Flux continuity and probability conservation in complexified Bohmian mechanics

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Recent years have seen increased interest in complexified Bohmian mechanical trajectory calculations for quantum systems as both a pedagogical and computational tool. In the latter context, it is *essential* that trajectories satisfy probability conservation to ensure they are always guided to where they are most needed. We consider probability conservation for complexified Bohmian trajectories. The analysis relies on time-reversal symmetry considerations, leading to a generalized expression for the conjugation of wave functions of complexified variables. This in turn enables meaningful discussion of complexified flux continuity, which turns out *not* to be satisfied in general, though a related property is found to be true. The main conclusion, though, is that even under a weak interpretation, probability is *not* conserved along complex Bohmian trajectories.

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I. INTRODUCTION

Trajectory interpretations of quantum mechanics have been of interest since the earliest days of quantum theory. Indeed, they even predate the Schrödinger equation itself—as one finds, e.g., by considering the Bohr-Sommerfeld quantization rule. Although the latter was discovered to be an incorrect description of quantum theory, it survives today in the form of the Jeffrey-Wentzel-Kramers-Brillouin (JWKB) approximation, or more generally, semiclassical mechanics [1]. In this approach, a time-evolving quantum pure state is treated as a statistical ensemble of classical trajectories that "carry" approximate quantum information—i.e., complex amplitudes. There are many reasons, both pedagogical and practical, why semiclassical and even classical trajectory methods may be regarded as beneficial. Surely, though, one of these must be the fact that the differential probability $\rho(x)dx$ is *conserved* along any given trajectory—a well-known property of classical statistical ensembles. This alone ensures that the ensemble trajectories travel to where they are "most needed"—i.e., to where the probability density is largest—a consideration that is especially important for localized wave packet propagation in the limit of large system dimensionality.

Starting with Madelung in the same year as the Schrödinger equation itself [2] (based on matter wave ideas of de Broglie) and evolving into a full-fledged interpretation of quantum theory with Bohm in the early 1950s [3,4], an *exact* trajectory formulation of quantum mechanics was also developed. Over the ensuing decades, the resultant "Bohmian mechanical" trajectory ensembles have been relied upon to provide interpretational or "analytical" insight into previously solved time-dependent quantum wave packet propagation problems, such as the fundamental double-slit experiment [5–9]. More recently, innovations spearheaded by members of the chemical physics community have led to the use of quantum trajectory methods (QTMs) as a "synthetic" tool—i.e., to solve the time-dependent Schrödinger equation (TDSE) itself [10–12].

Though it is of great interest to compare and contrast the behavior of quantum trajectories with their classical counterparts, we shall do so here only as it relates to the present goals, as a detailed discussion would take us too far afield. Most important in the present context is the fact that Bohmian quantum trajectories *also* satisfy probability conservation [Eq. (9)]—an extremely beneficial property for the "synthetic" application of QTMs, and again, a chief reason for their utility. On the other hand, standard Bohmian mechanical trajectories—which we shall henceforth refer to as "real-valued Bohmian trajectories" for reasons that will become clear—suffer from certain apparent drawbacks as well, some of which can cause severe numerical difficulties for the synthetic approach [10]. In particular, for nondegenerate stationary states, all quantum trajectories are stationary fixed points—in stark contrast to the corresponding classical trajectory orbits.

To circumvent the above problems, one approach is to follow the semiclassical prescription of adopting a multipolar expansion of the wave function Ψ [13,14]. This leads to a correspondence between individual (real-valued) quantum and classical trajectories in the classical limit. A second approach, the focus of the present paper, involves a different generalization of Bohm's original prescription—i.e., allowing the coordinates x and trajectory velocities v to take on complex values. The resultant "complex-valued Bohmian trajectories" offer certain advantages; for instance, they are known not to be fixed-points, in general, for nondegenerate stationary states, so that it is possible to achieve nontrivial trajectory dynamics in this context. Although complex-valued Bohmian mechanics may still be in its infancy, interest has grown tremendously in the last few years [1,9,15–32]. The field appears to have started in the 1980s with a paper by Leacock and Padgett [15] and a less well known (and very brief) article by Tourenne [16]. More recent authors have explored the complex Bohmian approach both for time-independent (stationary) and time-dependent (wave packet propagation) problems, in both analytical and synthetic contexts [17–32].

Remarkably, the all-important *issue of trajectory probability conservation does not yet appear to have been addressed* in the literature. Yet as stated previously, this is an

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essential requirement if the complex-valued synthetic TDSE methods currently under development are to have general utility for systems larger than two or three dimensions d. These methods *already* require special root-finding procedures to single out the subset of complex trajectories that happen to arrive on the d-dimensional real "axis" x at a desired final time t_f—since at other times, this trajectory ensemble is described by some nontrivial d-dimensional manifold embedded in the $2d$-dimensional complex coordinate space. Alternatively, one could in principle avoid the root search by simultaneously propagating trajectories over the entire complex coordinate space, but only at the expense of doubling the dimensionality of the trajectory ensemble space and thus enormously increasing the required number of trajectories to compute. Such an approach would be highly redundant from an information theory perspective, but perhaps feasible—much like coherent-state representations [1].

Though daunting, it may be possible to overcome the above "d-doubling problem" [31] for large systems, but *only* if complex quantum trajectories turn out to satisfy probability conservation, at least approximately. This paper thus considers the issue of probability conservation for complexified Bohmian trajectories. The analysis ultimately relies on time-reversal symmetry considerations, leading to a generalized definition of the conjugation operation for functions of complexified variables, which in turn leads naturally to a discussion of complexified flux continuity and probability conservation. Analytical properties of complex trajectory dynamics are then considered, and finally, several $d=1$ examples are discussed.

