Systematic elimination of Stokes divergences emanating from complex phase space caustics

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Stokes phenomenon refers to the fact that the asymptotic expansion of complex functions can differ in different regions of the complex plane, and that beyond the so-called Stokes lines has an unphysical divergence. An important special case is when the Stokes lines emanate from phase space caustics of a complex trajectory manifold. In this case, symmetry determines that to second order there is a double coverage of the space, one portion of which is unphysical. Building on the seminal but laconic findings of Adachi, we show that the deviation from second order can be used to rigorously determine the Stokes lines and therefore the region of the space that should be removed. The method has applications to wavepacket reconstruction from complex valued classical trajectories. With a rigorous method in hand for removing unphysical divergences, we demonstrate excellent wavepacket reconstruction for the Morse, Quartic, Coulomb and Eckart systems.

Keywords: semiclassics, complex trajectories, caustics, Stokes phenomenon

Introduction

Classical mechanics exhibits caustics, i.e. the focusing or coalescence of phase space trajectories when projected onto coordinate, momentum or any mixed subspace. For real trajectories, this phenomenon is well understood [1][3] but in complex classical dynamics fundamental questions remain unanswered. Extending the notion that caustics are stationary points of real trajectory manifolds, Adachi [4] and Rubin and Klauder [5] noted that caustics are second order saddle points of the complex trajectory manifold. Unlike in purely real dynamics, an unphysical type of divergence arises in extended regions of the trajectory manifold that is connected to the caustics. This type of divergence is called Stokes phenomenon, and the so-called Stokes lines, which emanate from the caustics in the complex space, define the boundary of the divergent contribution. [6][7].

Stokes divergences are a major obstacle in semiclassical wavepacket propagation methods that employ complex trajectories. Significant progress has been made towards eliminating such divergences in discrete time systems based on Adachi’s work on the Principle of Exponential Dominance (PED) [4][8][9][10]. However the PED requires comparison of trajectory pairs which can only be found numerically via a root search in the complex trajectory manifold. In continuous time dynamics such a root search is quite challenging and has been successful so far only for relatively short times [5][11][13]. Long time dynamics where the trajectory manifold is plagued by a multitude of caustics, remains elusive.

In this Communication, we provide a practical and rigorous procedure for removing Stokes divergences in continuous time complex trajectory manifolds. Building on the seminal but laconic work of Adachi, we perform a local expansion around the caustics. We show that the deviation from symmetry beyond second order can be used to rigorously determine the position of the Stokes lines and therefore the divergent region of the space that should be removed. Combining the method with the final value coherent state propagator (FINCO) approach [13] we calculate wavepacket dynamics for the Morse, Quartic, Coulomb and Eckart systems in excellent agreement with the quantum results.

Double-valuedness in the neighborhood of caustics

Consider a complex valued Lagrangian manifold of initial conditions, \( p_0(\nu), q_0(\nu) \in \mathbb{C} \) at time \( t_0 \), where \( \nu \) is the manifold label. An important example is the (possibly non-linear) manifold determined through a complex function \( S(\nu) \) by \( q_0(\nu) = \nu, p_0(\nu) = \frac{\partial S(\nu)}{\partial \nu} |_{\nu=\nu} \). This manifold is propagated using Hamilton’s equations of motion leading to the manifold \( p_t(\nu), q_t(\nu) \in \mathbb{C} \) at time \( t \). Choosing parameters \( \alpha, \beta \in \mathbb{C} \), we define a map \( \xi(\nu) \):

\[
\xi(\nu) = \alpha q(\nu) + \frac{1}{\hbar} \beta p(\nu) .
\]

For example \( \alpha = 1, \beta = 0 \) defines a map onto coordinate space at time \( t \).

The map Eq. \( \xi \) has a caustic at \( \nu^* \) if

\[
\xi^{(1)}(\nu^*) \equiv \left. \frac{d\xi(\nu)}{d\nu} \right|_{\nu=\nu^*} = 0 .
\]

Such locations always exist independent of \( \alpha \) and \( \beta \) if the manifold \( p_t(\nu), q_t(\nu) \) is a nonlinear function of \( \nu \). Higher order caustics may also exist but will not be considered in this Communication.

