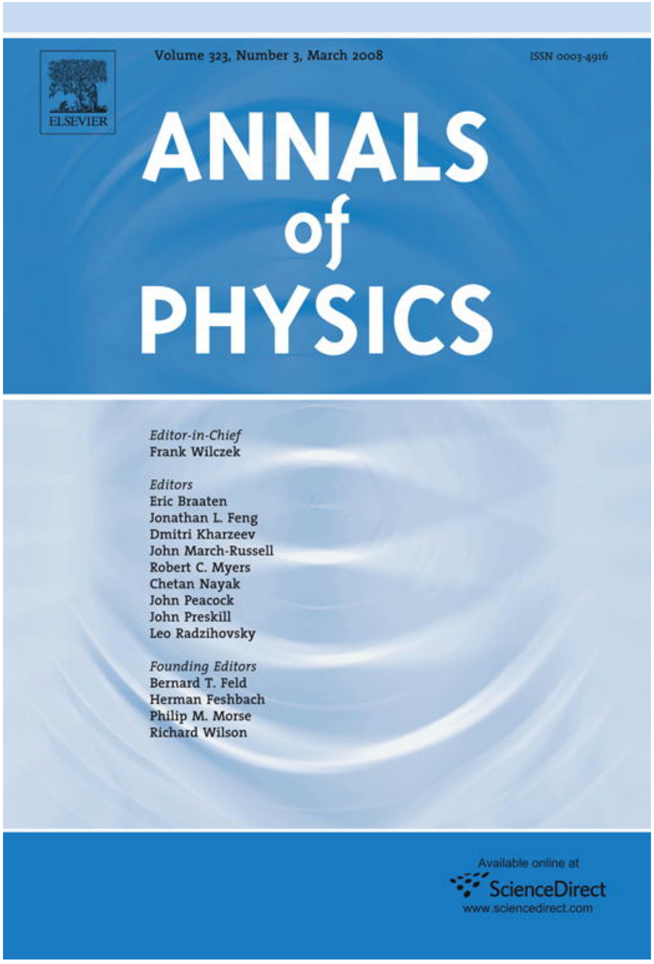
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Controlling phase space caustics in the semiclassical coherent state propagator

A.D. Ribeiro [a,b], M.A.M. de Aguiar [b,*]

[a] *Instituto de Física, Universidade de São Paulo, CP 66318, 05315-970 São Paulo, SP, Brazil*
[b] *Instituto de Física "Gleb Wataghin", Universidade Estadual de Campinas, 13083-970 Campinas, SP, Brazil*

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Abstract

The semiclassical formula for the quantum propagator in the coherent state representation $\langle \mathbf{z}''|e^{-i\hat{H}T/\hbar}|\mathbf{z}'\rangle$ is not free from the problem of caustics. These are singular points along the complex classical trajectories specified by $\mathbf{z}'$, $\mathbf{z}''$ and T where the usual quadratic approximation fails, leading to divergences in the semiclassical formula. In this paper, we derive third order approximations for this propagator that remain finite in the vicinity of caustics. We use Maslov's method and the dual representation proposed in Phys. Rev. Lett. 95, 050405 (2005) to derive uniform, regular and transitional semiclassical approximations for coherent state propagator in systems with two degrees of freedom.

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1. Introduction

Semiclassical methods are the fundamental tool in the study of the quantum-classical connection. In the limit where typical actions S become much larger than Planck's constant $\hbar$, it is possible to use classical ingredients, usually classical trajectories, to produce

* Corresponding author.
E-mail address: aguiar@ifi.unicamp.br (M.A.M. de Aguiar).

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approximations to quantum mechanical objects, like matrix elements, wavefunctions and propagators. In Feynman's path integral approach to quantum mechanics, semiclassical approximations consist in realizing that the classical paths become dominant as $S \gg \hbar$ and it suffices to add together the contributions of a small set of neighboring paths in the vicinity of the classical one. This apparently simple procedure, however, has two well known caveats that make the application of such formulas difficult: the existence of non-contributing classical solutions and the presence of focal points or caustics.

The first of these issues, which is not going to be further discussed in this paper, is closely related to the *Stokes Phenomenon*, which is the abrupt change in the number of contributing solutions to an asymptotic formula when a certain boundary in parameter space is crossed [1–3]. Although a general criterion to decide whether a trajectory should be included or not as a true contribution to the formula exists, it is usually hard to verify in practice. An example of a careful study of these solutions can be found in [4]. More generally, one resorts to a simple *a posteriori* criterion: the contribution of each trajectory is computed and, if it leads to non-physical results, it is discarded. This kind of prescription has been widely used in the last years as, for example, in the semiclassical formula of the coherent state propagator in one [5] and two [6] spatial dimensions, in the momentum propagator [7] and in the semiclassical evolution of gaussian wave packets [8].

Singularities due to caustics are the other recurrent problem in semiclassical formulas. In the WKB theory [9] the semiclassical wavefunction in the position representation diverges at the turning points $\dot{q} = 0$. In the momentum representation the equivalent problem occurs at the points where $\dot{p} = 0$. In addition, for the Van-Vleck propagator, which is a semiclassical formula of the propagator in the coordinate representation, $\langle q''|\mathrm{e}^{-\mathrm{i}\hat{H}T/\hbar}|q'\rangle$, singularities occur at the focal points [10]. These are points along the trajectory from $q(0) = q'$ to $q(T) = q''$ where an initial set of trajectories issuing from the same initial point $q(0)$ but with slightly different momenta, get together again, focusing at the same point $q(t)$.

The failure of the semiclassical approximation at these points, and the reason why a singularity develops there, is that the usual quadratic approximation used to derive such formulas becomes degenerate and third order contributions around the stationary points become essential. The standard procedure to obtain improved formulas valid at caustics is due to Maslov [11] and it consists in changing to a dual representation where the singularity does not exist [11,12]. For a singularity in coordinates, one uses the momentum representation and vice-versa. The trick is that, when transforming back to the representation where the singularity exists, one should go beyond the quadratic approximation, otherwise the singularity re-appears.

The subject of the present paper is the treatment of singularities due to caustics in the semiclassical formula of the coherent state propagator in two spatial dimensions $K(\mathbf{z}''^{*}, \mathbf{z}', T) \equiv \langle \mathbf{z}''|\mathrm{e}^{-\mathrm{i}\hat{H}T/\hbar}|\mathbf{z}'\rangle$. In spite of the fact that this is a phase space representation, where no turning points exist, this propagator is not free from caustics [5,6,13,14], although earlier works on the subject indicated so [15–18]. These points have termed *phase space caustics*.

The caustics in $K_{\mathrm{SC}}(\mathbf{z}''^{*}, \mathbf{z}', T)$ have the same origin as the focal point divergence in the Van-Vleck propagator, namely, the breakdown of the quadratic approximation. Therefore, it is natural to look for a dual representation as in Maslov's method to derive higher order approximations. However, since both coordinates and momenta are used in the coherent states, there seems to be no room for a natural dual representation. In a recent paper [19] we have proposed the construction of an application between $f(z^*) = \langle z|\psi\rangle$ and an associate function $\tilde{f}(w)$ that plays the role of the dual representation for the coherent state propagator. Using this auxiliary mapping we were able to derived a uniform approximation for the propagator of one-dimensional systems that is finite at phase space caustics. In this paper, we use such a representation to derive regular, transitional and uniform semiclassical approximation for the coherent state propagator of two-dimensional systems, which is the simplest case where conservative chaos is possible. The resulting formulas involve, as expected, the Airy function and the third derivatives of the action function.

This article is organized as follows: in Section 2, we review the semiclassical formula for the coherent state propagator in two dimensions and discuss its singularities. In Section 3, we review the dual representation proposed in Ref. [19] and generalize it for two-dimensional systems. In Section 4, we use this representation and the Maslov method to derive regular, transitional and uniform approximations for the coherent state propagator. Our conclusions and final remarks are presented in Section 5.

2. The semiclassical limit of the coherent state propagator

In this section, we briefly discuss the usual semiclassical formula for the propagator in the coherent state representation. The 2-D *non-normalized* coherent state $|\mathbf{z}\rangle$ is the direct product of two 1-D states, $|\mathbf{z}\rangle \equiv |z_x\rangle \otimes |z_y\rangle$, where

$$\begin{aligned} |z_r\rangle &= e^{z_r \hat{a}_r^\dagger}|0\rangle, \\ \hat{a}_r^\dagger &= \frac{1}{\sqrt{2}}\left(\frac{\hat{q}_r}{b_r} - i\frac{\hat{p}_r}{c_r}\right), \\ z_r &= \frac{1}{\sqrt{2}}\left(\frac{\bar{q}_r}{b_r} + i\frac{\bar{p}_r}{c_r}\right). \end{aligned} \tag{1}$$

The index r assumes the values x or y. $|0\rangle$ is the ground state of a harmonic oscillator of frequency $\omega_r = \hbar/(mb_r^2)$, $\hat{a}_r^\dagger$ is the creation operator and $\bar{q}_r$, $\bar{p}_r$ are the mean values of the position $\hat{q}_r$ and momentum $\hat{p}_r$ operators, respectively. The widths in position b_r and momentum c_r satisfy $b_r c_r = \hbar$. In addition, the complex number z_r is eigenvalue of $\hat{a}_r$ with eigenvector $|z_r\rangle$.

The coherent state propagator $K(\mathbf{z}''^*, \mathbf{z}', T) \equiv \langle \mathbf{z}''|e^{-i\hat{H}T/\hbar}|\mathbf{z}'\rangle$ represents the probability amplitude that the initial coherent state $|\mathbf{z}'\rangle$ evolves into another coherent state $|\mathbf{z}''\rangle$ after a time T, according to the Hamiltonian $\hat{H}$. Notice that, since the initial and final coherent states are non-normalized, all the propagators considered in this paper should be multiplied by $e^{-\frac{1}{2}|\mathbf{z}'|-\frac{1}{2}|\mathbf{z}''|^2}$ to get the usual propagators with normalized bras and kets.

