} F\right\}, \qquad (3)$$

where M_{vv} and F depend on (generally complex) classical trajectories. These trajectories are best represented in terms of the variables u and v, instead of the canonical variables q and p, defined by

$$u = \frac{1}{\sqrt{2}}\left(\frac{q}{b} + i\frac{p}{c}\right) \quad \text{and} \quad v = \frac{1}{\sqrt{2}}\left(\frac{q}{b} - i\frac{p}{c}\right). \qquad (4)$$

The sum in Eq. (3) runs over all trajectories governed by the complex Hamiltonian $\tilde{H}(u, v) \equiv \langle v|\hat{H}|u\rangle$ and satisfying the boundary conditions $u(0) \equiv u' = z_0$ and $v(T) \equiv v'' = z_f^*$. Notice that q and p are complex variables, while the propagator labels, q_0, p_0 for the initial state and q_f, p_f for the final one, are real. In Eq. (3), F is given by

$$F(v'', u', T) = S(v'', u', T) + \mathcal{G}(v'', u', T) - \frac{\hbar}{2}\sigma, \qquad (5)$$

where S, the complex action of the trajectory, and $\mathcal{G}$ are given by

$$S(v'', u', T) = \int_0^T \left[\frac{i\hbar}{2}(\dot{u}v - u\dot{v}) - \tilde{H}\right] dt - \frac{i\hbar}{2}\left[u''v'' + u'v'\right],$$

$$\mathcal{G}(v'', u', T) = \frac{1}{2}\int_0^T \frac{\partial^2 \tilde{H}}{\partial u \partial v} dt.$$

Finally M_{vv}, and its phase σ, are elements of the tangent matrix defined by

$$\begin{pmatrix} \delta u'' \\ \delta v'' \end{pmatrix} = \begin{pmatrix} M_{uu} & M_{uv} \\ M_{vu} & M_{vv} \end{pmatrix} \begin{pmatrix} \delta u' \\ \delta v' \end{pmatrix}, \qquad (6)$$

where δu and δv are small displacements around the complex trajectory. We use a single (double) prime to indicate initial time $t = 0$ (final time $t = T$). The elements of the tangent matrix can also be written in terms of second derivatives of the action (see Ref. [12]). Note that Eq. (5) differs from the formula given in [12] because we are using non-normalized coherent states.

Phase space caustics occur when $M_{vv} = 0$, causing the semiclassical propagator to diverge. Close to these points the semiclassical formula provides only a poor approximation to the quantum propagator. For a discussion of the mechanisms that lead to caustics in systems with 1 degree of freedom, see [6,13,14].

Caustics in the semiclassical propagator in a given representation can usually be circumvented by applying the Maslov method. This requires the calculation of the semiclassical propagator in the respective conjugate representation, followed by the transformation back to the original one, with this last step performed with an approximation better than quadratic. For the case of coherent states, although there is no natural dual representation to be used with $K(v'', u', T)$, the complex action $S(v'', u', T)$ satisfies the relations

$$u(T) = \frac{i}{\hbar}\frac{\partial S}{\partial v''} \quad \text{and} \quad v(0) = \frac{i}{\hbar}\frac{\partial S}{\partial u'}, \qquad (7)$$

which suggests a Legendre transformation $S \to \tilde{S}$ by the change of variables $v'' \to (i/\hbar)(\partial S/\partial v'')$. The transformed function $\tilde{S}$ depends on u' and u'', instead of u' and v'',

$$\tilde{S}(u'', u', T) = S(v'', u', T) + i\hbar u''v'', \qquad (8)$$

and satisfies the relations

$$v'' = -\frac{i}{\hbar}\frac{\partial \tilde{S}}{\partial u''} \quad \text{and} \quad v' = \frac{i}{\hbar}\frac{\partial \tilde{S}}{\partial u'}. \qquad (9)$$

These properties, on the other hand, suggest the following definition for the dual representation of the semiclassical propagator:

$$\tilde{K}(u'', u', T) = \frac{1}{\sqrt{2\pi i}}\int_C K(v'', u', T)e^{-u''v''}dv'', \qquad (10)$$

where the path C will be specified below.