II. BACKGROUND

Real-valued Bohmian mechanics begins with the Madelung-Bohm ansatz for the wave function [2–4],

$$\Psi(x,t) = R(x,t)e^{iS(x,t)/\hbar}. \tag{1}$$

The decomposition above is essentially unique, by virtue of the fact that R and S are taken to be real valued and $R>0$. By substituting Eq. (1) into the TDSE and gathering real and imaginary terms separately, one obtains the following two real-valued equations:

$$\frac{\partial R}{\partial t} = \frac{-1}{2m}(2R'S' + RS''), \tag{2}$$

$$\frac{\partial S}{\partial t} = -\left[\frac{S'^2}{2m} + V - \frac{\hbar^2}{2m}\frac{R''}{R}\right], \tag{3}$$

where the primes denote spatial differentiation. Equation (3) is the "quantum Hamilton-Jacobi equation" [3], which imparts a classical-field-theory-like [33] interpretation to quantum wave packet propagation, provided that (a) $S'(x,t)$ is interpreted as trajectory momentum and (b) an additional "quantum potential" $Q(x,t)=-(\hbar^2/2m)(R''/R)$ is added to the true potential $V(x)$ to determine the trajectory dynamics.

Equation (2) is the flux continuity equation, which under the above interpretations is identical to trajectory probability conservation. In particular, Eq. (2) can be rewritten as

$$\frac{\partial \rho(x,t)}{\partial t} = -j'(x,t), \tag{4}$$

where

$$\rho(x,t) = R^2(x,t) \text{ is the probability density}, \tag{5}$$

$$j(x,t) = \rho(x,t)v(x,t) \text{ is the probability flux}, \tag{6}$$

$$v(x,t) = S'(x,t)/m \text{ is the trajectory velocity}. \tag{7}$$

Note that the flux $j(x,t)$ above accords with the usual quantum definition—i.e.,

$$j = \frac{\hbar}{2im}(\Psi^*\Psi' - \Psi'^*\Psi). \tag{8}$$

Note also that the flux is independent of potential energy as is reasonable; i.e., $V(x)$ enters *only* into the dynamical equation for trajectory evolution, Eq. (3). In any case, Eq. (4) implies conservation of differential probability along a trajectory—i.e.,

$$\frac{d[\rho(x,t)dx]}{dt} = 0, \tag{9}$$

where d/dt refers to the total (hydrodynamic) time derivative. For simplicity, the above equations have been written as if the dimensionality is $d=1$, but they are meant to refer also to the multidimensional case, as the $d>1$ generalizations are straightforward.

In complex Bohmian mechanics, an altogether different ansatz is employed:

$$\Psi(x,t) = e^{iS(x,t)/\hbar}. \tag{10}$$

In effect, the real-valued amplitude R of the decomposition of Eq. (1) is "subsumed" into the exponent to form the imaginary part of the now-*complex*-valued action, S. Substitution into the TDSE now yields the *single*, complex-valued equation

$$\frac{\partial S}{\partial t} = -\left[\frac{S'^2}{2m} + V - \frac{i\hbar}{2m}S''\right], \tag{11}$$

which can be interpreted as a complex quantum Hamilton-Jacobi equation. Equation (11) is the starting point for the quantum Hamilton-Jacobi formalism, regarded as one of the nine fundamental formulations of quantum mechanics [15,18,34].

Unlike the real-valued equation (3), Eq. (11) contains *all* of the information present in Ψ, leading some authors to conclude that the complex version is the more fundamental [18]. On the other hand, in going from real- to complex-valued formulations we have apparently lost the flux continuity relation altogether. Thus, if there is indeed a probability conservation property for complex trajectories, it is neither manifest in, nor independent from, Eq. (11). Note that in certain contexts, it is possible to extract a complex energy-momentum conservation relation from Eq. (11) [18,35]. However, this is not directly useful for synthetic applications in relation to the guidance of trajectories to high-probability regions where they are needed most.

III. COMPLEXIFICATION: TIME-REVERSAL SYMMETRY AND GENERALIZED COMPLEX CONJUGATION

To make progress with regard to probability conservation, it seems clear that Eq. (11) must be written in a different, but mathematically equivalent, form. In comparing Eq. (1) to Eq. (10), which emphasizes the action S over amplitude R, it seems clear that the opposite procedure should be applied to emphasize the latter; i.e., the real-valued S of Eq. (1) should be "pulled down" from the exponent to form a complex-valued amplitude R. But this would simply yield Ψ itself as the appropriate quantity to work with. Thus, the TDSE in its standard form (i.e., in terms of Ψ) should be a reasonable starting point for analyzing flux continuity—albeit a *complexified* version, with $x \in \mathcal{R}$ replaced with $z \in \mathcal{C}$. Complexification of the TDSE *per se* offers no inherent difficulty provided that $V(x)$ and the initial wave packet $\Psi(x,t=0)$ are both analytic functions, as everything can then be uniquely lifted from the real x axis to the complex z plane in accordance with the usual rules of analytic continuation [36]. On the other hand, establishing a complexified probability density $\rho(z)$ does pose a bit of a problem, as the traditional definition $\rho(x)=\overline{\Psi(x)}\Psi(x)$ in terms of the conjugate function $\bar{\Psi}(x)=\Psi^*(x)=[\Psi(x)]^*$ is in general *not* analytic when x is replaced with z.

Two straightforward candidates for a complexified $\rho(z)$ quantity are presented below.

(i) Define $\rho(z)=\Psi^*(z)\Psi(z)$.

(ii) Define $\rho(z)$ as the analytic continuation of $\rho(x)$.

Option (i) has the presumed advantage that $\rho(z)$ is positive and real valued everywhere in the complex plane, but suffers from the severe drawback that $\rho(z)$ is not an analytic function. This approach is being considered by other authors [32]. Option (ii) offers analyticity, but yields complex-valued probability densities off of the real axis and bypasses the more fundamental issue of nonanalytic conjugate wave functions, which must still be resolved. Analyticity is an enormous advantage, for it means that familiar expressions such as $\int_{-\infty}^{+\infty}\rho(z)dz=1$ represent true contour integrations with path-independent meaning. Thus, integration contours may be deformed away from the real axis—which is especially important for synthetic TDSE applications, given that the contour is essentially the (time-evolving) trajectory ensemble manifold. In any case, complex probability values are likely unavoidable in complexified space, for even if the density $\rho(z)$ is real valued, the differential probability itself, $\rho(z)dz$, need not be.

