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Bohmian mechanics without pilot waves

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ABSTRACT

In David Bohm's causal/trajectory interpretation of quantum mechanics, a physical system is regarded as consisting of *both* a particle *and* a wavefunction, where the latter "pilots" the trajectory evolution of the former. In this paper, we show that it is possible to discard the pilot wave concept altogether, thus developing a complete mathematical formulation of time-dependent quantum mechanics directly in terms of real-valued trajectories alone. Moreover, by introducing a kinematic definition of the quantum potential, a generalized action extremization principle can be derived. The latter places very severe *a priori* restrictions on the set of allowable theoretical structures for a dynamical theory, though this set is shown to include both classical mechanics and quantum mechanics as members. Beneficial numerical ramifications of the above, "trajectories only" approach are also discussed, in the context of simple benchmark applications.

1. Introduction

The quantum theory of nature has been with us for about a century, yet its interpretation continues to generate as much controversy today as when it was first introduced [1–22]. At heart is the issue of how to interpret the wavefunction, Ψ, which, even for a single particle system, is a complex-valued field over all space and time, meant to predict the outcomes of experimental measurements that describe reality in localized particle-like terms. Of course in practice, Ψ can do so only statistically, thus prompting many to search for a more fundamental descriptive theory [2–5,12,14,16,19]. A number of such descriptive interpretations of quantum mechanics have been proposed. However, with few but important exceptions (such as Bell's inequality [2–5,23]), to the extent that such theories are mathematically consistent with the TDSE, they cannot be distinguished or tested via experiment.

There is therefore no objective empirical way to decide which of these competing viewpoints or interpretations is the "correct" or "preferred" description of reality. Without wishing to engage very deeply into this debate, it seems apparent that each of the major interpretations of quantum mechanics currently entertained [6] – e.g., deBroglie-Bohm [10–15], ensemble [16–18], many worlds [19–21], and to a certain extent, even Copenhagen [7–9] – has its own unique philosophical advantages and disadvantages. It is also abundantly clear that the variety of mathematical formulations of quantum mechanics – including matrix-mechanics [9], path-integral [1,24], and Wigner-Weyl [25], to mention a few, and to say nothing of approximate theories such as semiclassical mechanics [26–34] – provide enormous practical benefit as well. There is thus a tremendous benefit in having a plethora of such methods to choose from, and knowing when it is appropriate to use each – as has been often pointed out, e.g., by E. Pollak. Indeed, Pollak's own series approach to the forward–backward initial value representation (FB-SCIVR) [34] is just such a case in point, enabling large-scale dynamical calculations to be performed, yet providing a rigorous, built-in characterization of the method's own level of quality, together with a systematic means of improvement.

In this paper, the author develops a mathematical formulation of quantum mechanics that is shown to present some unique benefits, both from a formal theoretical perspective, as well as the practical computational one. At this stage, the primary focus is the mathematical formulation itself. Although new interpretative ramifications may well be suggested by the approach, discussion of such topics (particularly measurement) is primarily deferred to later papers, and perhaps other authors. Similarly, whereas a few specific one-dimensional (1D) models and numerical examples are worked out in this publication, a more detailed assessment of the numerical methods proposed will be presented in future publications. This includes the generalization for multidimensional applications, which has already been worked out in some detail, as a primary motivation for the present work is the development of efficient computational methods for solving the TDSE for realistic multidimensional molecular systems. In this context the new

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approach may offer some substantial numerical advantages, as will be discussed.

The present approach is an outgrowth of Bohmian Mechanics – i.e., the "pilot wave" interpretation of quantum mechanics, pioneered by de Broglie in the early days of the quantum theory, and developed into a full-fledged theory by Bohm in the 1950's [10–15]. Bohm's interest was primarily philosophical and interpretive – although the computational benefits of his approach have come to be greatly appreciated in recent years [13,35–38], especially by members of the chemical quantum dynamics community [13,39–53]. In Bohm's pilot wave theory, a system comprises both a wave *and* a particle [12]. The former is the usual quantum mechanical wavefunction, Ψ. The latter has a well-defined position and velocity at every point in time, thus defining a "quantum" trajectory, $\vec{x}(t)$, which evolves deterministically or causally over time, much like its classical counterpart. The forces that determine the quantum trajectory evolution stem from the usual classical potential $V(\vec{x})$, plus a "quantum potential" correction, $Q(\vec{x},t)$, which in turn derives from the wavefunction, $\Psi(\vec{x},t)$. Thus does the wavefunction "pilot" the particle trajectory. The classical similarities and deterministic appeal of the quantum trajectory portion of Bohm's theory are obvious; moreover, the "collapse" of Ψ upon measurement of the particle's position is not regarded as random, but rather, must coincide with the actual particle position as specified by $\vec{x}(t)$. On the other hand, some aspects that have been seen as "distasteful" include the asymmetric treatment of *non*-position measurements, and also the fact that the influence of Ψ on $\vec{x}(t)$ is not balanced by a reciprocal influence of $\vec{x}(t)$ on Ψ – though counters to each of these charges have been offered [3,12,14,15].

The present work was motivated by another, slightly distasteful feature of the pilot wave interpretation: why should a *global* field function, operating in principle throughout all (x,t), only ever be ever called into practical use at a single x for a given t? In electromagnetic (EM) field theory, for instance, one can in principle distribute multiple point charges throughout space to "feel" the effects of the EM field whereever desired. In comparison, Bohm's pilot wave seems rather wasteful. The situation is further compounded by a fact well-known to numerical practitioners – namely, that the same $\Psi(\vec{x},t)$ can be used to reconstruct an entire *ensemble* of quantum trajectories, all adhering to the same dynamical laws, but only one of which is regarded as physically "real." This begs the following question: is it possible to regard the *trajectory ensemble itself as the fundamental quantum entity*, thus removing the need for a pilot wave altogether? To the author's best knowledge, this is not a question that Bohm or his followers have ever seriously considered from a fundamental viewpoint. In particular, the earliest calculations of quantum trajectories were always performed in a manner consistent with the logically causal relationships of Bohm's theory itself – i.e., $\Psi(\vec{x},t)$ was computed *first*, only after which the quantum trajectory (or trajectory ensemble) was constructed from $\Psi(\vec{x},t)$. Such an approach, now called "analytical," [13,37,36,38] stands in stark contrast to more recent "synthetic" quantum trajectory methodologies (QTM's) [13,39–53], in which both the trajectories and the wavefunction are computed numerically on-the-fly, each affecting the propagation of the other, like electric and magnetic fields in an EM wave.

Taking this trend to its logical conclusion, a *complete inversion* of Bohm's original causal relationship is proposed in this paper, by demonstrating that the *trajectory ensemble itself* – specifically, the real-valued field $\vec{x}(\vec{x}_0,t)$ [where $\vec{x}_0 = \vec{x}(\vec{x}_0, t=0)$ denotes initial values] – can be propagated solely in accord with its *own partial differential equation* (PDE), making no explicit or implicit reference to an external pilot wave (though a trajectory density weighting is required). Once solved, the resultant $\vec{x}(\vec{x}_0,t)$ field can be used to reconstitute $\Psi(\vec{x},t)$, essentially uniquely, if desired; however, the latter step is certainly not necessary – neither logically, nor computationally. In any event, a primary ramification is that $\Psi(\vec{x},t)$ need not be regarded as more fundamental than $\vec{x}(\vec{x}_0,t)$ – at least not mathematically speaking, insofar as propagation of the TDSE is concerned. From an interpretive standpoint, a trajectories-only approach would also seem to offer many potential advantages, by avoiding the conceptual headaches associated with wavefunctions in general (e.g., complex-valued amplitudes), as well as the specific distasteful aspects of pilot waves discussed above. Moreover, by bringing the quantum trajectories to the fore, such an approach highlights the most attractive feature of Bohmian mechanics – i.e., its causal, trajectory-based description of quantum reality. Yet at the same time, it clearly suggests an interpretation altogether different from that of the pilot wave.