In the semiclassical limit this integral can be solved by the steepest descent method [15] and an explicit expression for $\tilde{K}$ can be obtained. Inserting Eq. (3) into (10) we find the saddle point condition

$$\frac{\partial}{\partial v''}[S + i\hbar u''v''] = 0 \quad \text{or} \quad u'' = \frac{i}{\hbar}\frac{\partial S}{\partial v''}, \qquad (11)$$

where we have considered that $\mathcal{G}$ varies slowly in comparison with S (see Ref. [12]). Equation (11) says that the stationary trajectory satisfies $u(0) = u'$ and $u(T) = u''$, i.e., the saddle point value v_c'' of the integration variable is equal to $v(T)$ of a trajectory satisfying these boundary conditions. This imposes that the integration path C must coincide with (or be deformable into) a steepest descent path through v_c''. Expanding the exponent up to second order around this trajectory and performing the Gaussian integral we obtain

$$\tilde{K}(u'', u', T) = \sqrt{\frac{i}{|M_{uv}|}} e^{(i/\hbar)\tilde{S}(u'',u',T) + (i/\hbar)\tilde{\mathcal{G}}(u'',u',T) - (i/2)\tilde{\sigma}}. \qquad (12)$$

We emphasize that $\tilde{K}$ depends on classical trajectories satisfying $u' = u(0)$ and $u'' = u(T)$. M_{uv} is given by Eq. (6), $\tilde{\sigma}$ is its phase, $\tilde{\mathcal{G}}(u'', u', T)$ is the function $\mathcal{G}$ calculated at the new trajectory, and $\tilde{S}(u'', u', T)$ is given by Eq. (8). The PSC affecting $\tilde{K}$ correspond to trajectories for which $M_{uv} = 0$, which generally do not coincide with the PSC of K.

The inverse transformation of Eq. (10) is given by

$$K(v'', u', T) = \frac{1}{\sqrt{2\pi i}}\int_{\tilde{C}} \tilde{K}(u'', u', T)e^{u''v''}du''. \qquad (13)$$

Replacing Eq. (12) into (13) and doing the integral again by the steepest descent approximation up to second order gives back the original propagator of Eq. (3).

The pairs of Eqs. (3)–(12) and (10)–(13) look very much like the corresponding transformation for the propagators in coordinates and momenta, $K(x_f, x_0, T)$ and $K(p_f, x_0, T)$. In that case the classical trajectory goes from x_0 to x_f in one case and from x_0 to p_f in the other. However, although the coherent states define a true quantum mechanical representation [9], and the propagator $K(z_f^*, z_0, T)$ corresponds to the matrix element $\langle z_f|e^{-i\hat{H}T/\hbar}|z_0\rangle$, there is no representation such that $\tilde{K}(z_f, z_0, T)$ also corresponds to a similar matrix element. $\tilde{K}$ would involve two kets, $|z_0\rangle$ and $|z_f\rangle$ instead of a ket $|z_0\rangle$ and a bra $\langle z_f|$.

Therefore, since $\tilde{K}$ is *not* a matrix element of the evolution operator we must formalize its quantum mechanical definition so that the previous transformations make precise sense. This is done as follows: given a ket $|f\rangle$ and its Bargmann representation $f(z^*) = \langle z|f\rangle$ [9], for each coherent-state ket $|w\rangle$ we define the application

$$\tilde{f}(w) = \frac{1}{\sqrt{2\pi i}} \int_\gamma \frac{\langle z|f\rangle}{\langle z|w\rangle} dz^* = \frac{1}{\sqrt{2\pi i}} \int_\gamma f(z^*) e^{-z^* w} dz^*. \tag{14}$$

The path γ must be chosen in such a manner that the integral becomes a Laplace transform. This definition is suggestive of the need to, so to speak, "cancel the bra $\langle z|$ and replace it by a ket $|w\rangle$." At the same time it provides just the right Legendre transform we need in the semiclassical limit when $|f\rangle = e^{-iHT/\hbar}|z_0\rangle$. The inverse transformation is defined as

$$f(z^*) = \frac{1}{\sqrt{2\pi i}} \int_{\gamma'} \tilde{f}(w)\langle z|w\rangle dw = \frac{1}{\sqrt{2\pi i}} \int_{\gamma'} \tilde{f}(w) e^{z^* w} dw, \tag{15}$$

with γ' chosen so that the integral is a Mellin transform.