Since \( \xi^{(1)}(\nu^*) = 0 \), the function \( \xi(\nu) \) is locally quadratic at the caustic, \( \xi(\nu) = \xi(\nu^*) + \frac{1}{2} \xi^{(2)}(\nu^*)(\nu - \nu^*)^2 + O((\nu - \nu^*)^3) \). This implies the existence of values \( \nu_1, \nu_2 \) in the vicinity of \( \nu^* \) for which \( \xi(\nu_1) = \xi(\nu_2) \), i.e. \( \xi(\nu) \) is a double cover near \( \nu^* \) [4][12]. Conversely, the inverse function \( \nu(\xi) \) is double valued near \( \xi^* = \xi(\nu^*) \).

Consider a function \( L(\xi) \) defined through the trajectory manifold in the form

\[
L(\xi) = \sum_j \phi_j(\xi(\nu_j)) e^{\sigma_j(\xi(\nu_j))} ,
\]

where \( \phi_j(\nu) \) and \( \sigma_j(\nu) \) are complex valued and the sum is over all trajectories in the manifold for which \( \xi(\nu_j) = \xi \).
Since the trajectory manifold $\xi(\nu)$ is a double cover in the vicinity of a caustic, the sum in Eq. (3) for a given $\xi$ contains two terms corresponding to the manifold labels $\nu_1$ and $\nu_2$. Sums of the form Eq. (3) occur in semiclassical expressions for the quantum mechanical propagator where the sum is over root trajectories, [16], as well as in semiclassical methods for calculating wavepacket evolution [12, 13, 17, 19]

**Stokes divergences** Since each of the two classical trajectories represents a distinct root trajectory, the dependence of $\{\sigma_1, \nu_1\}$ and $\{\sigma_2, \nu_2\}$ on $\xi$ and $\nu$ may be very different globally. Specifically, in regions of the complex $\xi$ plane where the saddle point approximation used to obtain Eq. (3) is invalid, unphysical divergences of $\phi(\xi) e^{\sigma_1(\xi)}$ may appear, known as Stokes phenomenon. This convergence of the validity of the approximation [8, 17] can be characterized by the difference of the exponents of the two terms

$$F(\xi) = \sigma_1(\xi) - \sigma_2(\xi). \quad (4)$$

Starting from a central point $\xi^*$ where $F(\xi^*) = 0$, the surrounding space is divided into sectors by the Stokes lines, the locus of points where $\Im F(\xi) = 0$, and the anti-Stokes lines, the locus of points where $\Re F(\xi) = 0$, [19]. By definition, on the anti-Stokes lines $\Re \sigma_1 = \Re \sigma_2$ and thus the exponential part of the two terms in Eq. (3) is of equal magnitude $|e^{\sigma_1}| = |e^{\sigma_2}|$. On the Stokes lines, on the other hand, $\Im \sigma_1 \neq \Im \sigma_2$ and the exponential parts $e^{\sigma_1}$ and $e^{\sigma_2}$ are of equal phase but differ in magnitude.

If one of the contributions to Eq. (3) diverges unphysically in a certain region of the complex $\xi$ plane, this contribution needs to be excluded and the sum in Eq. (3) is reduced to the other term. The most straightforward way to eliminate the Stokes divergence is simply to discard trajectories with $\Re \sigma(\xi) > 0$, corresponding to the invalid complex integration contour [11, 20]. However, simply removing trajectories with $\Re \sigma(\xi) > 0$ leads to inaccurate numerical results, due to the rapidly fluctuating phase $e^{i\Im \sigma(\xi)}$ at the boundary $\Re \sigma(\xi) = 0$. A number of criteria have been proposed to remove divergences based on the value of $\sigma(\xi)$ or components thereof [11, 12, 15, 20], but these are empirical at best and do not lead to satisfactory results for long time propagation.