To derive the trajectory-based PDE described above requires a bit of work. In particular, it requires a general overhaul of the quantum potential concept, as a consequence of which the traditional Ψ-based definition is replaced with a *kinematic*, trajectory-based form. Not only does this turn out to be possible, but one can also show that the new form of the quantum potential satisfies a generalized action extremization principle. The latter is particularly relevant, for it places very severe restrictions on the set of allowable mathematical structures that can be considered for a quantum dynamical theory. As a consequence, for example, it may be possible to *derive* the TDSE PDE (or its trajectory-based equivalent) from more fundamental considerations, though such an exercise is beyond the scope of this first effort.

The remainder of this paper is organized as follows. Section 2 discusses the special case of one-dimensional (1D) stationary scattering states. All of the key physical ideas and developments, including the generalized action extremization principle, manifest in this 1D special case, which therefore serves as a convenient starting point. Section 3 then deals with the more general case of time-dependent wavepacket dynamics in 1D. Sections 2 and 3 both include analytical and numerical examples, and a discussion of the numerical implementation. Concluding remarks, including speculative comments regarding potential ramifications for new interpretations of quantum theory, are provided in Section 4.

2. Stationary scattering states in one dimension

2.1. Background

The mathematical formulation of quantum mechanics presented in this paper can be applied to completely general multidimensional time-dependent wavepacket applications, as will be explained in later papers. However, the simplest special case of the stationary Hamiltonian eigenstates in 1D serves as a convenient venue for introducing all of the key aspects of the new approach in as clear a light as possible. Note that stationary *bound* states (even in many dimensions) are characterized by trivial quantum trajectories for which $\vec{x} = 0$ everywhere [12,13]. Thus, in order to observe non-trivial trajectory dynamics, we consider only 1D stationary *scattering* states.

Substitution of the Madelung-Bohm ansatz [10,11,54],

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

(where $R(x)$ and $S(x)$ are the real-valued amplitude and action fields, respectively) into the time-independent Schrödinger equation (TISE) yields the following coupled real-valued ordinary differential equations (ODE's) in x:

$$2\frac{dR}{dx}\frac{dS}{dx}+R\frac{d^2S}{dx^2}=0, \tag{2}$$

$$\frac{1}{2m}\left(\frac{dS}{dx}\right)^2+V(x)+Q(x)=E, \tag{3}$$

$$\text{where}\quad Q(x)=-\frac{\hbar^2}{2m}\left(\frac{d^2R}{dx^2}\right)\Big/R, \tag{4}$$

is the quantum potential. Under the usual association with the velocity field, i.e.,

$$m\dot{x}=\frac{dS}{dx}, \tag{5}$$

Eqs. (2) and (3) can be rewritten as follows:

$$\rho(x)\dot{x}=\text{const}, \tag{6}$$

$$\frac{1}{2}m\dot{x}^2+V(x)+Q(x)=E, \tag{7}$$

where $\rho(x)=R^2(x)=|\Psi(x)|^2$ is the probability density.

Eq. (6) is the continuity equation for steady-state fluid flow, or the condition of invariant flux [49], which must hold for any system exhibiting both probability conservation and stationarity. This is true regardless of the particular potential, $V(x)$ – or, for that matter, of the particular dynamical law (e.g., classical or quantum mechanics). Eq. (3) is the quantum stationary Hamilton–Jacobi equation, determining the forces that govern the quantum trajectory dynamics. For the stationary state case above, we find in Eq. (7) that the total energy – i.e., the sum of trajectory kinetic energy plus classical potential energy plus quantum potential energy –is the same throughout space, and equal to the corresponding energy eigenvalue. Equivalently, since $x=x(t)$ represents a quantum trajectory, we find that the total energy along a trajectory is conserved.

Having obtained the TISE solution, $\Psi(x)$, and the corresponding dS/dx, the resultant quantum trajectory ensemble may be constructed via explicit time-integration of Eq. (5). We denote the ensemble of specific solutions of this ODE in time as $x(x_0,t)$, where the initial values, $x_0=x(x_0,t=0)$, may also be regarded as individual quantum trajectory *labels*, which are relevant over *all* values of time. The entire trajectory ensemble is thus represented as the set of all $-\infty<x_0<\infty$.

The above is the most *direct* way to compute $x(x_0,t)$ from $\Psi(x)$; a more dynamical, but indirect, approach stems from the quantum version of Newton's second law, i.e.,

$$-\left[\frac{dV(x)}{dx}+\frac{dQ(x)}{dx}\right]=m\ddot{x}, \tag{8}$$

obtained from Eq. (7). The wavefunction enters Eq. (8) through the quantum potential driving term, $Q(x)$. Traditional treatments of Bohmian mechanics emphasize Eq. (8), because of its obvious dynamical significance, and undoubtedly also because Bohm himself did [10–13]. However, several compelling arguments [14,15] suggest that Eq. (5) is actually more fundamental. An additional supporting argument, relevant to the present trajectory-based formulation, is also introduced below.

This argument is based on yet another, slightly distasteful observation about Bohm's theory. Note that Eq. (5) provides a *complete* characterization of $x(x_0,t)$, in that all possible values of x_0 – i.e., all members of the trajectory ensemble – are associated with a single TISE solution $\Psi(x)$. In contrast, Eq. (8) is a higher-order ODE in time, requiring additional unspecified initial conditions. Specifically, for a given x_0, mathematical solutions of Eq. (8) for $x(x_0,t)$ exist for all values of $\dot{x}_0$ – but *only one of these* actually corresponds to $\Psi(x)$. In semiclassical mechanics, one might argue that a different set of $\dot{x}_0$ values corresponds to a different, possibly non-L^2-integrable solution $\Psi(x)$. This argument does not apply in Bohmian mechanics however, because changing the solution $\Psi(x)$ changes Eq. (8) itself – i.e., gives rise to a completely different ODE and trajectory solutions – because of the Q dependence on Ψ.

2.2. First derivation of the new ODE

Thus far in this section, we have presented nothing new, or outside the purview of standard Bohmian mechanics; it is from here, however, that we will diverge from the traditional deBroglie-Bohm formulation. Our first departing step will be to recognize that $x(x_0,t)$ provides an (essentially) unique coordinate transformation from x to t. Since the Eq. (5) ODE does not depend explicitly on t, the trajectory solutions for different x_0 values must all be equivalent to each other, apart from an immaterial time delay. In principle, there might be non-overlapping families of equivalent trajectories. However, that does not occur, because it would require that the quantum trajectories stop moving, or change direction, i.e., that $\dot{x}=0$ for certain values of (x_0,t), which in turn would imply a nonexistent divergence of Ψ via Eq. (6). All quantum trajectories must therefore move with finite speed and in the same direction over all time, and are all related to each other via an appropriate time delay, as indicated in Fig. 1. For definiteness, we take $\dot{x}>0$, and focus on a single reference trajectory $x(t)=x(x_0,t)$, for which x_0 represents a specific initial value. Under such conditions, the function $x(t)$ clearly satisfies the necessary conditions for a smooth, invertible (one-to-one and onto) coordinate transformation from t to x, with associated inverse transform, $t(x)$.