To illustrate the transformation we apply it to the harmonic oscillator. Let $|f\rangle$ be an eigenstate $|m\rangle$ of the Hamiltonian operator. Then $\langle z|m\rangle \equiv \phi_m(z^*) = (z^*)^m/\sqrt{m!}$ and

$$\tilde{\phi}_m(w) = \frac{1}{\sqrt{2\pi i m!}} \int_\gamma (z^*)^m e^{-z^* w} dz^*. \tag{16}$$

Writing $w = |w|e^{i\theta}$ and $z^* = re^{-i\alpha}$, the path γ is defined by $\alpha = \theta$ with r varying from 0 to ∞. This produces

$$\tilde{\phi}_m(w) = \frac{1}{\sqrt{2\pi i}} \frac{\sqrt{m!}}{w^{m+1}}. \tag{17}$$

The inverse transformation is given by

$$\check{\phi}_m(z^*) = \frac{\sqrt{m!}}{2\pi i} \int_{\gamma'} \frac{e^{z^* w}}{w^{m+1}} dw. \tag{18}$$

Writing $z = |z|e^{i\phi}$ and choosing γ' so that $w = (-\alpha + it)e^{i\phi}$, with $\alpha > 0$ fixed and t varying from $-\infty$ to $+\infty$, we can solve the integral by the method of residues and we find exactly $\check{\phi}_m(z^*) = \phi_m(z^*)$. For the propagator we set $|f\rangle = e^{-iHT/\hbar}|z_0\rangle$ and obtain

$$K(z_f^*, z_0, T) \equiv \langle z_f|e^{-i\hat{H}T/\hbar}|z_0\rangle = e^{z_0 z_f^* e^{-i\omega T} - i\omega T/2} \tag{19}$$

and

$$\tilde{K}(w, z_0, T) = \frac{1}{\sqrt{2\pi i}} \frac{e^{-i\omega T/2}}{w - z_0 e^{-i\omega T}}. \tag{20}$$

Eqs. (14) and (15) show that the semiclassical propagator $\tilde{K}$ given by Eq. (12) is the semiclassical approximation of a true quantum mechanical function, namely, Eq. (14) with $f(z^*) = K(z^*, z_0, T)$. This function, although not a matrix element in a mixed representation like $K(p_f, x_0, T) = \langle p_f|e^{-iHT/\hbar}|x_0\rangle$, is well defined provided the integral over γ converges. The application defined by Eqs. (14) and (15) can be thought of as conjugate to the Bargmann representation, and they provide the tools to the application of the Maslov method to the coherent-state propagator.

The connection between the propagator, Eq. (3), and its conjugate function, Eq. (12), via the steepest descent approximation with quadratic expansion of the exponent works only in the regions where both M_{uv} and M_{vv} are nonzero. Close to caustics, where two stationary trajectories coalesce and $M_{vv} = 0$, $\tilde{K}$ is still well defined and K can be obtained by doing the inverse transform (13) using a uniform approximation [16]. The basic idea is to map the function in the exponent of the integrand into an auxiliary cubic function of a new variable X. The new function is chosen in such a way that its stationary points coincide with those of the original function. Inserting Eq. (12) into Eq. (13) we define the new integration variable $X = X(u'')$ by

$$\frac{1}{\hbar}[\tilde{S} + \tilde{R}] - iu''v'' \equiv A - BX + X^3/3, \tag{21}$$

where $\tilde{R} = \tilde{\mathcal{G}} + (i \ln|M_{uv}| - \tilde{\sigma})\hbar/2$ contains the slowly varying terms and A and B are functions of u', v'', and T. Differentiating both sides with respect to X and discarding the variation of $\tilde{R}$ yields

$$\left[\frac{1}{\hbar}\frac{\partial \tilde{S}}{\partial u''} - iv''\right]\frac{\partial u''}{\partial X} = i[v(T) - v'']\frac{\partial u''}{\partial X} = -B + X^2. \tag{22}$$