Adachi [11] observed that a divergent region of the complex $\xi$ plane contains a Stokes line where $\Re \sigma_2(\xi)$ is maximal and $\Re \sigma_1(\xi)$ is minimal. He noted that removing all trajectories up to the neighboring Stokes lines on either side, where $\Re \sigma_2(\xi)$ is minimal and $\Re \sigma_1(\xi)$ is maximal, results in minimum discontinuity because the removed contribution $e^{\sigma_2(\xi)}$ is masked by the exponentially larger term $e^{\sigma_1(\xi)}$ at the Stokes line. The discontinuity can be removed entirely by using Berry’s smoothing factor $S(F(\xi)) = \text{erf} \left\{ \frac{\Im F(\xi)}{\sqrt{2\Im F(\xi)}} \right\}$, derived from asymptotic analysis [21];

$$\tilde{\phi}(\xi) = \phi_1(\xi) e^{\sigma_1(\xi)} + S(F(\xi)) \phi_2(\xi) e^{\sigma_2(\xi)} \quad (5)$$

where $\text{erf}(\tau) = \frac{2}{\sqrt{\pi}} \int_{-\infty}^{\tau} ds e^{-s^2}$ is the error function. As illustrated below in Fig. 2, in Berry’s procedure trajectories are removed completely only from the divergent Stokes line to the adjacent anti Stokes lines followed by a continuous transition from excluded to included in the neighboring anti Stokes sector.

Below we combine Adachi’s removal of the diverging contribution with Berry’s smoothing factor. But the procedure requires knowing the location of the Stokes lines. A brute force approach is to use a root search to determine for each trajectory $\nu_1, \xi(\nu_1)$ its conjugate trajectory $\nu_2$ fulfilling $\xi(\nu_1) = \xi(\nu_2)$, from which one can locate the Stokes lines. This procedure was apparently applied in Refs. [8, 9, 13, 14, 22], but becomes cumbersome for long propagation times as the number of caustics proliferates [9]. The main achievement of this paper is to provide a practical procedure to locate the boundary between included and excluded contributions. This is the subject of the next section.

**Systematic elimination of the Stokes divergence by identifying the double cover** A much more efficient approach to eliminate the Stokes divergence exploits an analytic expansion of the Stokes variable $F$ in terms of $\nu$ and $\xi$. This expansion provides $F(\xi)$ without the need to search for conjugate trajectories.

The condition for the double cover $\xi(\nu_1) = \xi(\nu_2)$ implicitly defines a relationship $\nu_2(\nu_1)$ for the conjugate manifold label $\nu_2$. Combining $\nu_2(\nu_1)$ with the map $\xi(\nu)$, we transform the Stokes variable from $\xi$ space to $\nu$ space

$$F(\nu_1) = \sigma(\nu_1) - \sigma(\nu_2(\nu_1)) \quad (6)$$

Whereas previously it was necessary to distinguish between $\sigma_1(\xi)$ and $\sigma_2(\xi)$ since $\xi(\nu)$ is a double cover, as a function of $\nu$, $\sigma(\nu)$ is single-valued.

Since $\sigma(\nu)$ and $\xi(\nu)$ are single-valued functions, we can use their Taylor expansions at the caustic $\nu^*$ to construct an approximation to Eq. (6) and determine Stokes lines and anti Stokes lines from that. Without loss of generality, in the following we will assume $\nu^* = 0$ and $\xi(\nu^*) = 0$.

The first step is to obtain an explicit form for the conjugate point $\nu_2(\nu_1)$. Since $\xi(\nu)$ is a double cover in the vicinity of the caustic, a straightforward inversion is impossible. Instead, we note that the second order Taylor expansion $\xi(\nu(\nu))$ is symmetric. Thus we define the estimate conjugate label $\nu^\prime = -\nu_1$, and obtain corrections to that estimate using a local inversion of $\xi(\nu)$ at $\nu^\prime$. The approach is illustrated in Fig. 1.

The conjugate point $\nu_2$ follows from the Taylor expansion of $\nu(\xi)$ (the inverse of $\xi(\nu)$) at $\xi^\prime \equiv \xi(\nu^\prime)$

$$\nu_2(\nu_1) = \nu^\prime + \sum_{i=1}^{\infty} \frac{\nu^{(i)}(\xi^\prime)}{i!} (\Delta \xi(\nu_1))^i , \quad (7)$$

where the deviation $\Delta \xi(\nu_1)$ is defined as:

$$\Delta \xi(\nu_1) = \xi(\nu_1) - \xi(\nu^\prime) = \frac{\xi^{(3)}(\nu^\prime)}{3} \nu_1^3 + \mathcal{O}(\nu_1^5). \quad (8)$$
The derivatives of the inverse $\nu^{(i)}(\xi')$ are obtained from the derivatives of the Taylor series evaluated at $\nu'$