We will resolve the matter by directly addressing the more general and fundamental issue of wave function conjugation on complexified spaces. One approach to this problem is to invoke charge–parity–time-reversal (CPT) symmetry [37]—an idea that was introduced previously in the specific context of non-Hermitian Hamiltonian operators [18,38,39]. Similar ideas can be applied in the present case of complexified Hermitian Hamiltonians, although for general potentials, only time-reversal symmetry is relevant. Let $\Psi(z,t)$ be a solution of the complexified TDSE ($z \in \mathcal{C}$, but $t \in \mathcal{R}$):

$$i\hbar\frac{\partial\Psi(z,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(z,t)}{\partial z^2} + V(z)\Psi(z,t). \tag{12}$$

Complex conjugating both sides and applying explicit time reversal, i.e., $t \to -t$, yields

$$i\hbar\frac{\partial[\Psi(z,-t)]^*}{\partial t} = -\frac{\hbar^2}{2m}\left[\frac{\partial^2\Psi(z,-t)}{\partial z^2}\right]^* + [V(z)]^*[\Psi(z,-t)]^*. \tag{13}$$

The above is the usual means of deriving the effect of the antiunitary time-reversal operator on a wave function for real-valued coordinates [37]. For the complexified case, however, it is clear that Eq. (12) is *not* equivalent to Eq. (13), because $[V(z)]^*=V^*(z)$ is not equivalent to $V(z)$ off of the real axis. Instead, we must introduce the additional and final step of replacing the coordinate z with its complex conjugate z^*. From the Schwartz reflection principle [36], $V^*(z^*)=V(z)$, because $V(x)$ is real valued. Thus,

$$i\hbar\frac{\partial\Psi^*(z^*,-t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi^*(z^*,-t)}{\partial z^2} + V(z)\Psi^*(z^*,-t), \tag{14}$$

so $\Psi^*(z^*,-t)$ is also a solution of the TDSE, the proper manifestation of time-reversal symmetry on the complexified space. Note that the final step above is also consistent with the approach of Hüber, Heller, and Littlejohn [40], which may be regarded as a semiclassical approximation to complexified Bohmian mechanics. In fact, there is a very close connection between the present approach and complex semiclassical mechanics, with the latter emerging as the first-order truncation of an infinite series expansion of the former, as elucidated by Goldfarb *et al.* [23–26].

Following the approach of Bender *et al.* [38,39], the corresponding conjugation operation is therefore

$$\overline{f(z)} = f^*(z^*) = g(z). \tag{15}$$

Note that along the real axis—i.e., $z=x$—Eq. (15) is equivalent to the standard conjugation operation. Most importantly however, we find that $f^*(z^*)$ is an *analytic function* in the original variable z, in that it satisfies the Cauchy-Reimann conditions [36]—unlike, say, $f(z^*)$ or $f^*(z)$. Equation (15) also satisfies the mathematical definition of a conjugate linear map [36], unlike $f(z^*)$ or $f^*(z)$. Note that $f^*(z^*)$ is *not* equivalent to $f(z)$ in general. We will therefore sometimes refer to $f^*(z^*)$ as "$g(z)$" to emphasize both its distinctness from $f(z)$ and also its analyticity. The latter property can be demonstrated explicitly from a Taylor expansion:

$$f(z) = \sum_{k=0}^{\infty} C_k z^k, \quad g(z) = \sum_{k=0}^{\infty} C_k^* z^k. \tag{16}$$

Having shown that $\overline{f(z)}$ is analytic, it follows trivially that the complexified inner product integration

$$\langle f|h\rangle = \int_{-\infty}^{+\infty} g(z)h(z)dz \tag{17}$$

is contour path independent, as the integrand itself is analytic [assuming analytic $h(z)$]. In particular, this implies that

$$\rho(z) = \overline{\Psi(z)}\Psi(z) \tag{18}$$

is analytic and, moreover, is equivalent to option (ii) described above.

Note that both $f(z)=V(z)$ and $f(z)=\rho(z)$ share the special property that $\overline{f(z)}=g(z)=f(z)$. This is nothing but the Schwartz reflection principle and is true whenever $f(z)$ is analytic and $f(x)$ is real. We find it convenient to refer to such a function as a RE function—even though it is understood that $f(z)$ is not real valued off of the real axis. Similarly, an IM analytic function $f(z)$ is defined such that $\overline{f(z)}=g(z)=-f(z)$ and is pure imaginary valued along the real axis, but not necessarily elsewhere. Any analytic function $f(z)$ can be decomposed into a sum of RE and IM parts, which we demonstrate via explicit construction:

$$f(z) = f_{\mathrm{RE}}(z) + f_{\mathrm{IM}}(z), \tag{19}$$

where

$$f_{\mathrm{RE}}(z) = \left[\frac{f(z)+f^*(z^*)}{2}\right],$$

$$f_{\mathrm{IM}}(z) = \left[\frac{f(z)-f^*(z^*)}{2}\right].$$

Note that $f_{\mathrm{RE}}(z)$ and $f_{\mathrm{IM}}(z)$ are themselves analytic—unlike, say, $\mathrm{Re}[f(z)]$ and $\mathrm{Im}[f(z)]$ (although $f_{\mathrm{RE}}(x)=\mathrm{Re}[f(x)]$, etc.) Note also that the analytic derivative $f'(z)=df(z)/dz$ of a RE (IM) function $f(z)$ is also RE (IM). Finally, the product of a RE and RE (or IM and IM) pair of functions is RE, whereas the product of RE and IM functions is IM.