The stationary condition $v(T) = v''$ has generally two solutions, u''_+ and u''_-, in the vicinity of a caustic. These two stationary points, that coalesce at the caustic, are mapped into $X_\pm = \pm B^{1/2}$, while the caustic itself corresponds to $X = 0$. Substituting $X = X_\pm$ in (21) and solving for A and B we find

$$\begin{aligned} A &= \frac{1}{2\hbar}(S_+ + \tilde{R}_+ + S_- + \tilde{R}_-), \\ B &= \left[-\frac{3}{4\hbar}(S_+ + \tilde{R}_+ - S_- - \tilde{R}_-)\right]^{2/3}, \end{aligned} \tag{23}$$

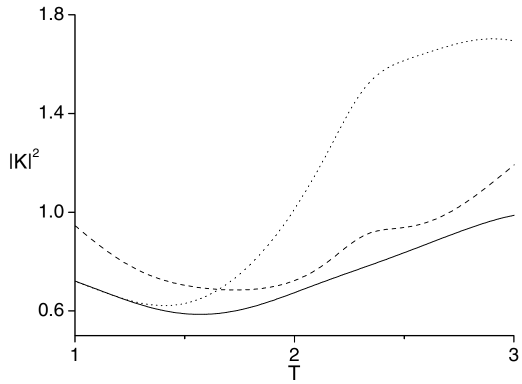

FIG. 1. Square modulus of diagonal propagator for fixed z. The lines correspond to the exact result (full line), bare semiclassical (dotted line), and uniform (dashed line).

where $S_{\pm}$ is the action $S = \tilde{S} - i\hbar u'' v''$ calculated at the stationary trajectories defined by $u''_{\pm}$.

The change of variables from u'' to X also produces a Jacobian $f(X) \equiv \partial u''/\partial X$. Since the X intervals that contribute significantly to integral are those close to the stationary points, we need to specify the Jacobian only in these regions. Writing $f(X) = C + G(X - B^{1/2}) + H(X + B^{1/2})$ and defining $f_{\pm} = f(X_{\pm})$ we find

$$f(X) = (f_+ + f_-)/2 + X(f_+ - f_-)/2B^{1/2}. \qquad (24)$$

Differentiating (22) with respect to X once again and calculating at $X_{\pm}$ we obtain

$$f_{\pm} = \left(\pm \frac{2M^{\pm}_{uv} B^{1/2}}{iM^{\pm}_{vv}} \right)^{1/2}. \qquad (25)$$

Putting everything together we find the following uniform approximation for the propagator:

$$K(u', v'', T) = \frac{1}{\sqrt{2\pi}} \int f(X) e^{i(A - BX + X^3/3)} dX. \qquad (26)$$

Far from the caustic, where the contribution of each stationary trajectory can be computed separately, $f(X)$ reduces to $f_{\pm}$ and the integral can be written in terms of an Airy function. In this case the Airy function can be evaluated by the method of steepest descent, with the integration path chosen according to the phase of its argument $z = -B$. Therefore the argument of z automatically indicates whether the two stationary points of the exponent contribute to the propagator or if only one of them do. Expanding the exponent to second order about the contributing points [X_+ or X_- or both, depending on the $\arg(z)$], and doing the resulting Gaussian integral recovers the quadratic approximation Eq. (3).

As an illustration we consider the Hamiltonian $\hat{H} = (a^\dagger a + 1/2)^2$. Figure 1 shows the square modulus of the diagonal propagator $\langle z | e^{-i\hat{H}T} | z \rangle$ ($b = c = \hbar = 1$) as a function of T for $z = 1/(2\sqrt{2})$. The dotted line displays the bare semiclassical result, showing a large increase for $T \gtrsim 2.0$, due to a nearby caustic. The exact result is the full line and the uniform approximation is shown by the dashed line, which is indeed uniformly good at all times. Detailed numerical applications will be published elsewhere.

Equation (26) and the definition of the conjugate application and its inverse, Eqs. (14) and (15), constitute the main results of this Letter. Although the idea of a conjugate application to the Bargmann representation is used here just as a tool to derive the above uniform approximation, it may be useful in other situations. For instance, a transitional approximation, valid only close to the caustics, can also be derived. In addition, the Fourier frequencies of the transformed propagator are the eigenvalues of the Hamiltonian, and it might be simpler to extract those eigenvalues from the transformed propagator than from the Bargmann propagator. This is certainly the case for the Harmonic oscillator, since the time dependence of $\tilde{K}(w, w, T)$, see Eq. (20), is trivial.

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