The semiclassical approximation for this propagator was firstly considered by Klauder [20–22] and Weissman [23]. More recently, however, a detailed derivation was presented for systems with one degree of freedom [24]. The expression for two-dimensional systems is [6]

$$K_{SC}^{(2)}(\mathbf{z}''^*, \mathbf{z}', T) = \sum_{\text{traj.}} \sqrt{\frac{1}{|\det M_{\mathbf{vv}}|}} \exp\left\{\frac{i}{\hbar}\mathcal{F}\right\}, \tag{2}$$

where the index (2) was inserted to indicate explicitly that this formula was obtained by means of a second order saddle point approximation. The factors $M_{\mathbf{vv}}$ and $\mathcal{F}$ depend on (generally complex) classical trajectories. These trajectories are best represented in terms of new variables **u** and **v**, instead of the canonical variables **q** and **p**, defined by

$$u_r = \frac{1}{\sqrt{2}}\left(\frac{q_r}{b_r} + \mathrm{i}\frac{p_r}{c_r}\right) \quad \text{and} \quad v_r = \frac{1}{\sqrt{2}}\left(\frac{q_r}{b_r} - \mathrm{i}\frac{p_r}{c_r}\right). \tag{3}$$

The sum in Eq. (2) runs over all trajectories governed by the complex Hamiltonian $\tilde{H}(\mathbf{u},\mathbf{v}) \equiv \langle \mathbf{v}|\hat{H}|\mathbf{u}\rangle$. They must satisfy the boundary conditions $\mathbf{u}(0) \equiv \mathbf{u}' = \mathbf{z}'$ and $\mathbf{v}(T) \equiv \mathbf{v}'' = \mathbf{z}''^{*}$. Notice that q_r and p_r are complex variables, while the propagator labels ($\bar{q}'_r$, $\bar{p}'_r$ for the initial state and $\bar{q}''_r$, $\bar{p}''_r$ for the final one) are real. In Eq. (2), $\mathcal{F}$ is given by

$$\mathcal{F}(\mathbf{v}'',\mathbf{u}',T) = \mathcal{S}(\mathbf{v}'',\mathbf{u}',T) + \mathcal{G}(\mathbf{v}'',\mathbf{u}',T) - \frac{\hbar}{2}\sigma_{\mathbf{vv}}, \tag{4}$$

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

$$\mathcal{S}(\mathbf{v}'',\mathbf{u}',T) = \int_0^T \left[\frac{\mathrm{i}\hbar}{2}(\dot{\mathbf{u}}\mathbf{v} - \mathbf{u}\dot{\mathbf{v}}) - \tilde{H}\right]\mathrm{d}t - \frac{\mathrm{i}\hbar}{2}[\mathbf{u}''\mathbf{v}'' + \mathbf{u}'\mathbf{v}'], \tag{5}$$

$$\mathcal{G}(\mathbf{v}'',\mathbf{u}',T) = \frac{1}{2}\int_0^T \left(\frac{\partial^2 \tilde{H}}{\partial u_x \partial v_x} + \frac{\partial^2 \tilde{H}}{\partial u_y \partial v_y}\right)\mathrm{d}t. \tag{6}$$

The matrix $M_{\mathbf{vv}}$ is a block of the tangent matrix defined by

$$\begin{pmatrix} \delta\mathbf{u}'' \\ \delta\mathbf{v}'' \end{pmatrix} = \begin{pmatrix} M_{\mathbf{uu}} & M_{\mathbf{uv}} \\ M_{\mathbf{vu}} & M_{\mathbf{vv}} \end{pmatrix}\begin{pmatrix} \delta\mathbf{u}' \\ \delta\mathbf{v}' \end{pmatrix}, \tag{7}$$

where $\delta\mathbf{u}$ and $\delta\mathbf{v}$ 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 be written in terms of second derivatives of the action (see Ref. [6]). Finally, $\sigma_{\mathbf{vv}}$ is the phase of $\det M_{\mathbf{vv}}$.

The classical trajectories contributing to the propagator are functions of nine real parameters: four initial labels $\bar{q}'_x$, $\bar{q}'_y$, $\bar{p}'_x$ and $\bar{p}'_y$, four final labels $\bar{q}''_x$, $\bar{q}''_y$, $\bar{p}''_x$ and $\bar{p}''_y$, and the propagation time T. As one changes one of these parameters continuously, it might happen that two independent solutions become very similar to each other. In the limit situation they might coalesce into a single trajectory, characterizing a phase space caustic, or a bifurcation point. At the immediate neighborhood of the caustic these solutions will satisfy identical boundary conditions. Therefore, close to the caustic, we can set small initial displacements $\delta\mathbf{u}' = 0$ and $\delta\mathbf{v}' \neq 0$ in such a manner that, after the time T, $\delta\mathbf{u}'' \neq 0$ and $\delta\mathbf{v}'' = 0$. Eq. (7) then reduces to

$$\begin{pmatrix} \delta\mathbf{u}'' \\ 0 \end{pmatrix} = \begin{pmatrix} M_{\mathbf{uu}} & M_{\mathbf{uv}} \\ M_{\mathbf{vu}} & M_{\mathbf{vv}} \end{pmatrix}\begin{pmatrix} 0 \\ \delta\mathbf{v}' \end{pmatrix}, \tag{8}$$

implying that $\det M_{\mathbf{vv}} = 0$. Therefore, at the caustic the pre-factor of the Eq. (2), $|\det M_{\mathbf{vv}}|^{-1/2}$, diverges and the semiclassical formula cannot be used. The main purpose of this paper is to correct the semiclassical formula in these situations, replacing the singular pre-factor by a well behaved Airy-type function.

As mentioned in Section 1, in addition to the divergence of the pre-factor, the semiclassical formula (2) can exhibit other peculiarities, which we shall not address here. For example, for some complex trajectories the imaginary part of $\mathcal{F}$ can be large and negative, giving unreasonably large contributions to the propagator. This problem is related to the

Stokes Phenomenon, and lead to the exclusion of some trajectories from the sum in Eq. (2) in order to eliminate the unphysical results they produce [4–8,13].

3. Dual representation for the coherent state propagator

The main difficulty in dealing with phase space caustics is the lack of a dual representation for the coherent state propagator. Caustics in position representation can be removed by changing to the momentum representation and vice-versa. For the coherent state propagator, since both position and momentum are being used, it is not clear what to do to bypass the phase space caustics. In Ref. [19] we defined an application that plays the role of a dual representation for the coherent state basis and used it to find a uniform formula for the semiclassical propagator for one-dimensional systems. The purpose of this section is to extend the formalism of Ref. [19] for systems with two degrees of freedom.

Based on the relations

$$\mathbf{u}(T) \equiv \mathbf{u}'' = \frac{\mathrm{i}}{\hbar}\frac{\partial \mathcal{S}}{\partial \mathbf{v}''} \quad \text{and} \quad \mathbf{v}(0) \equiv \mathbf{v}' = \frac{\mathrm{i}}{\hbar}\frac{\partial \mathcal{S}}{\partial \mathbf{u}'}, \tag{9}$$

which can be demonstrated by differentiating the complex action of Eq. (5), we perform a Legendre transform on $\mathcal{S}(\mathbf{v}'', \mathbf{u}', T)$ replacing the independent variable $\mathbf{v}''$ by $\mathbf{u}'' = (\mathrm{i}/\hbar)(\partial\mathcal{S}/\partial\mathbf{v}'')$. The transformed function $\tilde{\mathcal{S}}$ depends on the variables $\mathbf{u}'$ and $\mathbf{u}''$, instead of $\mathbf{u}'$ and $\mathbf{v}''$,

$$\tilde{\mathcal{S}}(\mathbf{u}'', \mathbf{u}', T) = \mathcal{S}(\mathbf{v}'', \mathbf{u}', T) + \mathrm{i}\hbar\mathbf{u}''\mathbf{v}'', \tag{10}$$

and satisfies the relations

$$\mathbf{v}'' = -\frac{\mathrm{i}}{\hbar}\frac{\partial \tilde{\mathcal{S}}}{\partial \mathbf{u}''} \quad \text{and} \quad \mathbf{v}' = \frac{\mathrm{i}}{\hbar}\frac{\partial \tilde{\mathcal{S}}}{\partial \mathbf{u}'}. \tag{11}$$

With these properties in mind we define a dual representation $\tilde{K}(\mathbf{u}'', \mathbf{u}', T)$ for the propagator $K(\mathbf{v}'', \mathbf{u}', T)$ by

$$\tilde{K}(\mathbf{u}'', \mathbf{u}', T) = \frac{1}{2\pi}\int_C K(\mathbf{v}'', \mathbf{u}', T)\mathrm{e}^{-\mathbf{u}''\mathbf{v}''}\mathrm{d}^2\mathbf{v}'', \tag{12}$$

$$K(\mathbf{v}'', \mathbf{u}', T) = \frac{1}{2\pi}\int_{\tilde{C}} \tilde{K}(\mathbf{u}'', \mathbf{u}', T)\mathrm{e}^{\mathbf{u}''\mathbf{v}''}\mathrm{d}^2\mathbf{u}'', \tag{13}$$

where C and $\tilde{C}$ are convenient paths that, as specified in [19], are chosen in such a way that Eqs. (12) and (13) are a Laplace and a Mellin transform, respectively. The analogy between these two expressions and the corresponding coordinate and momentum representations is not complete. This is because, while $K(\mathbf{v}'', \mathbf{u}', T)$ is the quantum propagator, $\tilde{K}(\mathbf{u}'', \mathbf{u}', T)$ does not seem to correspond to an explicit quantum matrix element. It is a mathematical artifice that allows for the continuation of the propagator in an auxiliary phase space, rather than a quantity with a direct physical interpretation.