IV. FLUX CONTINUITY AND PROBABILITY CONSERVATION

Our next goal is to define a complexified flux from which to derive a corresponding flux continuity relation. We start with the velocity field $v(z,t)$, which from Eqs. (7) and (10) is given by [15,17,18,23]

$$v(z,t) = -\frac{i\hbar}{m}\frac{\Psi'(z,t)}{\Psi(z,t)}. \tag{20}$$

In general, $v(z,t)$ is neither RE nor IM. Along the real axis, $v_{\mathrm{RE}}(x,t)$ is the "flow velocity" (i.e., the standard velocity field of real-valued Bohmian mechanics, closely related to hydrodynamics), whereas $v_{\mathrm{IM}}(x,t)$ is known as the "Einstein osmotic velocity," associated with wave packet spreading, or diffusion in stochastic quantum mechanics [10,41–43]. However, $v_{\mathrm{IM}}(x,t)$ is not used in the stochastic context to generate trajectories *per se* or otherwise venture off of the real coordinate axis. Hirschfelder *et al.* did use the imaginary velocity to create real-valued trajectories or "streamlines," but only along the real axis, by replacing t with it [44]. In complexified Bohmian mechanics, the imaginary velocity is directly responsible for transporting the complex trajectories off of the real axis. Of key significance for the present approach is that *both velocity components can be given significance off of the real axis*, due to the decomposition of Eq. (19) and the fact that $v_{\mathrm{RE}}(z,t)$ and $v_{\mathrm{IM}}(z,t)$ are analytic functions, provided $v(z,t)$ is (at least locally) analytic. Note that global analyticity of $\Psi(z,t)$ does not necessarily imply the same property for $v(z,t)$ (Sec. V).

The complexified flux is naturally defined from Eqs. (18) and (20), and the analytic continuation of Eq. (6), as

$$j(z,t) = v(z,t)\rho(z,t) = -\frac{i\hbar}{m}\Psi^*(z^*)\Psi'(z), \tag{21}$$

which, based on the multiplication rules given in Sec. III, is again neither RE nor IM. Note that the conjugation operation of Eq. (15) commutes with spatial differentiation—i.e., $[df(z^*)/dz^*]^*=g'(z)$, where $g(z)=f^*(z^*)$. Thus, the meaning of expressions such as the following is unambiguous:

$$j_{\mathrm{RE}}(z,t) = v_{\mathrm{RE}}(z,t)\rho(z,t)$$
$$= -\frac{i\hbar}{2m}[\Psi^*(z^*)\Psi'(z) - \Psi(z)\Psi'^*(z^*)], \tag{22}$$

$$j_{\mathrm{IM}}(z,t) = v_{\mathrm{IM}}(z,t)\rho(z,t)$$
$$= -\frac{i\hbar}{2m}[\Psi^*(z^*)\Psi'(z) + \Psi(z)\Psi'^*(z^*)]. \tag{23}$$

Note that along the real axis, $j_{\mathrm{RE}}(x,t)$ is equivalent to the usual real-valued quantum flux of Eq. (8). The imaginary flux $j_{\mathrm{IM}}(z,t)$, in contrast, does not appear to have been considered previously in the literature, even when restricted to the real coordinate axis. Off of the real axis, j and v point in different directions.

A flux continuity relation should presumably involve the divergence of the flux. From Eqs. (22) and (23) the RE and IM components are found to be

$$j'_{\mathrm{RE}}(z,t) = -\frac{i\hbar}{2m}[\Psi^*(z^*)\Psi''(z) - \Psi(z)\Psi''^*(z^*)], \tag{24}$$

$$j'_{\mathrm{IM}}(z,t) = -\frac{i\hbar}{2m}[\Psi^*(z^*)\Psi''(z) + \Psi(z)\Psi''^*(z^*) + 2\Psi'^*(z^*)\Psi'(z)]. \tag{25}$$

To relate the above to the time derivative of $\rho(z,t)$ as defined in Eq. (18) requires the time-derivative of $\overline{\Psi(z,t)}$. By replacing $t\to -t$ in Eq. (14), this is found to be

$$i\hbar\frac{\partial\overline{\Psi(z,t)}}{\partial t} = +\frac{\hbar^2}{2m}\overline{\Psi(z,t)}'' - V(z)\overline{\Psi(z,t)}. \tag{26}$$

Multiplying Eq. (12) by $-(i/\hbar)\overline{\Psi(z,t)}$ and adding to $-(i/\hbar)\Psi(z,t)$ times Eq. (26) then yields the complexified flux continuity relation

$$\frac{\partial \rho(z,t)}{\partial t} = -j'_{\mathrm{RE}}(z,t). \tag{27}$$

The above procedure is similar to that used to derive the real-valued flux continuity equation; however, it only works here by virtue of the Schwartz reflection principle. Indeed, a continuity relation based on *any* definition of $\Psi(z,t)$ other than Eq. (15) would result in a *flux quantity that depends on the potential energy*—a highly unphysical scenario that we reject out of hand.

On the other hand, the continuity relation of Eq. (27) involves only the RE component of flux, rather than $j(z,t)$ itself. This makes perfect sense when one considers that ρ itself is RE, and therefore its time derivative must also be RE. However, this has nontrivial ramifications in relation to probability conservation for complex trajectories generated from $v(z,t)$ rather than from, say, $v_{\mathrm{RE}}(z,t)$. We will have more to say on this topic in a moment, but first we point out some additional noteworthy aspects of Eq. (27). In particular,

$$\int_{-\infty}^{+\infty} \frac{\partial \rho(z,t)}{\partial z} dz = 0, \tag{28}$$

i.e., the total probability conservation property, which has a contour-path-independent meaning; it is in any event clear that integration of Eq. (24) along the real axis is zero. In the specific case of nondegenerate stationary states, one can further show that $\partial \rho(z,t)/\partial t = 0$ everywhere. Thus, even though ρ has a nontrivial complex phase off of the real axis, this phase does not evolve over time, so that $\rho(z,t)$ is truly stationary everywhere. Note that without loss of generality, $\Psi(z,t) = \psi(z)e^{-i\omega t}$ with $\psi(z)$ RE in this case, implying that