The next step is to rewrite Eq. (7), using three substitutions. First, Eq. (4) is used to express $Q(x)$ in terms of $R(x)$ and its double spatial derivative. Second, $R(x)$ is expressed in terms of $\dot{x}$, via Eq. (6). Note that the value of the constant in Eq. (6) is immaterial, as $R(x)$ and $R''(x)$ appear in Eq. (4) as a ratio. Finally, the coordinate transform $x\to t$ is applied, so that all spatial derivatives are replaced with time derivatives, via

$$\frac{d}{dx}=\left(\frac{1}{\dot{x}}\right)\frac{d}{dt}. \tag{9}$$

The result is the following third-order ODE in time:

$$\frac{1}{2}m\dot{x}^2+V(x)+\frac{\hbar^2}{4m}\left(\frac{\dddot{x}}{\dot{x}^3}-\frac{5}{2}\frac{\ddot{x}^2}{\dot{x}^4}\right)=E. \tag{10}$$

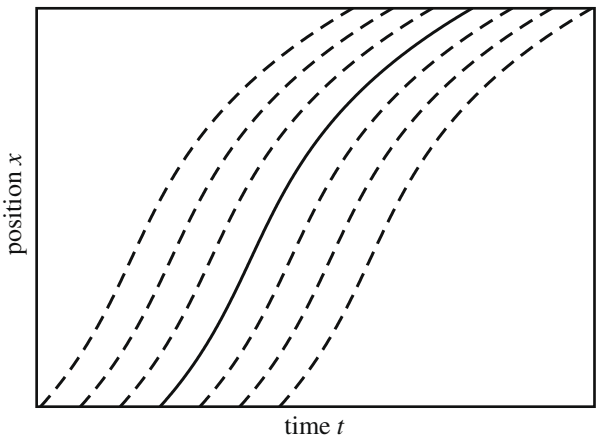

Fig. 1. Schematic indicating the ensemble of trajectories for a generic 1D stationary state application. The reference trajectory, $x(t)$ (solid curve), is identical to all other trajectories in the $x(x_0,t)$ ensemble (dashed curves), apart from a time shift. Also, $x(t)$ is monotonically increasing with t, and exhibits no turning points (i.e., points for which $\dot{x}=0$).

Note that Eq. (10) makes *no reference whatsoever* to the wavefunction, $\Psi(x)$, or associated fields, $R(x)$ and $S(x)$. It is a stand-alone, nonlinear, real-valued third-order ODE in time, that can be solved directly to obtain quantum trajectories, $x(t)$, for a given value of energy, E. The resultant quantum trajectories are identical to those of Bohm's theory, but are computed here without reference to any pilot wave, or external quantum driving terms of any kind. Of course, the ODE order is now even higher than Eq. (8). However, this is entirely appropriate in the new context, because treated as a functional of x and its time derivatives, Eq. (10) is the same for *all* TISE solution Ψ's for a given energy, E – unlike Eq. (7). Eq. (10) is thus "complete" in the sense that all solutions of this ODE are physically relevant, as we now discuss further.

Of the three real-valued initial values implied by Eq. (10), one is used as before, to specify x_0, i.e., the trajectory starting point. Since all trajectories associated with a given Ψ are equivalent apart from a time delay, this initial value is immaterial. The remaining two initial values are needed to specify the particular solution Ψ of interest. Note that if Ψ_1 and Ψ_2 are linearly independent TISE solutions at a given energy E, then a completely general solution may be written $\Psi = A(\Psi_1 + B\Psi_2)$, where A and B are arbitrary complex numbers. The value of A is completely immaterial, both in terms of the underlying physical quantum state of the system, as well as its effect on the quantum trajectory propagation of Eq. (10), as already stated. However, the two real-valued parameters associated with the complex number B correspond to physically distinct quantum states, and also to the remaining two parameters needed to specify the particular quantum trajectory solution. We thus find that *individual quantum states are associated with individual quantum trajectory orbits* in one-to-one fashion – a better correspondence, indeed, than for $\Psi(x)$, for which the immaterial overall scaling factor, A, results in a many-to-one correspondence with quantum states.

As additional confirmation that the trajectory representation described above is in fact a complete representation for 1D TISE quantum mechanics, we now demonstrate how the wavefunction may be uniquely reconstructed from a *single* trajectory solution $x(t)$, apart from the overall scaling factor, A. From $x(t)$ itself, one can reexpress the velocity field as a function of position, i.e., $\dot{x}(x)$. The spatial integral of $\dot{x}(x)$ then specifies the phase of $\Psi(x)$ via Eqs. (1) and (5), apart from an overall additive constant. Similarly, Eq. (6) specifies the wavefunction amplitude, $R(x)$, apart from an overall real-valued multiplicative constant. Together, these specify $\Psi(x)$ apart from the overall complex-valued scaling factor, A, as claimed.

It must be emphasized that, insofar as completeness of solutions is concerned, the key difference between Eqs. (7) and (10) lies in the new expression for the quantum potential used in the latter, i.e.,

$$Q(\dot{x},\ddot{x},\dddot{x}) = -\frac{\hbar^2}{2m}\left(\frac{5}{4}\frac{\ddot{x}^2}{\dot{x}^4} - \frac{1}{2}\frac{\dddot{x}}{\dot{x}^3}\right), \tag{11}$$

which has the same form for *all* TISE solutions – unlike Eq. (4), whose explicit form in terms of x depends on the particular solution, $\Psi(x)$. Eq. (11) is quite remarkable, in that it represents a completely trajectory-based, *local*, and *kinematic* (apart from the mass dependence) definition of the quantum potential. By "kinematic," we mean that no external force fields of *any* kind – not even the classical potential $V(x)$ – are involved. For homogeneous space as presumed here, kinematic expressions should exhibit no explicit dependence on position, depending only on $\dot{x}$ and higher time derivatives, and constants, as is the case for Eq. (11). By "local," in this context, we mean local in *time* – i.e., that Eq. (11) depends explicitly on only a *finite* number of x time derivative orders, in this case three.

Before proceeding, we derive the quantum equivalent of Newton's second law, using the new kinematic definition of Q. Substituting Eqs. (9) and (11) into Eq. (8) we obtain

$$-\frac{dV(x)}{dx} - m\ddot{x} - \frac{\hbar^2}{2m}\left(5\frac{\ddot{x}^3}{\dot{x}^6} - 4\frac{\ddot{x}\dddot{x}}{\dot{x}^5} + \frac{1}{2}\frac{\ddddot{x}}{\dot{x}^4}\right) = 0. \tag{12}$$

The last term on the left hand side above is a trajectory-based expression for the quantum force. Without it, one is left with the usual second-order classical ODE of Newton. Note that the single form of Eq. (12) applies to *all* TISE Ψ solutions, regardless of energy or boundary conditions. It is a fourth-order nonlinear ODE, all of whose solutions are physically relevant, with the four initial conditions serving as follows: one to specify initial point along trajectory orbit (as in classical mechanics, and discussed previously); one to specify solution energy (as in classical mechanics); two to specify particular quantum state for a given energy (as discussed above).

2.3. Second derivation of the new ODE: action extremization

The kinematic nature of Eq. (11) is particularly intriguing, in that it suggests that this definition is applicable to arbitrary *paths*, as opposed to just dynamical trajectories. By a "path," we mean essentially any smooth invertible function, $x(t)$ – i.e., an entity that *might* be a dynamical trajectory – whether or not it is actually a solution of Eq. (12). If the above interpretation is valid, one should be able to generalize the present approach for path-based methodologies. One such methodology is the Lagrangian formulation of classical mechanics [55], in which all paths that connect a fixed pair of endpoints in (x,t) space are considered. The path (or paths) which extremizes the action (i.e., the time-integral of the Lagrangian) is that which corresponds to the actual classical trajectory – i.e., the solution of the resultant Euler–Lagrange equation (Newton's second law in the simplest Cartesian case considered here). Action extremization is a fundamental principle of nature, that has found a home in virtually every field of physics; the present theory would be more compelling if it could be naturally formulated in such terms.

In classical mechanics, the Lagrangian is a functional of $x(t)$ and its time derivatives; in particular, x enters into the Lagrangian from the potential energy contribution, $V[x]$, whereas $\dot{x}$ enters in through the kinetic energy, $T[\dot{x}] = (1/2)m\dot{x}^2$. The quantum potential as expressed in Eq. (11) is also found to be of this form, i.e., $Q = Q[\dot{x},\ddot{x},\dddot{x}]$. This begs the question whether a similar action extremization principle can also be applied in quantum mechanics, and if so, whether it in fact leads to Eq. (12). Before addressing this question, we comment that a limited form of the action extremization principle is already known to hold for Bohmian quantum trajectories; a brief discussion is presented below.