$$\xi^{(i)}(\nu') \equiv \left. \frac{d^i \xi(\nu)}{d\nu^i} \right|_{\nu=\nu'} = \sum_{j=i}^{\infty} \frac{\xi^{(j)}(\nu)^*}{(j-i)!} (\nu' - \nu)^{j-i}$$

by applying the chain rule to the identity $\nu = \xi^{-1}(\xi(\nu))$. As an example, the first two of these evaluate to

$$\nu^{(1)}(\xi') = -[\xi^{(1)}(\nu') - \xi^{(2)}(\nu')]^{-1}$$

and

$$\nu^{(2)}(\xi') = -\frac{\xi^{(2)}(\nu') + O(\nu_1^2)}{[\xi^{(2)}(\nu') + O(\nu_1^2)]^3}.$$  

Note that the derivatives of the inverse involve the inverses of the derivatives. Inserting Eqs. (10) and (8) into Eq. (7) and re-expanding the quotients in terms of $\nu_1$ yields

$$\nu_2(\nu_1) = -\nu_1 + \varrho \nu_1^2 - \varrho^2 \nu_1^3 + O(\nu_1^4)$$

with $\varrho = -\xi^{(3)}(\nu^*) / 3\xi^{(2)}(\nu^*)$.

The second step is to insert Eq. (11) and the Taylor series of $\sigma(\nu)$ into Eq. (6) and we obtain the final result, the phase space caustic Stokes expansion (PCSE) in terms of the manifold label

$$F(\nu_1) = F^{(3)}(\nu_1^3) + O(\nu_1^4),$$

where $F^{(3)} = \frac{1}{2} \sigma^{(3)}(\nu^*) + \sigma^{(2)}(\nu^*) \varrho$.

Before discussing the use of $F(\nu_1)$ for locating Stokes lines, we describe some of its properties.

a) Assuming that $\sigma(\nu)$ has no explicit $\nu$ dependence, its first derivative $\sigma^{(1)}(\nu^*) = \frac{\partial \sigma(\xi)}{\partial \xi} \xi^{(1)}(\nu^*)$ vanishes because by definition Eq. (2), at the caustics $\xi^{(1)}(\nu^*) = 0$ vanishes. Moreover, due to the symmetry of $\sigma(\nu_1)$ and $\xi(\nu_1)$, Eq. (6) vanishes up to second order.

b) The dominant term in Eq. (12) is of third order. Hence there are six lines emanating from $\nu^*$ where $3F = 0$. In $\xi$ space, this leads to three Stokes lines enclosing angle $\frac{2\pi}{3}$. This term appears in a comment in Ref. [4] without derivation but correctly identifying the three Stokes lines.

c) The third order coefficient $F^{(3)}$ critically depends on the correction $\varrho \nu_1^2$ to the estimate $\nu' = -\nu_1$ in Eq. (11). Without it (equivalent to setting $\varrho = 0$), the direction of the Stokes lines predicted by Eq. (12) will be incorrect.

d) Due to symmetry, third order information at the caustic, i.e. $\xi^{(i)}(\nu^*), \sigma^{(i)}(\nu^*), i \in \{2, 3\}$ is sufficient for a fourth order accurate approximation. The fourth order coefficient is $F^{(4)} = -\frac{2}{3} \varrho^{(3)}(\nu^*)$.

e) The expansion in terms of the manifold label $\nu_1$ was derived using the expansion of $\xi(\nu)$ at the caustic. It turns out that for long propagation times and trajectories far from the caustic, it is more accurate to expand in terms of $\nu(\nu_1) = \pm \xi(\nu_1) = \xi(\frac{1}{2} \xi(\nu))^{1/2}$

$$\tilde{F}(\nu_1) = F^{(3)}(\nu_1)^3 + O(\nu^5)$$

with the sign of $\nu$ chosen such that $|\nu(\nu_1) - \nu_1|$ is minimal. The geometric interpretation of $\nu$ is given in Fig. 7.