In order to obtain a semiclassical formula for $\tilde{K}(\mathbf{u}'', \mathbf{u}', T)$, we insert Eq. (2) into (12),

$$\tilde{K}_{\mathrm{SC}}(\mathbf{u}'', \mathbf{u}', T) = \frac{1}{2\pi}\int_C \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\mathcal{S}(\mathbf{v}'', \mathbf{u}', T) + \frac{\mathrm{i}}{\hbar}\mathcal{G}(\mathbf{v}'', \mathbf{u}', T) - \frac{\mathrm{i}}{2}\sigma_{\mathbf{vv}} - \frac{1}{2}\ln|\det M_{\mathbf{vv}}| - \mathbf{u}''\mathbf{v}''}\mathrm{d}^2\mathbf{v}''. \tag{14}$$

Rigorously, Eq. (14) says that to calculate $\tilde{K}_{\mathrm{SC}}$ for a set of parameters $\mathbf{u}''$, $\mathbf{u}'$ and T, we need to calculate the contribution of the trajectory beginning at $\mathbf{u}(0) = \mathbf{u}'$ and ending at

$\mathbf{v}(T) = \mathbf{v}''$, and sum over all $\mathbf{v}''$ lying in the path C. Notice that, for each trajectory, the value of the variable $\mathbf{u}$ at time T is function of $\mathbf{u}'$, $\mathbf{v}''$ and T, namely, $\mathbf{u}(T) \equiv \mathbf{u}(\mathbf{v}'',\mathbf{u}',T)$. In the semiclassical limit this integral can be solved by the steepest descent method [3], according to which the critical value $\mathbf{v}''_c$ of the integration variable satisfies

$$\left\{\frac{\partial}{\partial \mathbf{v}''}[\mathcal{S} + \mathrm{i}\hbar \mathbf{u}''\mathbf{v}'']\right\}\bigg|_{\mathbf{v}''_c} = 0 \text{ or } \mathbf{u}'' = \frac{\mathrm{i}}{\hbar}\frac{\partial \mathcal{S}}{\mathbf{v}''}\bigg|_{\mathbf{v}''_c}, \tag{15}$$

where we have considered that $\mathcal{G}$ and $\ln|\det M_{\mathbf{vv}}|$ varies slowly in comparison with $\mathcal{S}$, since the former is of order $\hbar$ while the later is of order $\hbar^0$ (see Ref. [24]). Eq. (15) says that the critical trajectory satisfies $\mathbf{u}(0) = \mathbf{u}'$ and $\mathbf{u}(T) = \mathbf{u}(\mathbf{v}''_c, \mathbf{u}', T) = \mathbf{u}''$, i.e., the critical value $\mathbf{v}''_c$ of the integration variable is equal to $\mathbf{v}(T)$ of a trajectory satisfying these boundary conditions. This shows that the integration path C must coincide with (or be deformable into) a steepest descent path through $\mathbf{v}''_c$. Expanding the exponent up to second order around this trajectory and performing the resulting Gaussian integral we obtain

$$\tilde{K}^{(2)}_{\mathrm{SC}}(\mathbf{u}'', \mathbf{u}', T) = \sum_{\text{traj.}} \sqrt{\frac{1}{|\det M_{\mathbf{uv}}|}} \exp\left\{\frac{\mathrm{i}}{\hbar}\tilde{\mathcal{S}}(\mathbf{u}'', \mathbf{u}', T) + \frac{\mathrm{i}}{\hbar}\tilde{\mathcal{G}}(\mathbf{u}'', \mathbf{u}', T) - \frac{\mathrm{i}}{2}\sigma_{\mathbf{uv}}\right\}, \tag{16}$$

where, again, the index (2) is used to indicate the method of integration used. The sum over stationary trajectories was included because more than one of them may exist. To derive the last equation, we have also used the result

$$-\det\begin{pmatrix} \mathcal{S}_{v''_x v''_x} & \mathcal{S}_{v''_x v''_y} \\ \mathcal{S}_{v''_y v''_x} & \mathcal{S}_{v''_y v''_y} \end{pmatrix} = \hbar^2 \frac{|\det M_{\mathbf{uv}}|}{|\det M_{\mathbf{vv}}|} \mathrm{e}^{\mathrm{i}(\sigma_{\mathbf{uv}} - \sigma_{\mathbf{vv}})}, \tag{17}$$

with $\mathcal{S}_{\alpha\beta} \equiv \partial^2\mathcal{S}/\partial\alpha\partial\beta$, for $\alpha,\ \beta = v''_x$ or v''_y, and $\sigma_{\mathbf{uv}}$ is the phase of $\det M_{\mathbf{uv}}$. This last equation can be obtained by considering small variations of Eq. (9), rearranging the terms so as to write $\delta\mathbf{u}''$ and $\delta\mathbf{v}''$ as function of $\delta\mathbf{u}'$ and $\delta\mathbf{v}'$, and comparing with Eq. (7).

The new semiclassical propagator $\tilde{K}_{\mathrm{SC}}$ is a function of complex classical trajectories satisfying $\mathbf{u}' = \mathbf{u}(0)$ and $\mathbf{u}'' = \mathbf{u}(T)$. $M_{\mathbf{uv}}$ is given by Eq. (7), $\tilde{\mathcal{G}}(\mathbf{u}'', \mathbf{u}', T)$ is the function $\mathcal{G}$ calculated at the new trajectory, and $\tilde{\mathcal{S}}(\mathbf{u}'', \mathbf{u}', T)$ is given by Eq. (10). It is easy to see from Eq. (8) that, when $\det M_{\mathbf{vv}}$ is zero, $\det M_{\mathbf{uv}}$ is not. This is a fundamental property that one has to bear in mind when deriving approximations for $K(\mathbf{v}'', \mathbf{u}', T)$ inserting $\tilde{K}^{(2)}_{\mathrm{SC}}$ into Eq. (13). Three such approximations will be derived in the next section.

4. Coherent state propagator from its dual representation

Replacing Eq. (16) back into Eq. (13) we obtain

$$K_{\mathrm{SC}}(\mathbf{v}'', \mathbf{u}', T) = \frac{1}{2\pi}\int_{\tilde{C}} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\tilde{\mathcal{S}}(\mathbf{u}'',\mathbf{u}',T) + \frac{\mathrm{i}}{\hbar}\tilde{\mathcal{G}}(\mathbf{u}'',\mathbf{u}',T) - \frac{\mathrm{i}}{2}\sigma_{\mathbf{uv}} - \frac{1}{2}\ln|\det M_{\mathbf{uv}}| + \mathbf{u}''\mathbf{v}''} \mathrm{d}^2\mathbf{u}''. \tag{18}$$

To solve K_{SC} for the parameters $\mathbf{v}''$, $\mathbf{u}'$ and T, we need to sum the contributions of all trajectories beginning at $\mathbf{u}'$ and ending at $\mathbf{u}''$ lying in $\tilde{C}$. The saddle point $\mathbf{u}''_c$ of the exponent satisfies

$$\left\{\frac{\partial}{\partial \mathbf{u}''}[\tilde{\mathcal{S}} - \mathrm{i}\hbar \mathbf{u}''\mathbf{v}'']\right\}\bigg|_{\mathbf{u}''_c} = 0 \text{ or } \mathbf{v}'' = -\frac{\mathrm{i}}{\hbar}\frac{\partial \mathcal{S}}{\mathbf{v}''}\bigg|_{\mathbf{u}''_c}, \tag{19}$$

which says that the most contributing trajectories are those with boundary conditions $\mathbf{v}(T) = \mathbf{v}''$ and $\mathbf{u}(0) = \mathbf{u}'$, exactly as in Eq. (2). Therefore, expanding the exponent up to second order around the critical trajectory, solving the remaining Gaussian integral, and using the result (see Eq. (A.22) of the appendix)

$$-\det\begin{pmatrix}\tilde{S}_{u''_x u''_x} & \tilde{S}_{u''_x u''_y}\\ \tilde{S}_{u''_y u''_x} & \tilde{S}_{u''_y u''_y}\end{pmatrix} \equiv -\det\tilde{S}_{\mathbf{u}''\mathbf{u}''} = \hbar^2 \frac{|\det M_{\mathbf{vv}}|}{|\det M_{\mathbf{uv}}|} e^{i(\sigma_{\mathbf{vv}}-\sigma_{\mathbf{uv}})}, \tag{20}$$

we recover Eq. (2).

Clearly, the connection between the propagators of Eqs. (2) and (16) via steepest descent approximation with quadratic expansion of the exponent works only in the regions where both $\det M_{\mathbf{uv}}$ and $\det M_{\mathbf{vv}}$ are non-zero. Close to caustics, where $\det M_{\mathbf{vv}} = 0$, $\tilde{K}^{(2)}_{\mathrm{SC}}$ is still well defined and K_{SC} can be obtained by doing the inverse transform (18) but expanding the exponent to at least third order. There are, however, several ways to handle such an expansion, depending on how close to the caustic a given stationary trajectory is. In the next subsections, we show how to obtain three approximate formulas for the propagator:

In Section 4.1, we evaluate Eq. (18) by expanding its integrand up to third order around the stationary trajectories. As a result we find that each contribution already present in $K^{(2)}_{\mathrm{SC}}$ appears multiplied by a correction term $\mathcal{I}_{\mathrm{R}}$. This *regular formula* for the semiclassical propagator is good only if the stationary trajectories are not too close to caustics, so that second and third order terms contribute to the integral.