Based on the quantum potential as defined in Eq. (4), the "quantum Lagrangian" in standard Bohmian mechanics is given by [12]:

$$L_B[x,\dot{x},t] = \frac{1}{2}m\dot{x}^2 - V[x] - Q[x,t]. \tag{13}$$

For time-independent applications, Q has no explicit time dependence; Eq. (13) is written in more general form to accommodate the time-dependent case. Though ultimately it derives from Ψ, formally, Q enters into Eq. (13) in exactly the same manner as V. Since the potential energy function is arbitrary in classical mechanics, the Euler–Lagrange solution that extremizes the action obtained from the time-integral of Eq. (13) must be Eq. (8). Though encouraging, in a sense there is no new information here at all; so long as $Q = Q[x,t]$, one must obtain Eq. (8), even if an arbitrary non-classical law of dynamics [i.e., not necessarily the standard quantum case of Eq. (4)] were considered.

In contrast, the quantum Lagrangian implied by Eq. (11) takes on a completely different form:

$$L[x,\dot{x},\ddot{x},\dddot{x}] = \frac{1}{2}m\dot{x}^2 - V[x] - Q[\dot{x},\ddot{x},\dddot{x}]. \tag{14}$$

Like Eq. (11), Eq. (14) is a stand-alone expression that does not in any way rely upon the external $\Psi(x)$ fields, nor does it depend explicitly on time [which, incidentally, is even true for time-*dependent* applications, i.e., Eq. (25)]. Eq. (14) can thus be regarded as more fundamental than Eq. (13) from a physical theory standpoint, and perhaps more properly suited to an action extremization procedure. On the other hand, there is no *a priori* reason to imagine that the extremal $x(t)$ solution so obtained will actually satisfy the dynamically correct ODE, i.e., Eq. (12). Indeed, for a completely general form of the functional, $Q[\dot{x},\ddot{x},\dddot{x}]$ – i.e., if alternative laws of quantum dynamics were considered – it *could not* generally be true that the resultant action-extremized ODE would be consistent with Eq. (8). So if this property does indeed turn out to be true in the case of the TISE, it says something quite special about the latter.

In fact, the property is true, as we show below. First, because the quantum Lagrangian, L, depends on higher-order time derivatives than either L_B or the classical Lagrangian, we must apply the calculus of variations to derive a more generalized form of the Euler–Lagrange equations. Specifically, if $x, \dot{x}$, and $\ddot{x}$ are all held fixed at both path endpoints (in practice, the $\ddot{x}$ constraint is not needed), then the action-extremizing path is found to be that which satisfies the following generalized Euler–Lagrange equations:

$$\left[\frac{\partial L}{\partial x}\right] - \frac{d}{dt}\left[\frac{\partial L}{\partial \dot{x}}\right] + \frac{d^2}{dt^2}\left[\frac{\partial L}{\partial \ddot{x}}\right] - \frac{d^3}{dt^3}\left[\frac{\partial L}{\partial \dddot{x}}\right] = 0. \tag{15}$$

In the specific case where $Q[\dot{x},\ddot{x},\dddot{x}]$ is defined via Eq. (11), Eq. (15) is found to lead exactly to Eq. (12).

To conclude this subsection, we comment on some interesting ramifications of the above. First, we note that mathematically, one can construct $Q(x), R(x), S(x)$, and even $\Psi(x)$, directly from an arbitrary *path* $x(t)$, using the same techniques as were discussed previously for dynamical quantum trajectories. The resultant "kinematic" wavefunction is not a solution of the TISE, in general. To effect this reconstruction, the trajectory/path ensemble $x(x_0, t)$ is still presumed to be constrained such that all paths relate to the reference $x(t)$ via a time delay, as per Fig. 1. Also, probability conservation, as implied by Eq. (6) from the TISE, must still be employed. However, the *dynamical* part of the TISE, i.e., Eq. (7), is not invoked as of yet, as is appropriate for a path-based construction. Continuing further along the "reverse engineering" lines initiated above, though, one might consider *deriving* the quantum dynamical law (i.e., the precise form of the functional Q) from the action extremization principle, by stipulating that Eqs. (8) and (15) be equivalent. This intriguing idea cannot quite be fully realized, in the sense of uniquely resulting in the known TISE – any other value of Planck's constant would also do, for example, as would classical dynamics, i.e., $Q = 0$. However, it is clear that the action extremization principle imposes *extremely* severe restrictions on the form of any candidate for a quantum dynamical law.

2.4. Examples, and numerical considerations

From a numerical perspective, the fact that an entire quantum energy eigenstate, $\Psi(x)$ – of any desired boundary conditions and energy, E – may be computed exactly from a low-order ODE calculation of a *single* real-valued trajectory, is very advantageous. Using standard quantum trajectory methods (QTMs) for instance [13], an entire ensemble of trajectories would be propagated, together with commensurate Ψ field quantities. Moreover, the trajectories would communicate with one another, via explicit numerical differentiation across the quantum trajectory grid. Such "unstructured grid" calculations are exceedingly difficult to perform accurately – particularly when Ψ exhibits substantial interference, in which case standard QTM's become intractibly unstable (the "node problem" [13,50–52]). Alternatively, approximate methods employing *non-communicating* trajectories may also be used, such as the derivative propagation method (DPM) [47,48,50]. In the author's experience, however, very high orders of derivatives (much higher than that of the Eq. (12) ODE) are needed to maintain reasonable TISE stationarity (i.e., numerical accuracy) with DPM's, and in any case, trajectory ensembles are employed for a calculation that is still only approximate.

In contrast with standard QTMs – and in addition to the advantages listed above – propagation of Eq. (12) is extremely stable, because it is an ODE rather than a PDE, and therefore never requires that spatial differentiation be performed across unstructured grids. Even in cases where reflection interference is extremely strong (i.e., the deep tunneling regime), the author has observed no difficulty in accurately computing the exact solution $x(t)$. One might fear that the inverse powers of $\dot{x}$ could lead to singularities or approximate singularities in the ODE, but in fact this never happens, for reasons already discussed in Section 2.2, and further discussed in Section 3.4. A greater concern is the strong oscillatory behavior that can arise from substantial reflection interference; however, this situation is nowhere near as devastating as in the standard synthetic QTM case, and in fact can be easily and efficiently handled via modern adaptive time-step techniques.

It is also a straightforward matter, via judicious choice of initial conditions, to obtain the particular solution $x(t)$ that corresponds with any desired $\Psi(x)$, and to construct the latter from the former. For example, suppose that one wishes to compute the TISE eigenstate $\Psi(x)$ corresponding to energy E, and exhibiting left-incident boundary conditions. One would choose the "initial" (really final) position x_0 to be a point sufficiently far to the right of the scattering barrier interaction region, and propagate backwards in time. Assuming that $V(x)$ vanishes in the right asymptote, the energy determines the initial velocity value via $\dot{x}_0 = \sqrt{2E/m}$. Finally, left-incident boundary conditions imply that the right asymptote of $\Psi(x)$ is a plane wave, i.e., $\ddot{x}_0 = \dddot{x}_0 = 0$.

An example for a benchmark Eckart barrier [56,57] system is presented in Fig. 2. This is the "Eckart A" system from Ref. [58], i.e.,

$$V(x) = V_0\,\mathrm{sech}(\alpha x)^2, \tag{16}$$

with $V_0 = 400\ \mathrm{cm}^{-1}, \alpha = 3.0$ a.u., $m = 2000$ a.u., and $E = V_0$. With these parameter values, the system exhibits substantial reflection interference. The Eq. (12) ODE was solved using Mathematica's NDSolve routine, requiring a total of only 0.0805 s on a 2.26 GHz Quad-Core Intel Xeon CPU. The subsequently reconstructed $\Psi(x)$ agrees with analytical results to a relative accuracy of around 10^{-10}.