$$\rho(z,t) = [\psi(z)]^2. \tag{29}$$

Since the continuity relation in Eq. (27) is given in terms of $j_{\mathrm{RE}}(z,t) = v_{\mathrm{RE}}(z,t)\rho(z,t)$, it immediately follows via analytic continuation that $d[\rho(z,t)dz]/dt = 0$, provided the complex trajectories are obtained from $v_{\mathrm{RE}}(z,t)$ rather than $v(z,t)$. Along the real axis, the v_{RE} trajectories are just the standard real-valued Bohmian trajectories, so the orbit is the real axis itself. Off of the real axis, the $v_{\mathrm{RE}}(z,t)$ are quite nontrivial and might in principle be considered for dynamical purposes, with a ready-built trajectory probability conservation property. There are at least two drawbacks to this arrangement, however: (i) v_{RE} trajectories that start off of the real axis never intersect the real axis and (ii) nondegenerate stationary states still have $v_{\mathrm{RE}}(z,t) = 0$ everywhere in the complex plane. In any event, all of the previous literature on complexified Bohmian mechanics uses $v(z,t)$ rather than $v_{\mathrm{RE}}(z,t)$ trajectories. Note that for nondegenerate stationary states, $v(z,t) = v_{\mathrm{IM}}(z,t)$, so that *all* of the trajectory dynamics is due to the imaginary velocity in this case. Again, because $v_{\mathrm{IM}}(z,t)$ is not pure imaginary valued, this does *not* imply trivial "vertical" (parallel to imaginary axis) trajectory orbits in the complex plane. In general, stationary state orbits are vertical only where they intersect the real axis, about which the orbits display reflection symmetry; otherwise, they are quite arbitrary, often recrossing the real axis again at a different point (Sec. VI). The ground state of the harmonic oscillator system, for instance, is characterized by concentric circular orbits [10,17,18,20].

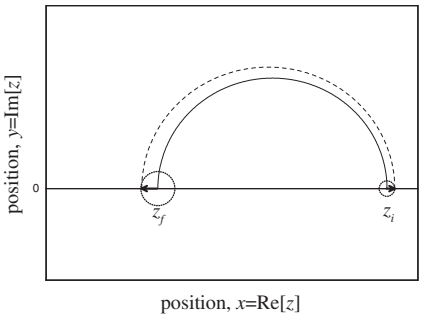

FIG. 1. Two closed complex trajectory orbits for a nondegenerate stationary state over half a period $\Delta t = T/2$. All units are atomic units. Solid curve denotes the main trajectory, starting at $(z_i = x_i, t_i)$ and ending at $(z_f = x_f, t_f)$. Dashed curve denotes neighboring trajectory, starting at $(x_i + dx_i)$. The function $f^{(t_i,t_f)}(z)$ maps z_i to z_f and the small differential circular disk $z_i + dz_i$ on the right to the small differential circular disk $z_f + dz_f$ on the left. Right and left arrows denote (directional) dx_i and dx_f intervals, respectively; note the change in sign.

For the more general case of nonstationary wave packet propagation, it is easily shown that $d[\rho(z,t)dz]/dt \neq 0$ in general, for trajectories obtained from $v(z,t)$. Thus, in a literal sense, probability conservation along trajectories is *not* satisfied. On the other hand, it might be argued that such a strong form of probability conservation should not be required. In particular, this relates to the fundamental question of how physical observables are to be interpreted in complexified space and how these relate to real measurements. The impression one derives from the literature is that observables are to have physical meaning *only* when evaluated along the real axis. On the other hand, a theory such as that presented here, which allows all quantities to be analytically continued, may shed additional light on this question, in that knowledge of said quantities along an essentially arbitrary d-dimensional manifold implies knowledge along the real axis.

Returning to the issue of probability conservation, if we presume that $\rho(z,t)dz$ has no direct physical meaning off of the real axis, then it may not be appropriate to impose Eq. (9) throughout the entire complex plane. Instead, let us imagine a particular $v(z,t)$ trajectory, $z(t)$, which crosses the real axis at time t_i and again at a later time t_f—i.e., $z(t_i) = x_i$ and $z(t_f) = x_f$ (Fig. 1). We stipulate on physical grounds that it should be sufficient to satisfy the following *weak* probability conservation condition:

$$\rho(x_i,t_i)dx_i = \rho(x_f,t_f)dx_f. \tag{30}$$

However, even Eq. (30) turns out not to be satisfied in general—even under the most favorable situation where Ψ is a nondegenerate stationary state and $v(z)$ is analytic.

V. ANALYTIC PROPERTIES AND TRAJECTORY DYNAMICS

To demonstrate that Eq. (30) is not satisfied, it is helpful to introduce the map $f^{(t_i,t_f)}(z_i) = z_f$, corresponding to the tra-

jectory that connects the initial point (z_i,t_i) to the final point (z_f,t_f) (Fig. 1). This in turn requires the trajectory guidance equation

$$\frac{dz}{dt} = v(z,t) = -\frac{i\hbar}{m}\frac{\Psi'(z,t)}{\Psi(z,t)}. \tag{31}$$

Regarded as a function of z_i, $f^{(t_i,t_f)}(z_i)$ is essentially a continuous composition of the generator map $v(z,t)$. Physically, it represents the effect of time evolution on the system, from the initial time t_i to the final time t_f, and is standard in classical field and semiclassical theories [1,33,45]. Note that the time evolution of $\Psi(z,t)$ is analogous to classical dynamics under a time-dependent potential, thus requiring *both* superscript time parameters t_i and t_f, rather than just the difference $\Delta t=(t_f-t_i)$.