In Section 4.2, we consider the situation where two contributing solutions are so close each other that, if we used the regular formula, the contributions would be counted twice. We therefore perform a *transitional* approximation, where the exponent of (18) is expanded around the trajectory that lies exactly at the phase space caustic. Since this trajectory is not generally stationary, this approach works only if the stationary solutions are sufficiently close to the caustic.

Finally, in Section 4.3, we derive a *uniform approximation*, which is applicable both near and far from the caustics but might not be so accurate as the two previous expressions.

4.1. Regular formula

The philosophy of the regular approximation is to correct the contribution of each stationary trajectory by including third order terms in the expansion of the exponent of Eq. (18). When this expansion is performed we obtain

$$K^{(3)}_{\mathrm{SC}}(\mathbf{v}'', \mathbf{u}', T) = \left\{\sqrt{\frac{1}{|\det M_{\mathbf{vv}}|}} e^{\frac{i}{\hbar}\mathcal{F}}\right\} \times \mathcal{I}_{\mathrm{R}}(\mathbf{v}'', \mathbf{u}', T), \tag{21}$$

where the quantities between brackets are the same as in Eq. (2), and the correction term $\mathcal{I}_{\mathrm{R}}$ is given by

$$\mathcal{I}_{\mathrm{R}} = \sqrt{-\frac{\det\tilde{S}_{\mathbf{u}''\mathbf{u}''}}{4\pi^2\hbar^2}} \int d^2[\delta\mathbf{u}''] e^{\frac{i}{\hbar}\{A\delta u''^2_x + B\delta u''_x u''_y + C\delta u''^2_y + D\delta u''^3_x + E\delta u''^2_x \delta u''_y + F\delta u''^2_y \delta u''_x + G\delta u''^3_y\}} \tag{22}$$

and

$$A = \frac{1}{2}\tilde{\mathcal{S}}_{u''_x u''_x}, \quad B = \tilde{\mathcal{S}}_{u''_x u''_y}, \quad C = \frac{1}{2}\tilde{\mathcal{S}}_{u''_y u''_y},$$
$$D = \frac{1}{6}\tilde{\mathcal{S}}_{u''_x u''_x u''_x}, \quad E = \frac{1}{2}\tilde{\mathcal{S}}_{u''_x u''_x u''_y}, \quad F = \frac{1}{2}\tilde{\mathcal{S}}_{u''_x u''_y u''_y} \quad \text{and} \quad G = \frac{1}{6}\tilde{\mathcal{S}}_{u''_y u''_y u''_y}. \tag{23}$$

All functions and constants in Eq. (21) are calculated at the critical trajectory. In Eq. (23), we define $\tilde{\mathcal{S}}_{\alpha\beta\gamma} \equiv (\partial^3\tilde{\mathcal{S}}/\partial\alpha\partial\beta\partial\gamma)$ and $\tilde{\mathcal{S}}_{\alpha\beta} \equiv (\partial^2\tilde{\mathcal{S}}/\partial\alpha\partial\beta)$, for $\alpha,\ \beta,\ \gamma = u''_x$ or u''_y. The integration contour of Eq. (22) is chosen to coincide with the steepest descent of the saddle point.

The integral (22) has no direct solution. However, it can be largely simplified in the coordinate system $(\delta u_+, \delta u_-)$ that diagonalizes the matrix of the quadratic terms,

$$\begin{pmatrix} A & B/2 \\ B/2 & C \end{pmatrix} = \frac{1}{2}\tilde{S}_{\mathbf{u}''\mathbf{u}''}. \tag{24}$$

Therefore, we perform the change of variables

$$\begin{bmatrix} \delta u''_x \\ \delta u''_y \end{bmatrix} = \frac{1}{B/2(\lambda_- - \lambda_+)}\begin{bmatrix} N_+(A-\lambda_-) & -N_-(A-\lambda_+) \\ N_+B/2 & -N_-B/2 \end{bmatrix}\begin{bmatrix} \delta u_+ \\ \delta u_- \end{bmatrix}, \tag{25}$$

where $N_\pm$ are normalization constants and $\lambda_\pm$ are eigenvalues of $\frac{1}{2}\tilde{S}_{\mathbf{u}''\mathbf{u}''}$,

$$N_\pm = \sqrt{(B/2)^2 + (A-\lambda_\pm)^2} \quad \text{and} \quad \lambda_\pm = \frac{\mathrm{tr}\tilde{S}_{\mathbf{u}''\mathbf{u}''}}{4}\left\{1 \pm \sqrt{1 - 4\frac{\det \tilde{S}_{\mathbf{u}''\mathbf{u}''}}{(\mathrm{tr}\tilde{S}_{\mathbf{u}''\mathbf{u}''})^2}}\right\}. \tag{26}$$

In the new variables Eq. (22) becomes

$$\mathcal{I}_{\mathrm{R}} = \sqrt{-\frac{\lambda_+\lambda_-}{\pi^2\hbar^2}}\int \mathrm{d}[\delta u_+]\mathrm{d}[\delta u_-]\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\{\lambda_+\delta u_+^2 + \lambda_-\delta u_-^2 + D'\delta u_+^3 + E'\delta u_+^2\delta u_- + F'\delta u_+\delta u_-^2 + G'\delta u_-^3\}}, \tag{27}$$

where the new coefficients, D', E', F' and G', are combinations of those in Eq. (23). Our final formula depends just on G', which amounts to

$$G' = \left(\frac{N_-}{\lambda_+ - \lambda_-}\right)^3\left[\left(\frac{A-\lambda_+}{B/2}\right)^3 D + \left(\frac{A-\lambda_+}{B/2}\right)^2 E + \left(\frac{A-\lambda_+}{B/2}\right)F + G\right]. \tag{28}$$

According to Eqs. (20) and (24), when $\det M_{\mathbf{vv}} \to 0$, $\det \tilde{S}_{\mathbf{u}''\mathbf{u}''}$ also tends to zero, causing the breaking down of the quadratic approximation. However, in terms of the variables δu_+ and δu_-, we see that $\det \tilde{S}_{\mathbf{u}''\mathbf{u}''} (= 4\lambda_+\lambda_-)$ goes to zero in a particular way: while λ_- vanishes, λ_+ generally remains finite. Therefore Eq. (27) is always of a gaussian type integral in the variable δu_+, since we are still able to neglect third order terms in this direction. Solving the integral in δu_+ leads to

$$\mathcal{I}_{\mathrm{R}} \approx \sqrt{\frac{-\mathrm{i}\lambda_-}{\pi\hbar}}\int \mathrm{d}[\delta u_-]\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\{\lambda_-\delta u_-^2 + G'\delta u_-^3\}}. \tag{29}$$

Now we perform a last changing of variables, $t = (\frac{3G'}{\hbar})^{1/3}[\delta u_- + \frac{\lambda_-}{3G'}]$, and obtain

$$\mathcal{I}_{\mathrm{R}} \approx 2\sqrt{\pi}\bar{w}\mathrm{e}^{\frac{2}{3}\bar{w}^6} f_i(\bar{w}^4), \tag{30}$$

where $\bar{w} = \frac{(-\mathrm{i}\lambda_-/\hbar)^{1/2}}{(3G'/\hbar)^{1/3}}$ and $f_i(w)$ is given by

$$f_i(w) = \frac{1}{2\pi}\int_{C_i} \mathrm{d}t \exp\left\{\mathrm{i}\left[wt + \frac{1}{3}t^3\right]\right\}, \tag{31}$$

for $i = 1, 2, 3$. The index i refers to three possible paths of integration C_i, giving rise to three different Airy's functions (see Ref. [3]). Rigorously the choice of the path should be done according to Cauchy's Theorem, since it must be obtained by a deformation of the original contour of integration. In practice, however, it might be very difficult to find the correct path in this way, and we have to use physical criteria to justify the choice of C_i.

Inserting (30) into Eq. (21) and considering the existence of more than one critical trajectory, we finally find the regular formula

$$K^{(3)}_{\mathrm{SC}}(\mathbf{v}'', \mathbf{u}', T) = \sum_{\mathrm{traj.}}\left\{\left[\sqrt{\frac{1}{|\det M_{\mathbf{vv}}|}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\mathcal{F}(\mathbf{v}'',\mathbf{u}',T)}\right] \times \left[2\sqrt{\pi}\bar{w}\mathrm{e}^{\frac{2}{3}\bar{w}^6} f_i(\bar{w}^4)\right]\right\}. \tag{32}$$

In this equation, each stationary trajectory gives a contribution which is that of the quadratic approximation multiplied by a correction factor $\mathcal{I}_{\mathrm{R}}$ that depends only on the parameter $\bar{w}$. Close to a caustic λ_- is very small but G' (generally) remains finite. Exactly at the caustic $|\bar{w}|$ is zero, getting larger and larger as we move away from it. Therefore we expect that $\mathcal{I}_{\mathrm{R}}$ should go to 1 as $|\bar{w}|$ goes to infinity, since the regular expression should recover $K^{(2)}_{\mathrm{SC}}$ in this limit. To verify this assertion, we look at the asymptotic formulas for the Airy's functions [25],

$$\begin{aligned} f_1(w) &\sim \frac{1}{2\sqrt{\pi}} w^{-1/4}\mathrm{e}^{-\frac{2}{3}w^{3/2}}, \\ f_2(w) &\sim \frac{-\mathrm{i}}{2\sqrt{\pi}} w^{-1/4}\mathrm{e}^{\frac{2}{3}w^{3/2}}, \\ f_3(w) &\sim \frac{\mathrm{i}}{2\sqrt{\pi}} w^{-1/4}\mathrm{e}^{\frac{2}{3}w^{3/2}}. \end{aligned} \tag{33}$$

Using these expressions in Eq. (30), we see that only $f_1(w)$ produces the desired asymptotic result, indicating that this is the proper choice of Airy function far from the caustic. However, this is so only because we have taken the principal root in the definition of $\bar{w}$. As the physical results should not depend on the arbitrariness of branches in the complex plane, the choice of a different root would lead to a different path C_i, so that physical results remain the same. A careful discussion about this point can be found in [4].