As a final example, we consider the free particle Hamiltonian, i.e., $V(x) = 0$. If the quantum potential were also zero, i.e., in the classical limit, Eq. (12) would reduce to $\ddot{x} = 0$, with classical solutions $x(t) = x_0 + v_0 t$. These straight-line trajectories are also *quantum* solutions of Eq. (12), which correspond to the plane wave free particle eigenstates. However, for a given energy E, the quantum free particle Hamiltonian also admits $\Psi(x)$ eigenstate solutions that correspond to linear superpositions of positive- and negative-momentum plane waves. These non-classical superposition states manifest interference as oscillations in the probability density, $\rho(x)$. From the perspective of quantum trajectory solutions, the superposition states correspond to quantum trajectories for which the initial conditions satisfy either $\ddot{x}_0 \neq 0$ or $\dddot{x}_0 \neq 0$, or both. We conclude this section with a couple of formal properties of Eq. (12). If $V(x)$ is a symmetric potential, then it can be shown that

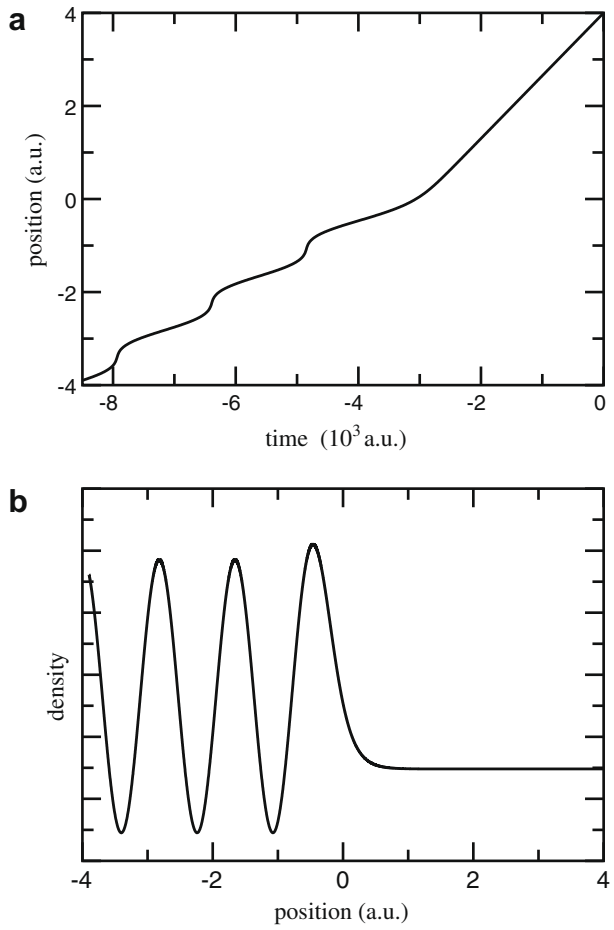

Fig. 2. Numerical solution of the 1D Eckart barrier system described in Section 2.4 (Eq. (16)). (a) Reference trajectory, $x(t)$, obtained by solving the Eq. (12) ODE, with initial trajectory values corresponding to the $\Psi(x)$ TISE stationary state with energy $E = V_0$, and left-incident boundary conditions. The oscillations at early times correspond to reflection interference in $\Psi(x)$. (b) Computed wavefunction density, $\rho(x) = |\Psi(x)|^2$ (units arbitrary), obtained from solution trajectory $x(t)$, via Eq. (6).

$-x(t)$ is a quantum trajectory solution if $x(t)$ is. Also, for completely general $V(x)$ (i.e., not necessarily symmetric) it can be shown that $x(-t)$ is also a solution – corresponding to $\Psi^*(x)$, as might be expected based on time-reversal-symmetry arguments.

3. Time-dependent wavepacket dynamics in one dimension

Having tackled the special case of 1D stationary scattering states, we now move on to the more general case of time-dependent wavepacket dynamics in 1D. Our basic strategy will be similar to that of Section 2; however, the theoretical framework is now somewhat more involved. In particular, the action extremization principle now relies on a Lagrangian *density*, rather than Lagrangian, formulation.

3.1. First derivation of the new PDE

We start similarly to Section 2, by substituting Eq. (1) into the TDSE, to obtain

$$\left.\frac{\partial R}{\partial t}\right|_x = \frac{-1}{2m}\left(2\left.\frac{\partial R}{\partial x}\right|_t \left.\frac{\partial S}{\partial x}\right|_t + R\left.\frac{\partial^2 S}{\partial x^2}\right|_t\right), \tag{17}$$

$$\left.\frac{\partial S}{\partial t}\right|_x = -\frac{1}{2m}\left(\left.\frac{\partial S}{\partial x}\right|_t\right)^2 - V(x) - Q(x,t). \tag{18}$$

In the equations above, it is understood that $\Psi(x,t), R(x,t), S(x,t)$, and $Q(x,t)$, now all depend explicitly on t, as well as x, though we nevertheless find it convenient to explicitly denote which variables are held constant in the partial derivatives.

As before, the trajectory field is denoted $x(x_0,t)$, where $x_0 = x(x_0, t=0)$ denotes both the initial value of, and an identifying label for, each trajectory in the ensemble. The latter interpretation is particularly convenient, for it enables straightforward computation of the *total* (Lagrangian) time derivative of any quantity – namely,

$$\dot{\cdot} = (d/dt) = \left.\frac{\partial}{\partial t}\right|_x + \dot{x}\left.\frac{\partial}{\partial x}\right|_t = \left.\frac{\partial}{\partial t}\right|_{x_0}. \tag{19}$$

Applying the Eq. (5) relation, and transforming to the total time derivative, Eq. (17) becomes the continuity equation, which leads directly to

$$\rho(x,t) = \frac{\rho_0(x_0)}{x'}, \tag{20}$$

$$\text{where} \quad \rho_0(x_0) = \rho(x = x_0, t = 0), \tag{21}$$

$$\text{and} \quad x' = \left.\frac{\partial x}{\partial x_0}\right|_t. \tag{22}$$

Note that henceforth, $\dot{\cdot}$ and $'$ will refer to the appropriate time and space partial derivatives in the (x_0,t) coordinate system.

Eq. (20) implies that *probability* (i.e., $\rho(x)dx$) is conserved along any given trajectory, x_0, in the ensemble. This has important ramifications for the coordinate transformation, which in the TDSE case, is more natural to define between x and x_0, rather than x and t. Note that the quantum trajectories in the $x(x_0,t)$ ensemble are no longer related via a time delay, but are instead essentially all completely different (though interdependent). Thus, all values of x_0 must be considered explicitly, and x_0 is now to be regarded as a full-fledged *coordinate*, rather than a single initial value. A central idea of this section is that for a given value of the parameter t, the trajectory field $x(x_0,t)$ defines a unique, continuous, and invertible coordinate transformation between x_0 and x, with the inverse transformation denoted $x_0(x,t)$. These desirable attributes of the coordinate transformation follow from Eq. (20); in particular, the fact that quantum mechanics admits only nonnegative finite ρ values implies that x' is also always nonnegative. This is also closely related to a well-known property of quantum trajectory ensembles for time-dependent systems: individual trajectories never cross, as a result of which field functions such as $R(x,t)$, etc., are always single-valued. For time-independent states, as we have seen, the corresponding condition is that trajectories never change direction, which is why t is the appropriate transformational coordinate in that context, and x_0 is the appropriate coordinate here. In either context, the situation stands in marked contrast to classical and semiclassical trajectories, for which turning points and caustics (crossing trajectories) give rise to divergent probability densities, multivalued field functions, and various other headaches such as the double boundary value problem [26–33]. At least one quantum trajectory method has been developed specifically to exploit this property [59].