If $v(z,t)$ is presumed to be analytic, at least locally in the vicinity of some given trajectory, then $f^{(t_i,t_f)}(z_i)$ will also be locally analytic. *Globally*, however, $f^{(t_i,t_f)}(z_i)$ is usually *not* analytic even if $v(z,t)$ itself is globally analytic, due to branch cuts that can arise in the function $f^{(t_i,t_f)}(z_i)$. In most cases—e.g., when $\Psi(x,t)$ has nodes—$v(z,t)$ is not (globally) analytic, but "meromorphic," meaning that it is globally analytic apart from a discrete set of simple poles [36]. In this case, also, $f^{(t_i,t_f)}(z_i)$ is usually not meromorphic itself (though it must have simple poles), but also exhibits branch cuts. The branch cuts delineate regions of the z_i domain that get mapped discontinuously under $f^{(t_i,t_f)}(z_i)$ to different regions of the range. In the trajectory interpretation, two initially nearby trajectories, starting differentially close to each other at t_i, but on either side of a branch cut, wind up far apart at t_f. The branch cuts themselves must therefore correspond to "separatrix"-type trajectory orbits (Fig. 2).

On the other hand, for trajectories sufficiently far from a separatrix or simple pole, $f^{(t_i,t_f)}(z_i)$ may be regarded as locally analytic. Consequently, points $z=z_i+dz_i$ lying within a differentially small circle centered at z_i get mapped under $f^{(t_i,t_f)}(z)$ to another differentially small disk of points $f^{(t_i,t_f)}(z_i+dz_i)=z_f+dz_f$, as in Fig. 1. Due to local analyticity [36], the ratio of differentials—i.e., dz_f/dz_i—is independent of the magnitude or direction of dz_i:

$$\frac{dz_f}{dz_i} = f^{(t_i,t_f)'}(z_i). \tag{32}$$

Thus, the spatial derivative function $f^{(t_i,t_f)'}(z_i)$ specifies how the differential volume element dz is transformed via trajectory evolution over the specified time interval. For a given initial point (z_i,t_i), we can, by varying $t_f=t$, obtain a transformed dz for every point along the $z(t)$ trajectory. In particular,

$$\frac{dz}{dz_i} = f^{(t_i,t)'}(z_i) = r^{(z_i,t_i)}[z(t)], \tag{33}$$

where it is understood that the trajectory $z(t)$ passes through (z_i,t_i). Note the new quantity $r^{(z_i,t_i)}[z(t)]$, which—though equivalent to $f^{(t_i,t)'}(z_i)$—is introduced so as to be regarded as a function of the *final* trajectory point $z(t)$ (at arbitrary time t), rather than the initial point z_i. Note also that $r^{(z_i,t_i)}(z_i)=1$.

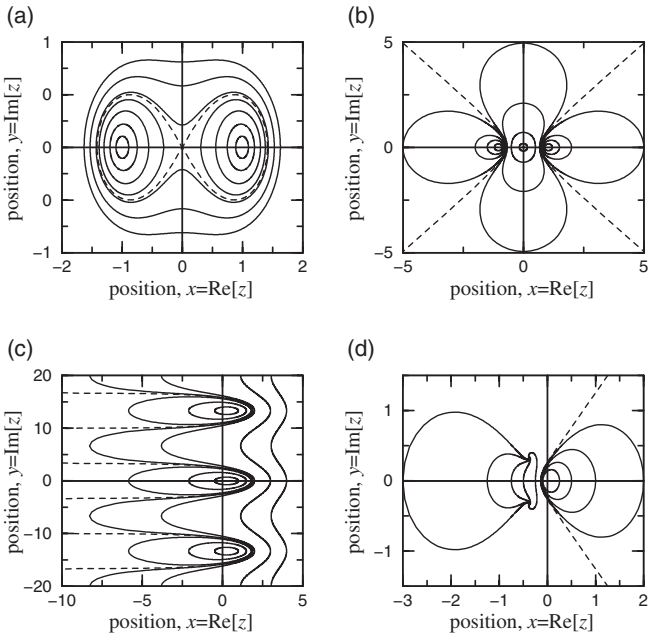

FIG. 2. Complex quantum trajectories for a representative sampling of one-dimensional nondegenerate stationary states for Hamiltonians of the form of Eq. (41). All units are atomic units. Dashed lines indicated separatrix trajectories, leading to branch cuts in the map $f^{T/2}(z)$. See text for additional discussion. Specific states are as follows: (a) system II, harmonic oscillator first excited state; (b) system III, symmetric double-peaked ground state; (c) system IV, Morse oscillator ground state; (d) system V, asymmetric single-peaked ground state.

For differentially small time increments $\Delta t=dt$, it can easily be shown using standard statistical or hydrodynamical arguments that $dz_f=[1+v'(z_i,t_i)dt]dz_i$ [10], implying that

$$\frac{dr^{(z_i,t_i)}[z(t)]}{dt} = v'[z(t),t]r^{(z_i,t_i)}[z(t)]. \tag{34}$$

The solution for $r^{(z_i,t_i)}[z(t)]$ is therefore found to be

$$r^{(z_i,t_i)}[z(t)] = \exp\left(\int_{t_i}^{t} v'[z(t'),t']dt'\right), \tag{35}$$

where the integration is along the trajectory.