Exactly at the caustic, $\bar{w} = 0$, the regular formula becomes

$$K^{(3)}_{\mathrm{SC}}(\mathbf{v}'', \mathbf{u}', T) = \sqrt{\frac{\mathrm{i}\hbar\pi}{\lambda_+(\det M_{\mathbf{uv}})}}\left(\frac{\hbar}{3G'}\right)^{1/3} f_i(0)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}[\mathcal{S}+\mathcal{G}]}, \tag{34}$$

where the sum was excluded because the critical trajectories coalesce at this point.

4.2. Transitional formula

Each contribution to the semiclassical propagator calculated in the last section (as well as those of Eq. (2)) has information about the critical trajectory plus its vicinity. If two trajectories are very close each other, like in the vicinity of a phase space caustic, their regions of influence might overlap. The regular formula cannot be used in these situations, since it assumes that the trajectories can still be counted independently. To find an approximation for $K(\mathbf{v}'', \mathbf{u}', T)$ valid in this scenario, we shall perform the integral (18) expanding the exponent about the (non-stationary) trajectory corresponding to the phase space caustic itself, defined by the point $\bar{\mathbf{u}}''$ where $|\det \tilde{S}_{\mathbf{u}''\mathbf{u}''}|$ and therefore $|\det M_{\mathbf{vv}}|$ [see Eq. (20)] are zero. Evaluating this single contribution to third order should be equivalent to include and sum over each stationary trajectory.

The condition $\det \tilde{S}_{\mathbf{u}''\mathbf{u}''} = 0$ leads to the PSC trajectory that begins at $\mathbf{u}(0) \equiv \mathbf{u}'$ and $\mathbf{v}(0) \equiv \mathbf{v}'$, and ends at $\mathbf{u}(T) \equiv \bar{\mathbf{u}}''$ and $\mathbf{v}(T) \equiv \bar{\mathbf{v}}''$, where $\bar{\mathbf{v}}''$ is assumed to be close to $\mathbf{v}''$. Expanding the exponent of Eq. (18) up to third order around this new trajectory yields

$$K_{\mathrm{SC}}^{\mathrm{PSC}}(\mathbf{v}'', \mathbf{u}', T) = (\det M_{\mathbf{uv}})^{-1/2} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\{\mathcal{S}(\bar{\mathbf{v}}'', \mathbf{u}', T) + \mathcal{G}(\bar{\mathbf{v}}'', \mathbf{u}', T) - \mathrm{i}\hbar \bar{\mathbf{u}}''(\mathbf{v}'' - \bar{\mathbf{v}}'')\}} \mathcal{I}_{\mathrm{T}}, \tag{35}$$

where

$$\mathcal{I}_{\mathrm{T}} = \frac{1}{2\pi} \int \mathrm{d}^2[\delta \mathbf{u}''] \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\{X\delta u''_x + Y\delta u''_y + A\delta u''^2_x + B\delta u''_x u''_y + C\delta u''^2_y + D\delta u''^3_x + E\delta u''^2_x \delta u''_y + F\delta u''^2_y \delta u''_x + G\delta u''^3_y\}}, \tag{36}$$

with $X = \partial \tilde{\mathcal{S}}/\partial u''_x - \mathrm{i}\hbar v''_x$ and $Y = \partial \tilde{\mathcal{S}}/\partial u''_y - \mathrm{i}\hbar v''_y$. The functions appearing in Eq. (35) and all the coefficients are calculated at the PSC trajectory.

We solve Eq. (36) using the same technique described in the last section, with the use of the transformation (25). However, as we deal with the PSC trajectory, $\lambda_+ = A + C$ and $\lambda_- = 0$. The integral $\mathcal{I}_{\mathrm{T}}$ becomes

$$\mathcal{I}_{\mathrm{T}} = \frac{1}{2\pi} \int \mathrm{d}[\delta u_+]\, \mathrm{d}[\delta u_-] \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\{a\delta u_+ + b\delta u_- + \lambda_+ \delta u_+^2 + D'\delta u_+^3 + E'\delta u_+^2 \delta u_- + F'\delta u_+ \delta u_-^2 + G'\delta u_-^3\}}, \tag{37}$$

where the only coefficients that appear in the final formula are

$$a = -\left(\frac{N_+}{\lambda_+ - \lambda_-}\right)\left[\left(\frac{A - \lambda_-}{B/2}\right)X + Y\right], \quad b = \left(\frac{N_-}{\lambda_+ - \lambda_-}\right)\left[\left(\frac{A - \lambda_+}{B/2}\right)X + Y\right] \tag{38}$$

with $\lambda_- = 0$ and G', given by Eq. (28).

The integral over δu_+ can be performed neglecting terms of third order. We obtain

$$\mathcal{I}_{\mathrm{T}} = \frac{1}{2\pi} \sqrt{\frac{\mathrm{i}\pi\hbar}{\lambda_+}} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\frac{a^2}{4\lambda_+}} \int \mathrm{d}[\delta u_-] \exp\left\{\frac{\mathrm{i}}{\hbar}\left[b\delta u_- + G'\delta u_-^3\right]\right\}. \tag{39}$$

By setting $t = (\frac{3G'}{\hbar})^{1/3}\delta u_-$, the last equation can be written as

$$\mathcal{I}_{\mathrm{T}} = \sqrt{\frac{\mathrm{i}\pi\hbar}{\lambda_+}} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\frac{a^2}{4\lambda_+}} \left(\frac{\hbar}{3G'}\right)^{1/3} f_i(\tilde{w}), \tag{40}$$

where $\tilde{w} = \frac{b/\hbar}{(3G'/\hbar)^{1/3}}$ and the function $f_i(w)$ refers to the Airy's functions (31). Finally, we write the transitional formula by combining Eq. (40) with Eq. (35),

$$K_{\mathrm{SC}}^{\mathrm{PSC}}(\mathbf{v}'', \mathbf{u}', T) = \sqrt{\frac{\mathrm{i}\hbar\pi}{\lambda_+(\det M_{\mathbf{uv}})}} \left(\frac{\hbar}{3G'}\right)^{1/3} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\frac{a^2}{4\lambda_+}} f_i(\tilde{w}) \mathrm{e}^{\frac{\mathrm{i}}{\hbar}[\mathcal{S} + \mathcal{G}] - \mathrm{i}\hbar \bar{\mathbf{u}}''(\mathbf{v}'' - \bar{\mathbf{v}}'')}. \tag{41}$$

Eq. (41) depends on the PSC trajectory, which satisfies $\mathbf{u}(0) = \mathbf{u}'$ and $\mathbf{v}(T) = \bar{\mathbf{v}}''$, and is valid only if $\bar{\mathbf{v}}''$ is close to $\mathbf{v}''$.

Far from the caustic Eq. (41) does not make sense, since the PSC trajectory becomes completely different from the actual stationary trajectories. On the other hand, when the propagator is calculated exactly at the PSC, Eqs. (41) and (32) should furnish the same result. This can be verified by setting $\bar{\mathbf{v}}'' = \mathbf{v}''$ and $a = b = \tilde{w} = 0$ in Eq. (41), which reduces directly to Eq. (34).

4.3. Uniform formula

The regular formula is good as long as one is not too close to a phase space caustic, whereas the transitional formula is good only very close to it. In either cases the expressions we derived cannot be used everywhere in the space spanned by the parameters $\mathbf{u}'$, $\mathbf{v}''$ and T. The uniform approximation provides such a global formula [26]. The basic idea is to map the argument of the exponential in (18) into a function having the same structure of saddle points as the original one, i.e., two saddle points that may coalesce on the phase space caustic depending on a given parameter.

In order to simplify our calculation, we shall use the variables u''_+ and u''_-, instead of the original u''_x and u''_y [see Eq. (25)]. In these variables the exponent of Eq. (18)

$$E(\mathbf{u}'', \mathbf{u}', T) = \frac{\mathrm{i}}{\hbar}\tilde{\mathcal{S}}(\mathbf{u}'', \mathbf{u}', T) + \frac{\mathrm{i}}{\hbar}\tilde{\mathcal{G}}(\mathbf{u}'', \mathbf{u}', T) - \frac{\mathrm{i}}{2}\sigma_{\mathbf{uv}} - \frac{1}{2}\ln|\det M_{\mathbf{uv}}| + \mathbf{u}''\mathbf{v}'', \tag{42}$$

becomes

$$\mathcal{E}(u''_+, u''_-) \equiv E[\mathbf{u}''(u''_+, u''_-), \mathbf{u}', T], \tag{43}$$

where we omit the dependence on the variables $\mathbf{u}'$ and T because they are not being integrated. The integral (18) then becomes

$$\frac{1}{2\pi}\int \mathrm{e}^{\mathcal{E}(u''_+, u''_-)}\,\mathrm{d}u''_+\,\mathrm{d}u''_-. \tag{44}$$

Since the main contributions to this integral come from the neighborhood of the saddle points, we can map the exponent $\mathcal{E}(u''_+, u''_-)$ into a new function $N(x,y)$, where $x = x(u''_+)$ and $y = y(u''_-)$. We restrict ourselves to the case where there are only two critical points, $\mathbf{u}''_1 = (u''_+, u''_-)_1$ and $\mathbf{u}''_2 = (u''_+, u''_-)_2$, which, depending on the parameters $\mathbf{u}'$ and T, may coalesce at the phase space caustic. Then

$$\frac{1}{2\pi}\int \mathrm{e}^{\mathcal{E}(u''_+, u''_-)}\,\mathrm{d}u''_+\mathrm{d}u''_- \approx \frac{1}{2\pi}\int J(x, y,)\mathrm{e}^{N(x,y)}\,\mathrm{d}x\,\mathrm{d}y. \tag{45}$$