We next adopt the kinematic viewpoint, as in Section 2, wherein all possible trajectory/path ensemble fields $x(x_0,t)$ are considered, regardless of whether or not they correspond to a given $\Psi(x,t)$ TDSE solution. The only constraints imposed on $x(x_0,t)$ are those necessary to ensure a continuous invertible coordinate transformation between x and x_0 for all t, as discussed above. Analogous to Section 2, we interpret Eq. (20) kinematically, which provides a unique specification of $\rho(x,t)$, in terms of $x(x_0,t)$ and $\rho_0(x_0)$. Though the latter can be thought of as the initial probability density, it is more correct to regard $\rho_0(x_0)$ as the *trajectory density weighting*. As such, it is an essential element in the formulation – i.e., it is assigned a fundamental significance, along with $x(x_0,t)$,

even though $\Psi(x,t)$ is not. As implied by Eq. (20), $\rho_0(x_0)$ must behave as a true probability density under coordinate transformations. Indeed, by such arguments it can be shown that $\rho_0(x_0,t)=\rho_0(x_0)$, i.e., that the weighting for a given trajectory is *conserved over time*, where $\rho_0(x_0,t)$ is the Ψ-based probability density, as referred to the coordinate x_0 rather than x. Only at the initial time, $t=0$, does $\rho(x,t)=\rho_0(x_0,t)$, because $x_0=x$ at $t=0$, and $x'(t=0)=1$. In practice, we work directly with $R_0(x_0)=\sqrt{\rho_0(x_0)}$, rather than $\rho_0(x_0)$ itself. No constraints are imposed on $R_0(x_0)$, other than that it be positive (see Section 3.4), finite, and square-integrable (for definiteness, $\int R_0^2(x_0)\,dx_0=1$ is presumed). Together with the above constraints on $x(x_0,t)$, one can regard this as constituting a *derivation* of the finiteness and unit normalization of $\Psi(x,t)$, rather than the other way around.

As before, it is possible to associate a unique $\Psi(x,t)$ (apart from the scaling factor) with a given $x(x_0,t)$ and $R_0(x_0)$, by employing $R(x,t)$ as obtained above, and spatially integrating the Eq. (5) relation to obtain $S(x,t)$. Our immediate aim, however, is to use $R(x,t)$ to construct a kinematic expression for the quantum potential. This can be achieved by transforming Eq. (4) from the (x,t) to the (x_0,t) representation. Thus,

$$R(x_0,t)=R[x(x_0,t),t]=R_0(x_0)x'^{-1/2}(x_0,t), \tag{23}$$

(where the last step follows from Eq. (20)), and the spatial derivative becomes

$$\left.\frac{\partial}{\partial x}\right|_t=\left(\frac{1}{x'}\right)\left.\frac{\partial}{\partial x_0}\right|_t. \tag{24}$$

This yields the following kinematic expression for Q:

$$Q[x',x'',x''',x_0]=\left[\frac{Q_0(x_0)}{x'^2}\right]+\frac{\hbar^2}{m}\left[\frac{R_0'(x_0)}{R_0(x_0)}\right]\left(\frac{x''}{x'^3}\right)-\frac{5\hbar^2}{8m}\left(\frac{x''^2}{x'^4}\right)+\frac{\hbar^2}{4m}\left(\frac{x'''}{x'^3}\right), \tag{25}$$

$$\text{where}\quad Q_0(x_0)=-\frac{\hbar^2}{2m}\left[\frac{R_0''(x_0)}{R_0(x_0)}\right]. \tag{26}$$

Note that Eq. (25) is expressed solely in terms of $R_0(x_0)$, and the spatial derivatives of $x(x_0,t)$. There is no explicit time-dependence whatsoever, and the only explicit spatial dependence (really trajectory dependence) is through $R_0(x_0)$, which is reasonable. As expected, there is no dependence on $\Psi(x,t)$ or the associated field functions. The lack of dependence on the time derivatives of x is quite interesting, and bears comment, particularly as Eq. (25) is more fundamental than Eq. (11). Basically, this implies that *no* quantum effects can be attributed to the behavior of a *single* trajectory alone. Rather, all quantum behavior in nature is due to an interaction amongst the different trajectories within a given ensemble, with the entire ensemble needed to characterize a single quantum state.

Having arrived at a Ψ-free, kinematic expression for the quantum potential, the final step is to derive a dynamical PDE, which can be solved directly to obtain the quantum trajectory field, $x(x_0,t)$. This is achieved by substituting Eqs. (5) and (25) into the quantum Hamilton–Jacobi equation (Eq. (18)), and spatially differentiating both sides with respect to x, via Eq. (24). The result is:

$$-\left.\frac{\partial V(x)}{\partial x}\right|_t-m\ddot{x}-\left(\frac{1}{x'}\right)Q'(x',x'',x''',x_0)=0,\quad\text{or} \tag{27}$$

$$-\left.\frac{\partial V(x)}{\partial x}\right|_t-m\ddot{x}-\left(\frac{Q_0'}{x'^3}\right)+\left[4Q_0+\frac{\hbar^2}{m}\left(\frac{R_0'}{R_0}\right)^2\right]\left(\frac{x''}{x'^4}\right)+\frac{3\hbar^2}{m}\left(\frac{R_0'}{R_0}\right)\left(\frac{x''^2}{x'^5}\right)-\frac{\hbar^2}{m}\left(\frac{R_0'}{R_0}\right)\left(\frac{x'''}{x'^4}\right)-\frac{5\hbar^2}{2m}\left(\frac{x''^3}{x'^6}\right)+\frac{2\hbar^2}{m}\left(\frac{x''x'''}{x'^5}\right)-\frac{\hbar^2}{4m}\left(\frac{x''''}{x'^4}\right)=0. \tag{28}$$

Solution of the Eq. (28) PDE will be discussed in some detail in Section 3.3.

3.2. Second derivation of the new PDE: action extremization

The action extremization principle that applies to $x(x_0,t)$ for arbitrary time-dependent wavepacket propagation is similar in spirit to the classical field equations for continuous elastic media [55], as can be modeled discretely, e.g., via a crystal lattice system with elastic deformations. One defines a Lagrangian *density*, $\mathscr{L}$, with units of energy per unit length, such that the action for a given trajectory field, $x(x_0,t)$, is given by

$$S=\int_0^T\int_{-\infty}^{\infty}\mathscr{L}[x,\dot{x},\ddot{x},\ldots,x',x'',\ldots]\,dx_0\,dt. \tag{29}$$

In continuous media, x represents displacements of differential mass elements from their equilibrium positions, x_0, and the spatial derivative contributions to $\mathscr{L}$ are associated with the (usually elastic) interactions of neighboring elements (or crystal lattice sites), which in turn relate to the Young's modulus of the material [55]. In the present quantum context, these spatial derivative contributions are associated with the kinematic quantum potential of Eq. (25). In classical field theory, the kinetic and external potential energy contributions to the Lagrangian density are generally expressed per unit mass (or per unit charge), and then multiplied by the mass density of the material (mass per unit length), which need not be uniform. In the present quantum context, mass density per se is not relevant; however, trajectory density *is* relevant, as we have seen. In any case, careful consideration of the total Lagrangian for a discretely-spaced set of trajectories, in the limit that the trajectory spacing, Δ_{x_0}, approaches zero, results in the following expression for the quantum Lagrangian density:

$$\mathscr{L}[x,\dot{x},x',x'',x''',x_0]=\rho_0(x_0)\left(\frac{1}{2}m\dot{x}^2-V[x]-Q[x',x'',x''',x_0]\right), \tag{30}$$

where $Q[x',x'',x''',x_0]$ is given by Eq. (25).