The general global solution to Eq. (35) above is not straightforward; in particular, it is not apparent how to obtain $r^{(z_i,t_i)}$ values for (z,t) points off of the $z(t)$ trajectory. However, this is easily achieved for the specific case of nondegenerate stationary states, on which we will focus for the remainder of this paper. In this context, $v(z,t)=v(z)$ is independent of (final) time, and similarly, $r^{(z_i,t_i)}=r^{z_i}$ is independent of initial time, as appropriate for the resultant "time-independent potential" dynamics. A simple change of variables in Eq. (35) above then leads to

$$r^{z_i}(z) = \frac{v(z)}{v(z_i)}. \tag{36}$$

Since $v(z)=v_{\mathrm{IM}}(z)$ is pure IM, for trajectories initiating on the real axis, $z_i=x_i$, the function $r^{x_i}(z)$ is pure RE. Thus, whenever the trajectory $z(t)$ recrosses the real axis, at $(z_f=x_f,t_f)$, the initial real-valued volume element $dz_i=dx_i$ is transformed to a final volume element $dz_f=dx_f$ that is *also* real valued (Fig. 1)—a nontrivial but essential prerequisite for any relation of the same type as Eq. (30), since $\rho(x_i,t_i)$ and $\rho(x_f,t_f)$ are also real valued. In particular, we obtain

$$\frac{dx_i}{v_{\mathrm{IM}}(x_i)} = \frac{dx_f}{v_{\mathrm{IM}}(x_f)}. \tag{37}$$

However, it is not necessary to restrict oneself to x_f values that are connected to x_i via trajectories; in fact, the above relation is true for completely general values of x_i and x_f.

Substituting Eq. (20) into Eq. (37), and exploiting Eq. (29), we derive the following relation:

$$\frac{\rho(x_i)}{\rho'(x_i)}dx_i = \frac{\rho(x_f)}{\rho'(x_f)}dx_f. \tag{38}$$

Equation (38) above is similar to, but clearly distinct from, the desired probability conservation condition, Eq. (30). The latter is thus satisfied if and only if $|\rho'(x_i)|=|\rho'(x_f)|$, which—though not true in general—is true for the special case of symmetric analytic velocity fields $[v(-z)=-v(z)]$ with a single stationary point at the origin.

Note that for nondegenerate stationary states, $f^{(t_i,t_f)}(z_i)=f^{\Delta_t}(z_i)$ depends only the time interval Δ_t. It is of interest to relate $v(z)$ to $f^{\Delta_t}(z_i)$ via $r^{x_i}(z_f)$. With $z=z_i$ and $f=f^{\Delta_t}(z_i)=z_f$, one obtains

$$\frac{df}{dz} = r^{x_i}(z_f) = \frac{v(f)}{v(z)}, \tag{39}$$

$$w(f) = w(z) + \mathrm{const}, \tag{40}$$

where $w(y)$ is the integral $\int dy/v(y)$. Clearly, $w(y)$, and thus $f^{\Delta_t}(z)$, will not in general be globally analytic, even if $v(z)$ itself is.

The role of stationary points—i.e., z_0 such that $v(z_0)=0$—is important in trajectory dynamics. These occur where $\psi'(z)=0$—i.e., the non-node zeros of $\rho'(z)=0$. When $\psi(z)$ has nodes, it is easy to demonstrate that $v(z)$ has a simple pole at each node and is therefore meromorphic at best. Conversely, node-free analytic wave functions $\psi(z)$ can often lead to globally analytic velocity fields. In the vicinity of nodes, $v(z)$ directs initially neighboring trajectories to very different final destinations, thus leading to separatrix-like trajectories and branch cuts in $f^{\Delta_t}(z)$ (Fig. 2). However, unlike separatrix orbits in classical phase space, $v(z)$ does not approach zero as the node is approached—because the poles are not themselves stationary points. Note that separatrix-like trajectories, and associated $f^{\Delta_t}(z)$ branch cuts, can arise even when $v(z)$ is globally analytic (Sec. VI).

In the neighborhood of stationary points, one can apply the standard velocity field linearization method [45] to determine the behavior of neighboring trajectories. In particular, $v(z)\approx A_1(z-z_0)$, where A_1 is a complex constant. If A_1 is pure imaginary, then the neighboring trajectories are circular and closed, with frequency $\omega=|A_1|$ and period $T=2\pi/|A_1|$. This is always the case for stationary points on the real axis—i.e., $z_0=x_0$—which we now consider in greater detail. Note that due to reflection symmetry about the real axis, the first crossing of the real axis occurs at time $T/2$, at location $x_f=x_0-(x_i-x_0)$, for differentially small (x_i-x_0). Thus, in some small neighborhood of x_0, the map $f^{T/2}(x)$ is real valued, which in turn implies that $f^{T/2}(z)$ is RE over the domain around x_0 for which $f^{T/2}(z)$ is analytic. This in turn implies that *all trajectories within the domain of analyticity have period T*, even well away from the neighborhood where the velocity field is linear and the trajectory orbits circular.

For stationary points off of the real axis, it may still be true that A_1 is pure imaginary, leading to closed neighboring trajectories and essentially "conservative" dynamics. However, A_1 may also be complex valued, resulting in aperiodic trajectories that spiral in or out, with the stationary point an attractor or repeller, respectively (with the former akin to dissipative dynamics). Such stationary points z_0 come in complex-conjugate pairs, with the A_1 of one the complex conjugate of the other, thus implying that one point of the pair is an attractor and the other a repeller. It is possible for trajectories to flow directly from an attractor to its conjugate repeller, crossing the real axis in a region without closed orbits.

VI. SPECIFIC EXAMPLES

To demonstrate the range of dynamical behaviors available, for both analytic and nonanalytic $v(z)$, we consider a representative sampling of $d=1$ systems, some of which have been considered in the previous literature [15,17,18,20,29]. In each case, the Hamiltonian is of the form

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + V(z), \tag{41}$$

with $m=\hbar=1$. All units may therefore be taken to be atomic units. Complex quantum trajectories for systems II–V are presented in Fig. 2. In every case, Eq. (38) has been confirmed numerically for those trajectories that recross the real axis. The velocity field $v(z)$ is obtained using Eq. (20); stationary points are obtained by solving $v(z_0)=0$; corresponding trajectory periods are obtained as per the end of Sec. V.