With Eq. (13) in hand, the following procedure removes Stokes divergences from the trajectory manifold without the need to find conjugate trajectories (dropping the subscript of $\nu_1$).

a) Construct the initial manifold $p_0(\nu), q_0(\nu)$.

b) Propagate to $p_t(\nu), q_t(\nu)$ and compute the final phase space map $\xi(\nu)$, the prefactors $\phi(\nu)$ and exponents $\sigma(\nu)$, and the stability matrix elements $M_{ab} = \frac{\partial \phi(\nu)}{\partial \nu_a} \phi(\nu)$ with $a, b \in \{p, q\}$.

c) Locate the caustics in the manifold as the roots of

$$d\xi(\nu) = (\alpha M_{qp} + \beta M_{pp}) \frac{\partial \sigma}{\partial \nu} + (\alpha M_{qq} + \beta M_{pq}) \frac{\partial \sigma}{\partial \nu}.$$  

for each caustic $\nu^*$.

i) Compute $\xi^{(i)}(\nu^*), \sigma^{(i)}(\nu^*), i \in \{2, 3\}$ via finite differencing with trajectories near $\nu^*$.

ii) Split the manifold into six sectors along the anti Stokes lines $\Re F(\xi(\nu)) = 0$. (See Fig. 2)

iii) Remove the sector that contains the Stokes line $\Im F(\xi(\nu)) = 0$ along which $\Re F(\nu) > 0$ diverges.

iv) Multiply all trajectory contributions $\phi(\nu) e^{\sigma(\nu)}$ in the two adjacent sectors by the Berry factor $S(F(\xi(\nu)))$ according to Eq. (5).

Application to wavepacket reconstruction. We illustrate this procedure by using it for wavepacket reconstruction in the context of the final value coherent state propagator method (FINCO) [15]. The initial manifold is derived from the analytic continuation of a wavefunction $\psi_0(x)$ according to $q_0(\nu) = \nu$ and $p_0(\nu) = \sigma(\nu)$.
In FINCO, a time evolved wavepacket is computed using a Gaussian basis \( g_{\gamma}(x, \xi) \) with \( \gamma = \frac{1}{2} \) (analogous to Eq. (16)) with coefficients given by Eq. (3)

\[
\psi_{\gamma}(x) = -\frac{1}{4\pi\gamma} \int d\xi g_{\gamma}(x, \xi) L(\xi) .
\]  

The sum over trajectories in \( L(\xi) \) is accounted for by transforming to \( \nu \) space

\[
\psi_{\gamma}(x) = -\frac{1}{4\pi\gamma} \int d\nu |J(\nu)| g_{\gamma}(x, \xi(\nu)) \phi(\nu) e^{i\sigma(\nu)} ,
\]

with the Jacobian \( |J(\nu)| = |\xi^{(1)}(\nu)|^{\frac{1}{2}} \) and prefactor \( \phi(\nu) = (8\gamma\pi)^{-\frac{1}{2}} [\xi^{(1)}(\nu)]^{-\frac{1}{2}} \) where \( \xi^{(1)}(\nu) \) is given by Eq. (14). The exponent \( \sigma(\nu) \) is defined in Eq. (15). For more details see Refs. 15, 20.

Trajectory based wavepacket reconstructions are compared with quantum results in Fig. 3. The initial wavepackets Eq. (16) with width \( \gamma_{0} = \frac{1}{2} \) are propagated for three classical periods of oscillation in the Morse, Quartic and Coulomb potentials and for about 1.5 times the classical turning point time in the Eckart potential. Potential functions and system parameters are given in Table I. The quality of the reproduction is semi-quantitative throughout.

Note that for the Morse, Coulomb and Eckart systems, imaginary time contour propagation is required to obtain all relevant contributions 14, 20, 24. A separate publication will give more details of the implementation and the phase space geometry of the caustics in the four prototypical potentials.

In summary, the present paper provides a practical and rigorous way to remove Stokes divergences emanating from caustics in complex trajectory manifolds. Besides its inherent conceptual interest it opens the door to accurate, longtime wavepacket propagation using complex valued classical trajectories.

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FIG. 3. Trajectory based wavefunctions (solid, green) and numerical quantum results (dashed, blue) at time $t = 3T_{cl}$ in a) Morse, b) Quartic and c) Coulomb potential. For the Eckart barrier d), only the transmitted part of the wavepacket is shown enlarged by a factor of 10 at $t \approx 1.5T_{cl}$. For parameters see Table I.

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