The simplest function with these properties is

$$N(x, y) = \mathcal{A} - \mathcal{B}y + \frac{y^3}{3} + \mathcal{C}x^2, \tag{46}$$

where $\mathcal{A}$, $\mathcal{B}$ and $\mathcal{C}$ may depend on $\mathbf{u}'$ and T. The mapping requires that the saddle points of $N(x,y)$, which are $(0, \pm\sqrt{\mathcal{B}})$, coincide with the critical points $\mathbf{u}''_{1,2}$:

$$\begin{aligned} \mathcal{E}(\mathbf{u}''_1) &\equiv \mathcal{E}_1 = N(0, \sqrt{\mathcal{B}}) = \mathcal{A} - \frac{2}{3}\mathcal{B}^{3/2}, \\ \mathcal{E}(\mathbf{u}''_2) &\equiv \mathcal{E}_2 = N(0, -\sqrt{\mathcal{B}}) = \mathcal{A} + \frac{2}{3}\mathcal{B}^{3/2}, \end{aligned} \tag{47}$$

implying that

$$\mathcal{A} = \frac{1}{2}(\mathcal{E}_1 + \mathcal{E}_2) \quad \text{and} \quad \mathcal{B} = \left[\frac{3}{4}(\mathcal{E}_2 - \mathcal{E}_1)\right]^{2/3}. \tag{48}$$

Another condition required to validate the method is to impose the equivalence between the vicinity of critical points of $N(x,y)$ and $\mathcal{E}(u''_+, u''_-)$,

$$\left\{\delta N + \frac{1}{2}\delta^2 N + \frac{1}{6}\delta^3 N + \ldots\right\}\Big|_{(0,\pm\sqrt{\mathcal{B}})} = \left\{\delta\mathcal{E} + \frac{1}{2}\delta^2\mathcal{E} + \frac{1}{6}\delta^3\mathcal{E} + \ldots\right\}\Big|_{\mathbf{u}''_{1,2}}. \tag{49}$$

This equation allows us to find how to transform an arbitrary infinitesimal vector $(\delta u''_+, \delta u''_-)$ into $(\delta x, \delta y)$, around the critical points. It provides, therefore, information about the Jacobian $J(x,y)$ of the transformation calculated at the critical points, namely, $J_1 \equiv J(0,\sqrt{\mathcal{B}})$ and $J_2 \equiv J(0,-\sqrt{\mathcal{B}})$.

As the first derivatives of $\mathcal{E}$ and N vanish at the critical points, Eq. (49) implies that

$$\frac{1}{2}\begin{pmatrix}\delta x & \delta y\end{pmatrix}\begin{pmatrix} \frac{\partial^2 N}{\partial x^2} + \frac{1}{3}\frac{\partial^3 N}{\partial x^3}\delta x & \frac{\partial^2 N}{\partial x\partial y} + \frac{\partial^3 N}{\partial y\partial x^2}\delta x \\ \frac{\partial^2 N}{\partial y\partial x} + \frac{\partial^3 N}{\partial x\partial y^2}\delta y & \frac{\partial^2 N}{\partial y^2} + \frac{1}{3}\frac{\partial^3 N}{\partial y^3}\delta y \end{pmatrix}\Bigg|_{(0,\pm\sqrt{\mathcal{B}})}\begin{pmatrix}\delta x \\ \delta y\end{pmatrix} \tag{50}$$

should be equal to

$$\frac{1}{2}\begin{pmatrix}\delta u''_+ & \delta u''_-\end{pmatrix}\begin{pmatrix} \frac{\partial^2\mathcal{E}}{\partial u''^2_+} + \frac{1}{3}\frac{\partial^3\mathcal{E}}{\partial u''^3_+}\delta u''_+ & \frac{\partial^2\mathcal{E}}{\partial u''_+\partial u''_-} + \frac{\partial^3\mathcal{E}}{\partial u''_-\partial u''^2_+}\delta u''_+ \\ \frac{\partial^2\mathcal{E}}{\partial u''_-\partial u''_+} + \frac{\partial^3\mathcal{E}}{\partial u''_+\partial u''^2_-}\delta u''_- & \frac{\partial^2\mathcal{E}}{\partial u''^2_-} + \frac{1}{3}\frac{\partial^3\mathcal{E}}{\partial u''^3_-}\delta u''_- \end{pmatrix}\Bigg|_{\mathbf{u}''_{1,2}}\begin{pmatrix}\delta u''_+ \\ \delta u''_-\end{pmatrix}. \tag{51}$$

Writing $\delta u''_+ = a_+\delta x$ and $\delta u''_- = a_-\delta y$ this equality results in

$$\begin{aligned}
&\left\{\left[\frac{\partial^2\mathcal{E}}{\partial u''^2_+} + \frac{1}{3}\frac{\partial^3\mathcal{E}}{\partial u''^3_+}(a_+\delta x)\right]a_+^2\right\}_{\mathbf{u}''_{1,2}} = 2\mathcal{C},\\
&\left\{\left[\frac{\partial^2\mathcal{E}}{\partial u''_+\partial u''_-} + \frac{\partial^3\mathcal{E}}{\partial u''_-\partial u''^2_+}(a_+\delta x)\right]a_+a_-\right\}_{\mathbf{u}''_{1,2}} = 0,\\
&\left\{\left[\frac{\partial^2\mathcal{E}}{\partial u''_-\partial u''_+} + \frac{\partial^3\mathcal{E}}{\partial u''_+\partial u''^2_-}(a_-\delta y)\right]a_+a_-\right\}_{\mathbf{u}''_{1,2}} = 0,\\
&\left\{\left[\frac{\partial^2\mathcal{E}}{\partial u''^2_-} + \frac{1}{3}\frac{\partial^3\mathcal{E}}{\partial u''^3_-}(a_-\delta y)\right]a_-^2\right\}_{\mathbf{u}''_{1,2}} = \pm 2\sqrt{\mathcal{B}} + \frac{2}{3}\delta y.
\end{aligned} \tag{52}$$

In the limit of small $\hbar$, $\mathcal{G}$ and $\det M_{\mathbf{uv}}$ vary slowly in comparison with $\mathcal{S}$ and the first and last of equations (52) become, respectively,

$$\begin{aligned}
&\frac{\mathrm{i}}{\hbar}\{[\lambda_+ + D'(a_+\delta x)]a_+^2\}|_{\mathbf{u}''_{1,2}} = \mathcal{C},\\
&\frac{\mathrm{i}}{\hbar}\{[\lambda_- + G'(a_-\delta y)]a_-^2\}|_{\mathbf{u}''_{1,2}} = \pm\sqrt{\mathcal{B}} + \frac{1}{3}\delta y.
\end{aligned} \tag{53}$$

Moreover, the second and third (52) imply that $E' = F' = 0$. We emphasize that D', E', F' and G' are the same coefficients as those of Section 4.1.

Eq. (53) can be solved if we neglect the terms containing δx and δy. We find

$$(a_+)|_{\mathbf{u}''_{1,2}} = \sqrt{\frac{-\mathrm{i}\hbar\mathcal{C}}{(\lambda_+)|_{\mathbf{u}''_{1,2}}}} \quad \text{and} \quad (a_-)|_{\mathbf{u}''_{1,2}} = \sqrt{\frac{\mp\mathrm{i}\hbar\sqrt{\mathcal{B}}}{(\lambda_-)|_{\mathbf{u}''_{1,2}}}}, \tag{54}$$

so that the Jacobian at the saddle points becomes

$$J_{1,2} = (a_+a_-)|_{\mathbf{u}''_{1,2}} = \sqrt{\frac{\mp\hbar^2\mathcal{C}\sqrt{\mathcal{B}}}{(\lambda_+\lambda_-)|_{\mathbf{u}''_{1,2}}}}. \tag{55}$$

The full Jacobian can therefore be conveniently written in the vicinity of the saddle points as

$$J(x,y) = J(y) = \frac{1}{2}(J_1 + J_2) - \frac{y}{2\sqrt{\mathcal{B}}}(J_2 - J_1), \tag{56}$$

and the uniform approximation for the propagator becomes

$$K_{\mathrm{SC}}^{\mathrm{UN}}(\mathbf{v}'', \mathbf{u}', T) = \frac{1}{2\pi}\int J(x,y)\mathrm{e}^{\mathcal{A}-\mathcal{B}y+y^3/3+\mathcal{C}x^2}\,\mathrm{d}x\,\mathrm{d}y. \tag{57}$$

Performing the integral over x we obtain the final expression

$$K_{\mathrm{SC}}^{\mathrm{UN}}(\mathbf{v}'', \mathbf{u}', T) = \mathrm{i}\sqrt{\pi}\mathrm{e}^{\mathcal{A}}\left\{\left(\frac{g_2 - g_1}{\sqrt{\mathcal{B}}}\right)f_i'(\mathcal{B}) + (g_1 + g_2)f_i(\mathcal{B})\right\}, \tag{58}$$

where f_i is given by Eq. (31), $f_i' = \mathrm{d}f_i/\mathrm{d}y$ and

$$g_{1,2} = \sqrt{\frac{\pm\hbar^2\sqrt{\mathcal{B}}}{(4\lambda_+\lambda_-)|_{\mathbf{u}''_{1,2}}}} = \sqrt{\mp\sqrt{\mathcal{B}}\left(\frac{\det M_{\mathbf{uv}}}{\det M_{\mathbf{vv}}}\right)\bigg|_{\mathbf{u}''_{1,2}}}. \tag{59}$$

Eq. (58) is the uniform formula for the two-dimensional coherent state propagator. As in Sections 4.1 and 4.2, the determination of the proper path of integration C_i is done by physical criteria.