Using the calculus of variations to extremize Eq. (29), with respect to the trajectory field $x(x_0,t)$, for a Lagrangian density of the form of Eq. (30), one obtains the following Euler-Lagrange-type equations:

$$\left[\frac{\partial L}{\partial x}\right]-\frac{d}{dt}\left[\frac{\partial L}{\partial\dot{x}}\right]-\left[\frac{\partial L}{\partial x'}\right]'+\left[\frac{\partial L}{\partial x''}\right]''-\left[\frac{\partial L}{\partial x'''}\right]'''=0. \tag{31}$$

Some comments on the derivation of Eq. (31) are in order, as it is somewhat non-standard. With regard to the time coordinate, since the Lagrangian density depends only on the first time derivative of x, the extremization is with respect to all trajectory fields for which the initial and final trajectory positions are fixed. The fixed initial value condition is satisfied automatically by the earlier stipulation that $x_0=x(x_0,t=0)$. If $x_T(x_0)=x(x_0,t=T)$ represents the final positions of the trajectories, then the extremization is taken over all possible $x(x_0,t)$ trajectory fields for a given fixed $x_T(x_0)$, as indicated in Fig. 3. Thus, action extremization allows one to obtain a solution $x(x_0,t)$ field for *any* desired *a priori* final locations, $x_T(x_0)$, which could have very important practical implications, e.g., in the quantum control field [60].

The spatial boundary conditions also merit discussion. In principle, for a Lagrangian density with third-order spatial derivative contributions, one would have to fix x,x', and x'' at both the left and right endpoints. For Eq. (30) however, since the endpoints are $\pm\infty$, and since $R_0(x_0)$ is square integrable, these boundary conditions (which arise from integration by parts) are found not to apply. Consequently, the solution $x(x_0,t)$ trajectory fields are spatially unconstrained, and only the initial and final value constraints, i.e., x_0 and $x_T(x_0)$ respectively, are applicable. In practice, the latter is

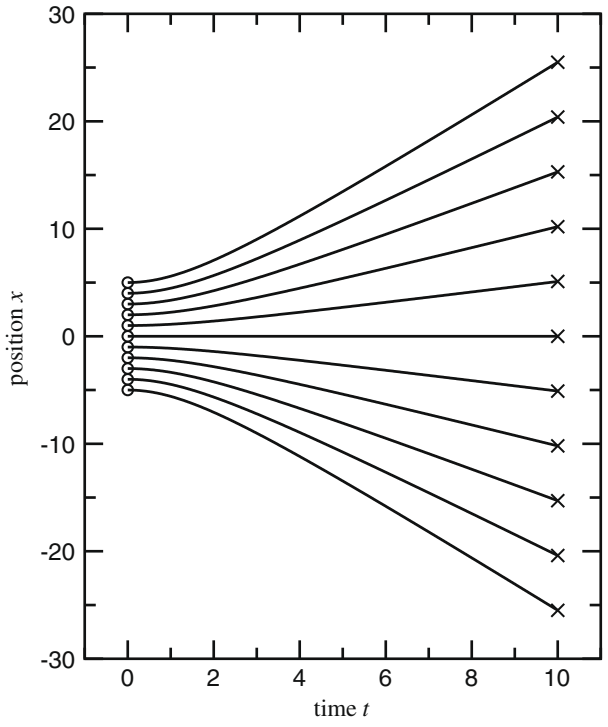

Fig. 3. Quantum trajectories for the time-evolving free particle Gaussian wavepacket application of Section 3.3, computed by solving the Eq. (37) PDE. The figure also serves as a schematic indicating the ensemble of trajectories for a generic 1D time-dependent wavepacket application, $x(x_0,t)$. Individual trajectories/paths can be varied independently and arbitrarily, except that they may not cross, and the initial ($\circ$) and final ($\times$) values must remain fixed.

replaced with a constraint on the initial velocity field, $\dot{x}_0(x_0)$, as the evaluation of Eq. (31) yields a PDE that is second-order in time.

We still have had not addressed whether the Eq. (31) PDE is equivalent to Eq. (28) or not – i.e., whether the action extremization procedure described above actually yields the correct quantum trajectories. As in Section 2.3, for a general quantum dynamical law – i.e., an arbitrary kinematic quantum potential functional, $Q[x',x'',x''',x_0]$ – the Eq. (31) PDE will *not* be consistent with the Eq. (27). For the TDSE case. however, it is in fact possible to show (with a bit of algebra) that Eq. (31) leads exactly to the rather complicated PDE of Eq. (28). It is highly unlikely that this is mere accident; again, the set of possible dynamical laws that obey this equivalence – though it includes both classical and quantum mechanics – must be very severely restricted. This issue will be explored more fully in future papers.

We conclude this subsection with a discussion of the "completeness" of the above equations, in the sense discussed in Section 2. We have already shown how to construct a legitimate $\Psi(x,t)$ from a given solution $x(x_0,t)$, but can *any* legitimate TDSE solution be so constructed? Likewise, are all of the $x(x_0,t)$ solutions physically relevant? Note that the TDSE PDE is first-order in time and second-order in space, but complex-valued. Eq. (28), on the other hand, has twice the order (second-order in time and fourth-order in space), but is real-valued; so the notion is at least reasonable, and in fact turns out to be correct. To demonstrate this, since the TDSE PDE is first-order in time, we need only consider the initial wavepacket, $\Psi_0(x_0)=\Psi(x,t=0)$, and whether that can be placed in one-to-one and onto correspondence with the Eq. (28) solutions. Note that the latter are already constrained by the initial condition $x_0=x(x_0,t=0)$. Thus, the $x(x_0,t)$ solutions of interest are uniquely specified by the initial velocity field, $\dot{x}_0(x_0)$, and the trajectory probability density field, $\rho_0(x_0)=R_0^2(x_0)$. But these latter two functions determine, respectively, the phase and amplitude of $\Psi_0(x_0)$, apart from immaterial constants as discussed previously. Again, we emphasize that the correspondence with physical quantum states is actually better for the $x(x_0,t)$ than for the $\Psi(x,t)$, because the immaterial constants render the latter correspondence many-to-one (even if unit normalization is presumed) rather than one-to-one.

3.3. Examples and numerical consideration

Eq. (28) is a stand-alone, nonlinear, real-valued PDE that can be solved directly to obtain the quantum trajectory ensemble, $x(x_0,t)$, for any TDSE wavepacket application in 1D. As in Section 2, the resulting trajectories are identical to those of Bohm's theory, but are computed here without reference to any pilot wave, or external quantum driving terms of any kind. Instead, it is the trajectories themselves – specifically, their interactions with each other – that give rise to all quantum dynamical effects.

From a numerical perspective, one still requires an ensemble of discrete, communicating trajectories in order to propagate Eq. (28), and in that respect, the situation is not improved over that of traditional QTM's. On the other hand, a tremendous numerical advantage is gained in the shift from x to x_0 as the spatial coordinate, which much more than offsets the increase in PDE order. Specifically, *x grids are moving (unstructured), whereas x_0 grids are fixed (structured).* Thus, once the x_0 grid points are initially determined – presumably in a desirably structured arrangement that makes strategic use of $\rho_0(x_0)$ – they remain fixed for all time. Moreover, since the probability of each trajectory (as well as the probability density, $\rho_0(x_0,t)$) remains constant over time, there should never be a need to add or remove grid points as the calculation progresses. Such an arrangement may eradicate the reflection interference node problem discussed previously, for it is well established that the resultant oscillations in *R per se* cause no special difficulty for spatial derivatives evaluated on fixed structured grids.