A. System I: Harmonic oscillator ground state

The relevant quantities are as fiollows:

Potential	$V(z)=z^2/2$
Wave function	$\psi(z)=\exp(-z^2/2)$
Velocity	$v(z)=iz$
Stationary point	$z_0=0$
Period	$T=2\pi$

This system conforms to the special symmetric case, discussed after Eq. (38), for which $|\rho'(x_i)|=|\rho'(x_f)|$. Due to

symmetry, $x_f=-x_i$ corresponds to the first real-axis crossing at time $T/2$. Consequently, $dx_f=-dx_i$, $\rho(x_i)=\rho(x_f)$, and weak probability conservation is satisfied. This is the *only* example considered for which Eq. (30) is correct. Also, rather uncharacteristically, $f^{\Delta t}(z)=e^{i\Delta t}z$ is globally analytic. The complex trajectory orbits are concentric circles centered at the origin that move counterclockwise.

B. System II: Harmonic oscillator first excited state

We use the following parameters:

Potential	$V(z)=z^2/2$
Wave function	$\psi(z)=z\exp(-z^2/2)$
Velocity	$v(z)=i(z^2-1)/z$
Node	$z=0$
Stationary point	$z_0=\pm 1$
Period	$T=\pi$

The first excited state of the harmonic oscillator has a node at the origin. As per the discussion at the start of Sec. V, this implies that the velocity field $v(z)$ is meromorphic, with a simple pole at the $z=0$ node. Through this node, separatrices partition two sets of closed trajectories (period π) around the two stationary points. Note that since these stationary points lie on the real axis, the nearby trajectories must be concentric circles (A_1 is pure imaginary). There are also larger trajectory orbits, also closed (period 2π), that surround both stationary points. Thus, trajectories on either side of the separatrices get mapped to very different locations, so for this example, $f^{T/2}(z)$ is not globally analytic, or even meromorphic.

C. System III: Symmetric double-peaked ground state

We use the following parameters:

Wave function	$\psi(z)=\exp(-z^4/2+z^2)$
Velocity	$v(z)=2iz(z^2-1)$
Stationary point	$z_0=0,\pm 1$
Period	$T=\pi,\pi/2$

There are no wave function nodes and therefore no simple poles in the velocity field $v(z)$ or in the trajectory map $f^{T/2}(z)$. Although $v(z)$ is globally analytic, $f^{T/2}(z)$ is not. All trajectories except for the separatrices are closed, each surrounding exactly one of the three stationary points. This is the first case considered for which there are separatrix trajectories when $v(z)$ itself is globally analytic.

D. System IV: Morse oscillator ground state

We use the following parameters:

Potential	$V(z)=\exp(-2\sqrt{2}z/3)-2\exp(-\sqrt{2}z/3)$
Wave function	$\psi(z)=618^{1/4}\exp(-3e^{-\sqrt{2}z/3}-5\sqrt{2}z/6)$
Velocity	$v(z)=i(5-6e^{-\sqrt{2}z/3})/3\sqrt{2}$
Stationary point	$z_0=3\ln(6/5)/\sqrt{2}+ik3\sqrt{2}\pi$ with k an integer
Period	$T=18\pi/5$

The velocity field $v(z)$ is globally analytic, but $f^{T/2}(z)$ is not. Also, $v(z)$ is periodic in the imaginary direction, over a distance $3\sqrt{2}\pi$. Thus, the stationary point along the real axis and surrounding "librational" closed trajectories are duplicated at regular intervals away from the real axis. In addition, there is a family of open, "hindered rotational" trajectories, on the right side of the figure, that traverse all unit cells.

E. System V: Asymmetric single-peaked ground state

We use the following parameters:

Wave function	$\psi(z)=\exp(-z^4-z^2/2-z^3)$
Velocity	$v(z)=i(z+3z^2+4z^3)$
Stationary point	$z_0=0,-3/8\pm i\sqrt{7}/8$
Period	$T=2\pi$

The velocity field $v(z)$ is globally analytic, but $f^{T/2}(z)$ is not. The stationary point at $z_0=0$ is surrounded by closed trajectories with period 2π on the right side of the figure. In addition, there is a pair of complex-conjugate stationary points off of the real axis, such that the one in the upper half plane is a repeller and the other an attractor. On the left side of the figure is a family of aperiodic, doubly spiraling trajectories that connect the repeller to the attractor. These trajectories cross the real axis only once.

VII. CONCLUSIONS

We conclude with a brief summary of what has been achieved here. First, it seems evident that any analysis of quantum probability flux on complexified space requires generalized complex conjugation of the form of Eq. (15). This results in analyticity of the requisite quantities such as probability density—but much more importantly, leads to complexified flux relations [e.g., Eq. (27)] that are physically relevant because they do not depend explicitly on the potential energy. On the other hand, the most straightforward complex generalization of the flux continuity relation to emerge from this work—i.e., Eq. (27)—corresponds to the $v_{\mathrm{RE}}(z,t)$ rather than the $v(z,t)$ velocity field. Even relaxing to the weaker condition of Eq. (30) is insufficient to achieve probability conservation for $v(z,t)$. Yet even if this condition were somehow satisfied, it might not be very useful for most multidimensional applications, because few if any trajectories recross all of the real coordinate axes simultaneously (even for separable systems, if the frequencies are incommensurate).

The above suggests that a different choice of complex velocity field might be more advantageous, though it is not

clear at present how to construct such a field. One possible approach, inspired by coherent-state initial-value representations [1], might be to regard z and z^* as completely independent quantities—e.g., in formulating partial derivative expressions for the flux and its divergence. This might in principle require a pair of distinct complex trajectories, one on z space and another on z^* space, which somehow get combined together to form the time-evolving probability density $\rho[z(t),z^*(t),t]$. Perhaps even two time coordinates would be involved.

On the other hand, there is still some hope for the $v(z,t)$ approach, as well. In particular, as per the discussion following Eq. (36), the fact that real dx_i implies real dx_f under $v(z,t)$ dynamics might turn out to be quite useful. Also, in certain special cases, it may turn out that Eq. (30) is *approximately* satisfied—well enough to enable calculations for large systems. In any event, it is hoped that this initial foray may enable subsequent developments toward achieving probability conservation for complex quantum trajectories, or at least, provide a useful framework for analysis of these important issues.

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