Eq. (59) shows us how the singularity in the coalescence point is controlled. When $\det M_{\mathbf{vv}}$ goes to zero, the difference between $\mathcal{E}_1$ and $\mathcal{E}_2$ also vanishes, so that the quotient $\sqrt{\mathcal{B}}/\det M_{\mathbf{vv}}$ [see also Eq. (48)] remains finite. Notice, however, that this fraction might become extremely fragile close to a caustic, because both numerator and denominator go to zero. Exactly at the caustic we can return to the second of Eq. (53) to find the correct value of a_-:

$$a_-^{\mathrm{PSC}} = \left(\frac{-\mathrm{i}\hbar}{3G'}\right)^{1/3} \Rightarrow J_{\mathrm{PSC}} = \left(\frac{-\mathrm{i}\hbar\mathcal{C}}{\lambda_+}\right)^{1/2}\left(\frac{-\mathrm{i}\hbar}{3G'}\right)^{1/3}. \tag{60}$$

One should also remember that, if $\hbar$ is not sufficiently small, the derivatives of $\mathcal{G}$ and $\det M_{\mathbf{vv}}$ may become important, specially when $\lambda_- \to 0$.

It is interesting to check that the uniform approximation (58) recovers the quadratic approximation away from the caustics, i.e., in the limit $\mathcal{B} \to \infty$. According to Eq. (33) we find that, for large w,

$$
\begin{aligned}
w^{-1/2}f_1'(w) &\sim \tfrac{-1}{2\sqrt{\pi}} w^{-1/4} e^{-\frac{2}{3}w^{3/2}},\\
w^{-1/2}f_2'(w) &\sim \tfrac{-i}{2\sqrt{\pi}} w^{-1/4} e^{\frac{2}{3}w^{3/2}},\\
w^{-1/2}f_3'(w) &\sim \tfrac{i}{2\sqrt{\pi}} w^{-1/4} e^{\frac{2}{3}w^{3/2}}.
\end{aligned}
\tag{61}
$$

Inserting Eqs. (33) and (61) into the uniform approximation results in

$$
K_{SC}^{UN}(\mathbf{v}'', \mathbf{u}', T) \approx \begin{cases} -ig_2 e^{\mathcal{A}-\frac{2}{3}\mathcal{B}^{3/2}}\mathcal{B}^{-1/4}, & \text{by using } f_1 \\ -g_1 e^{\mathcal{A}+\frac{2}{3}\mathcal{B}^{3/2}}\mathcal{B}^{-1/4}, & \text{by using } f_2 \\ \ \ g_1 e^{\mathcal{A}+\frac{2}{3}\mathcal{B}^{3/2}}\mathcal{B}^{-1/4}, & \text{by using } f_3 \end{cases}. \tag{62}
$$

It's easy to see that using the contour $C_1 + C_2$ we find $|K_{SC}^{UN}| = |K_{SC}^{(2)}|$.

Another way to arrive at the same conclusion is as follows: if $\mathbf{u}_1''$ and $\mathbf{u}_2''$ are not close each other, we can individually evaluate the contribution of each one through the second order saddle point method and sum the contributions at the end. Starting from Eq. (57) we get

$$
\begin{aligned}
K_{SC}^{UN}(\mathbf{v}'', \mathbf{u}', T) &= \tfrac{-i}{2\sqrt{\pi}} \int J(y) e^{\mathcal{A}-\mathcal{B}y+y^3/3}\, dy \\
&= \tfrac{-i}{2\sqrt{\pi}} \sum_{y_0=\pm\sqrt{\mathcal{B}}} \{J(y_0) e^{\mathcal{A}-\mathcal{B}y_0+y_0^3/3} \int e^{y_0(y-y_0)^2}\, dy\} \\
&= \frac{i\hbar e^{\mathcal{A}-\frac{2}{3}\mathcal{B}^{3/2}}}{\sqrt{\left(\det \tilde{S}_{\mathbf{u}''\mathbf{u}''}\right)_{\mathbf{u}_1''}}} + \frac{i\hbar e^{\mathcal{A}+\frac{2}{3}\mathcal{B}^{3/2}}}{\sqrt{\left(\det \tilde{S}_{\mathbf{u}''\mathbf{u}''}\right)_{\mathbf{u}_2''}}} = -K_{SC}^{(2)}(\mathbf{v}'', \mathbf{u}', T).
\end{aligned}
\tag{63}
$$

Finally we consider the uniform formula evaluated exactly at the caustic. To do so we rewrite Eq. (57) using the uniform Jacobian given by Eq. (60):

$$
K_{SC}^{UN}(\mathbf{v}'', \mathbf{u}', T) = \frac{1}{2\pi}\left[\left(\frac{i\pi\hbar}{\lambda_+}\right)^{1/2}\left(\frac{-i\hbar}{3G'}\right)^{1/3}\right] e^{\mathcal{A}} \int e^{y^3/3}\, dy. \tag{64}
$$

Since $\frac{(-i)^{1/3}}{2\pi}\int e^{y^3/3}\, dy = e^{-2\pi i/3} f_i(0)$, we find the same result as found previously with the formulas of the Sections 4.1 and 4.2 calculated at phase space caustics.

5. Final remarks

Semiclassical approximations for the evolution operator seem to be plagued by focal points and caustics in any representation. A relatively simple way to derive improved expressions that avoid the singularities of such quadratic approximations is provided by the Maslov method. The method explores the fact that, for example, the coordinate representation of the propagator, $\langle x|K(T)|x'\rangle$ can be written as the Fourier transform of the propagator in its dual representation, $\langle x|K(T)|x'\rangle = \int \langle x|p\rangle\langle p|K(T)|x'\rangle\, dp$. If the trajectory from x' to x in the time T corresponds to a focal point, we can still use this integral expression and the usual quadratic approximation for $\langle p|K(T)|x'\rangle$, as long as we perform the integral over p expanding the exponents to third order around the stationary point. This results in a well behaved approximation for the coordinate propagator in terms of an Airy function. In this paper, we have shown that a similar procedure can be applied to the coherent state representation and derived three similar third order formulas that can be used depending on how far the stationary trajectory is from the phase space caustics.

Although we have considered only systems with two degrees of freedom the extension to higher dimensions is immediate. We note that a uniform formula for the coherent state propagator was previously derived in [27] for a particular Hamiltonian.

The regular formula (32) is the simplest of our three approximations and consists of a sum over the same complex trajectories that enter in the quadratic approximation. The contribution of each trajectory is regularized by a term that avoids divergences at phase space caustics. We emphasize that this regularization deals just with the problem of caustics, so that we still need to identify contributing and non-contributing trajectories in order to get acceptable results. This approximation holds as far as the contributing trajectories are not too close to the caustics, otherwise the vicinities of different trajectories can start to overlap and their contributions would be miscounted. The transitional formula (41) works exactly in this situation. It involves the contribution of the PSC trajectory alone, and therefore is valid only very close to the caustic. Finally, the uniform formula (58) is valid everywhere, near of far a caustic. The formula we derived deals with the simplest topology of caustics [28].

All three semiclassical formulas derived here involve the calculation of third order derivatives of the action. We present an algorithm to evaluate these derivatives numerically in Appendix A. Numerical results using these expressions will presented in a future publication.

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Appendix A. Derivatives of the action $\tilde{\mathcal{S}}$

In this appendix, we show how second and third derivatives of $\tilde{\mathcal{S}}(\mathbf{u}',\mathbf{u}'',T)$ can be calculated for a given trajectory. This procedure can be used with any set of variables (for example, $(\mathbf{u}',\mathbf{v}'',T)$ or $(\mathbf{q}',\mathbf{q}'',T)$) with minor modifications.

A.1. The tangent matrix and the tangent tensor

The equations of motion in the $\mathbf{u}$ and $\mathbf{v}$ variables can be written in compact form as

$$\dot{r}_i = J_{ij}H'_j \tag{A.1}$$

where the vector $\mathbf{r}$ and the matrix J are given by

$$\mathbf{r} = \begin{pmatrix} u_x \\ u_y \\ v_x \\ v_y \end{pmatrix} \quad \text{and} \quad J = \begin{pmatrix} 0 & 0 & -\mathrm{i}/\hbar & 0 \\ 0 & 0 & 0 & -\mathrm{i}/\hbar \\ \mathrm{i}/\hbar & 0 & 0 & 0 \\ 0 & \mathrm{i}/\hbar & 0 & 0 \end{pmatrix}, \tag{A.2}$$

and

$$\tilde{H}'_i = \frac{\partial \tilde{H}}{\partial r_i}. \tag{A.3}$$

Expanding Eq. (A.1) up to second order around a reference trajectory $\bar{\mathbf{r}}(t)$, we obtain

$$\delta\dot{r}_i = J_{ij}H''_{jk}\delta r_k + \frac{1}{2}J_{ij}\delta r_l H'''_{lkj}\delta r_k, \tag{A.4}$$

where

$$\tilde{H}''_{ij} = \left.\frac{\partial^2 \tilde{H}}{\partial r_i \partial r_j}\right|_{\bar{\mathbf{r}}} \quad \text{and} \quad \tilde{H}'''_{ijk} = \left.\frac{\partial^3 \tilde{H}}{\partial r_i \partial r_j \partial r_k}\right|_{\bar{\mathbf{r}}}. \tag{A.5}$$

The solution of Eq. (A.4) can be expressed in terms of the initial displacement $\delta\mathbf{r}(0)$ as

$$\delta r_i(t) = M_{ij}(t)\delta r_j(0) + \delta r_k(0)U_{kli}(t)\delta r_l(0), \tag{A.6}$$

where the tangent matrix M and the tangent tensor U satisfy $M(0) = \mathbf{1}$ and $U(0) = 0$. Differentiating this equation with respect to t and by using Eq. (A.4), we obtain the differential equations satisfied by M and U directly:

$$\dot{M}_{ij}(t)\delta r_j(0) + \delta r_k(0)\dot{U}_{kli}(t)\delta r_l(0) = J_{ij}H''_{jk}M_{kl}\delta r_l(0) + J_{ij}H''_{jm}\delta r_k(0)U_{klm}\delta r_l(0) + \frac{1}{2}J_{ij}\delta r_k(0)M_{nk}H'''_{nmj}M_{ml}\delta r_l(0), \tag{A.7}$$

where we have discarded terms of third order in $\delta r_i(0)$. This leads to

$$\dot{M}_{ij} = J_{il}H''_{lk}M_{kj} \tag{A.8}$$

and

$$\dot{U}_{ijk} = J_{kl}H''_{lm}U_{ijm} + \frac{1}{2}J_{kl}M_{ni}H'''_{nml}M_{mj}. \tag{A.9}$$

These two sets of differential equations can be solved for a given reference trajectory $\bar{\mathbf{r}}(t)$ and boundary conditions $M(0) = \mathbf{1}$ and $U(0) = 0$.

A.2. Derivatives of $\tilde{\mathcal{S}}$

Here, we show how to obtain the second and third derivatives of $\tilde{\mathcal{S}}$ in terms of M and U. We start from Eq. (11), which can be written as

$$V_i = K_{ij}\tilde{\mathcal{S}}'_j, \tag{A.10}$$

where

$$\mathbf{V} = \begin{pmatrix} v'_x \\ v'_y \\ v''_x \\ v''_y \end{pmatrix}, \quad \mathbf{U} = \begin{pmatrix} u'_x \\ u'_y \\ u''_x \\ u''_y \end{pmatrix}, \quad K = \begin{pmatrix} \mathrm{i}/\hbar & 0 & 0 & 0 \\ 0 & \mathrm{i}/\hbar & 0 & 0 \\ 0 & 0 & -\mathrm{i}/\hbar & 0 \\ 0 & 0 & 0 & -\mathrm{i}/\hbar \end{pmatrix} \tag{A.11}$$

and $\tilde{\mathcal{S}}'_i = \partial\tilde{\mathcal{S}}/\partial U_i$.

Considering variations on Eq. (A.10) around the reference trajectory and expanding up to second order, we get

$$\delta V_i = K_{ij}\tilde{S}''_{jk}\delta U_k + \frac{1}{2}K_{ij}\delta U_l \tilde{S}'''_{lkj}\delta U_k, \tag{A.12}$$

where

$$\tilde{S}''_{ij} = \left.\frac{\partial^2 \tilde{\mathcal{S}}}{\partial U_i \partial U_j}\right|_{\bar{\mathbf{r}}} \quad \text{and} \quad \tilde{S}'''_{ijk} = \left.\frac{\partial^3 \tilde{\mathcal{S}}}{\partial U_i \partial U_j \partial U_k}\right|_{\bar{\mathbf{r}}}. \tag{A.13}$$

The idea now is to manipulate Eq. (A.12) so that final displacements are written in terms of the initial ones. To do this we write

$$\begin{aligned}\delta\mathbf{U} &= A\delta\mathbf{r}(0) + B\delta\mathbf{r}(T)\\ \delta\mathbf{V} &= C\delta\mathbf{r}(0) + D\delta\mathbf{r}(T)\end{aligned} \tag{A.14}$$

where A, B, C and D are 4×4 matrices that can be written in terms of 2×2 blocks as

$$A = \begin{pmatrix}\mathbf{1} & \mathbf{0}\\ \mathbf{0} & \mathbf{0}\end{pmatrix},\ B = \begin{pmatrix}\mathbf{0} & \mathbf{0}\\ \mathbf{1} & \mathbf{0}\end{pmatrix},\ C = \begin{pmatrix}\mathbf{0} & \mathbf{1}\\ \mathbf{0} & \mathbf{0}\end{pmatrix},\ D = \begin{pmatrix}\mathbf{0} & \mathbf{0}\\ \mathbf{0} & \mathbf{1}\end{pmatrix}. \tag{A.15}$$

Replacing Eqs. (A.14) into (A.12) and solving for $\delta\mathbf{r}(T)$ produces

$$\delta\mathbf{r}(T) = (D - K\tilde{S}''B)^{-1}(K\tilde{S}''A - C)\delta\mathbf{r}(0) + \frac{1}{2}\Lambda^{-1}\mathbf{w}, \tag{A.16}$$

where $\Lambda \equiv K^{-1}(D - K\tilde{S}''B)$ and

$$\begin{aligned} w_i &= \delta u_l \tilde{S}'''_{lmi}\delta u_m\\ &= [A\delta\mathbf{r}(0) + B\delta\mathbf{r}(T)]_l\ \tilde{S}'''_{lmi}[A\delta\mathbf{r}(0) + B\delta\mathbf{r}(T)]_m\\ &\approx [A\delta\mathbf{r}(0) + BM\delta\mathbf{r}(0)]_l\ \tilde{S}'''_{lmi}[A\delta\mathbf{r}(0) + BM\delta\mathbf{r}(0)]_m\\ &= [L\delta\mathbf{r}(0)]_l\ \tilde{S}'''_{lmi}[L\delta\mathbf{r}(0)]_m. \end{aligned} \tag{A.17}$$

In this expression, we have discarded terms of third order in $\delta\mathbf{r}(0)$ and we have defined the auxiliary matrix $L = A + BM$. Computing all these matrices explicitly, we find

$$(D - K\tilde{S}''B)^{-1} = \begin{pmatrix} \mathrm{i}\hbar\tilde{S}^{-1}_{\mathbf{u}'\mathbf{u}''} & 0\\ \tilde{S}_{\mathbf{u}''\mathbf{u}''}\tilde{S}^{-1}_{\mathbf{u}'\mathbf{u}''} & 1\end{pmatrix}, \tag{A.18}$$

$$(K\tilde{S}''A - C) = \begin{pmatrix} (\mathrm{i}/\hbar)\tilde{S}_{\mathbf{u}'\mathbf{u}'} & -1\\ -(\mathrm{i}/\hbar)\tilde{S}_{\mathbf{u}''\mathbf{u}'} & 0\end{pmatrix}, \tag{A.19}$$

$$L^{-1} = \begin{pmatrix} 1 & 0\\ -M^{-1}_{\mathbf{uv}}M_{\mathbf{uu}} & M^{-1}_{\mathbf{uv}}\end{pmatrix}, \qquad \Lambda = -\mathrm{i}\hbar\begin{pmatrix} -M^{-1}_{\mathbf{uv}} & 0\\ M_{\mathbf{vv}}M^{-1}_{\mathbf{uv}} & -1\end{pmatrix}. \tag{A.20}$$

Comparing linear terms of Eq. (A.16) with (A.6), we find

$$M = \begin{pmatrix} M_{\mathbf{uu}} & M_{\mathbf{uv}}\\ M_{\mathbf{vu}} & M_{\mathbf{vv}}\end{pmatrix} = \begin{pmatrix} -\tilde{S}^{-1}_{\mathbf{u}'\mathbf{u}''}\tilde{S}_{\mathbf{u}'\mathbf{u}'} & -\mathrm{i}\hbar\tilde{S}^{-1}_{\mathbf{u}'\mathbf{u}''}\\ (\mathrm{i}/\hbar)\left(\tilde{S}_{\mathbf{u}''\mathbf{u}''}\tilde{S}^{-1}_{\mathbf{u}'\mathbf{u}''}\tilde{S}_{\mathbf{u}'\mathbf{u}'} - \tilde{S}_{\mathbf{u}''\mathbf{u}'}\right) & -\tilde{S}_{\mathbf{u}''\mathbf{u}''}\tilde{S}^{-1}_{\mathbf{u}'\mathbf{u}''}\end{pmatrix} \tag{A.21}$$

or

$$\tilde{S}'' = \begin{pmatrix} \tilde{S}_{\mathbf{u}'\mathbf{u}'} & \tilde{S}_{\mathbf{u}'\mathbf{u}''} \\ \tilde{S}_{\mathbf{u}''\mathbf{u}'} & \tilde{S}_{\mathbf{u}''\mathbf{u}''} \end{pmatrix} = i\hbar \begin{pmatrix} M_{\mathbf{uv}}^{-1} M_{\mathbf{uu}} & -M_{\mathbf{uv}}^{-1} \\ -(M_{\mathbf{vv}} M_{\mathbf{uv}}^{-1} M_{\mathbf{uu}} + M_{\mathbf{vu}}) & M_{\mathbf{vv}} M_{\mathbf{uv}}^{-1} \end{pmatrix}. \tag{A.22}$$

Finally, comparing the quadratic terms,

$$\begin{aligned} \frac{1}{2}\Lambda_{ik}^{-1} w_k &= \frac{1}{2}\Lambda_{ij}^{-1} L_{nk}\delta r_k \tilde{S}'''_{nmj} L_{ml}\delta r_l \\ &\equiv \delta r_k U_{kli}\delta r_l \end{aligned} \tag{A.23}$$

or

$$\frac{1}{2}\Lambda_{ij}^{-1} L_{nk}\tilde{S}'''_{nmj} L_{ml} = U_{kli}. \tag{A.24}$$

Solving for the third derivatives of $\tilde{S}$ produces

$$\tilde{S}'''_{ijk} = 2L_{mi}^{-1}\Lambda_{kn} U_{mln} L_{lj}^{-1}, \tag{A.25}$$

where Λ and L^{-1} are given by (A.20).

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