Wyatt and coworkers [61] have explored one such strategy using structured grids over x, where the grid points themselves are fixed, but the grid truncation changes over time (the moving boundary truncation method). Their approach has the advantage of numerical stability in the presence of nodes, but efficiency is somewhat compromised because probability is not conserved for individual grid points. Traditional QTM's, in contrast, are characterized by extremely efficient, probability conserving grids, but numerically unstable propagation in the vicinity of nodes. The numerical propagation of Eq. (28) offers the best of both worlds, i.e., fixed structured grids *that are also* probability conserving. Thus, if the initial wavepacket has narrow extent over x_0, the same will be true of the grid, and for all time. However, one drawback that still remains in the present approach is that the *density* of grid points (if not their spatial extent) may still need to be high, in order to accommodate interference oscillations. This latter difficulty might be ameliorated in a bipolar treatment [49,53,58], as may be explored in the future.

From a numerical standpoint, the author is aware of two other, existing methods that bear some resemblance to the present approach. The first is a distributed approximating functional (DAF) approach of Wyatt, Kouri, and Hoffman [62,63], in which a new coordinate transformation is applied at each time step, in order to render the (1D) trajectory grid at that particular time uniform (i.e., regular). The transformed grid is then used to perform all spatial derivatives. Though spiritually similar to the present approach, the coordinate transformation used is not well-defined at interstitial x values, and the method does not generalize to multidimensional problems. Another related approach is the Monte Carlo (MC) IVR method of Makri and coworkers [48,64], which explicitly exploits the fact that the initial wavepacket is smooth and

localized, and therefore amenable to efficient MC sampling. Moreover, this approach makes explicit use of the x_0 spatial derivatives of $x(x_0,t)$ and $\rho_0(x_0)$. However, instead of evaluating the derivative expressions explicitly on the x_0 grid, they are propagated approximately using independent (non-communicating) trajectories, in a DPM-like scheme.

To test the behavior and numerical efficiency of the new method, we have applied Eq. (28), both analytically and numerically, to the problem of free particle propagation of the Gaussian wavepacket in 1D. The analytical TDSE solution is as follows [60]:

$$\Psi(x,t) = (2\pi)^{-1/4} \times \sqrt{\frac{\sigma_0}{\sigma_0^2 + i\hbar t/2m}} \exp\left[-\frac{\sigma_0^2 p_0^2}{\hbar^2}\right] \exp\left[-\frac{\left(x - 2i\sigma_0^2 p_0/\hbar\right)^2}{4\left(\sigma_0^2 + i\hbar t/2m\right)}\right]. \tag{32}$$

Setting $t = 0$ above, we obtain the following initial values for Eq. (28)

$$R_0(x_0) = (2\pi)^{-1/4}\sigma_0^{-1/2} \exp\left[-\frac{x^2}{4\sigma_0^2}\right], \tag{33}$$

$$\dot{x}_0(x_0) = \frac{p_0}{m}. \tag{34}$$

The solution trajectory ensemble is then found to be

$$x(x_0,t) = x_0\sqrt{1 + \left(\frac{\hbar t}{2m\sigma_0^2}\right)^2} + \frac{p_0}{m}t. \tag{35}$$

Eq. (35) is easily shown to satisfy Eq. (28), with $V(x)$ set to zero. In particular,

$$x' = \sqrt{1 + \left(\frac{\hbar t}{2m\sigma_0^2}\right)^2}, \tag{36}$$

is independent of x_0, so $x'' = x''' = x'''' = 0$, and Eq. (28) becomes

$$m\ddot{x} = -\frac{Q_0'(x_0)}{x'^3}. \tag{37}$$

Given that

$$Q_0(x_0) = -(\hbar^2/2m)\left[\frac{R_0''(x_0)}{R_0(x_0)}\right] = \frac{\hbar^2}{4m\sigma_0^2} - \left(\frac{\hbar^2}{8m\sigma_0^4}\right)x_0^2, \tag{38}$$

both sides of Eq. (37) are seen to be equal to

$$\left(\frac{\hbar^2}{4m\sigma_0^4}\right)x_0\left[1 + \left(\frac{\hbar t}{2m\sigma_0^2}\right)^2\right]^{-3/2}. \tag{39}$$

Numerical calculations were performed for the above system, setting $m = \hbar = \sigma_0 = 1$ and $p_0 = 0$. The coordinate ranges, $-3 \leqslant x_0 \leqslant 3$ and $0 \leqslant t \leqslant 10$, span all regions of significant probability, and a very substantial amount of dispersion dynamics. Eq. (37) was solved using Mathematica's NDSolve routine, specifying only the initial value conditions of Eqs. (33) and (34) (i.e., no boundary conditions were needed). The entire calculation required only 0.0184 s on a 2.26 GHz Quad-Core Intel Xeon CPU, with the resultant computed $x(x_0,t)$ values agreeing with those of Eq. (35) to a relative accuracy of around 10^{-11}. The computed quantum trajectories are presented in Fig. 3.

3.4. Behavior in the vicinity of nodes

Although Bohmian mechanics, strictly speaking, only makes use of a single quantum trajectory, numerical implementations generally involve a trajectory *ensemble*, identical to that of the present approach. As such, the formal properties of quantum trajectories are well-understood [13,12], especially in the vicinity of nodes. In particular, quantum trajectories may not cross each other (because the velocity fields are single-valued), and also, they may not pass through nodes. It is nevertheless instructive to consider the ramifications of these well-understood facts for the present formulation, with regard to the coordinate transformation aspect, as well as Eq. (28).

We begin with the stationary scattering state case. Since all mathematical and physical solutions exhibit invariant flux (i.e., the constant value of Eq. (6)), and $\rho(x)$ must be finite everywhere, then $\dot{x}(t) \neq 0$ for all t, provided the flux value is non-zero. This implies that the coordinate transformation, $x(t)$, is not only a continuous invertible (one-to-one and onto) mapping, but also a *diffeomorphism*. The corresponding $\Psi(x)$ – though in some cases highly oscillatory – exhibits no true nodes. Nodes occur only for those stationary solutions with zero flux, which include certain scattering state solutions, as well as all bound state solutions (in 1D Cartesian space). For these solutions, $\dot{x}(t) = 0$ *everywhere*, and so it is impossible to define an $x(t)$ transformation – the one situation in which the Section 2 analysis breaks down. However, the more general framework of Section 3 is still perfectly applicable in this case also, leading to the trivially well-behaved relation, $x(x_0,t) = x_0$ for all t.

For time-dependent wavepacket dynamics, true nodes definitely can develop, although their occurrence in practice is actually quite rare. Of interest are the ramifications for the coordinate transformation, $x(x_0,t)$. With t taken as a fixed positive parameter, this function therefore relates the initial position, x_0, to the final position, x. Three possibilities present themselves: (a) a node at $t = 0$ persists through to the final time; (b) a node at $t = 0$ vanishes by the final time; and (c) a node comes into being at the final time that did not exist at $t = 0$. In *all* cases, the $x(x_0,t)$ mapping is continuous and invertible. In case (a), this transformation is also generally a diffeomorphism, as $\rho(x,t) = \rho_0(x_0) = 0$ in Eq. (20) allows a finite, non-zero value for x'. This case includes the stationary bound states, for example, for which the nodes are of the less-problematic "type I" variety [49], with finite, well-behaved quantum potentials. The evolution of the nodes over time, though not quantum trajectories *per se*, can nevertheless be thought of as separatrices between adjacent quantum trajectory regions. Cases (b) and (c) are more problematic, in that either the forward- or reverse-time coordinate transform has a Jacobian of zero (e.g., $x' = 0$ in case (b)), implying that the transformation is *not* a diffeomorphism. In practical terms, this implies that the quantum potential and force can exhibit a singularity at the node. However, even in this context, the singularity does not belong to any given quantum trajectory, because $\rho = 0$ at the node, and all nearby trajectories are driven away.

In applications, one has the freedom to choose $\rho_0(x_0)$ as desired. In practice, one would almost always choose this function to be node-free, so that only case (c) need be considered. The birth of nodes therefore corresponds *not* to $x' = 0$, but to x' *singularities*. Thus in Eq. (28), for instance, the inverse x' powers *per se* never cause difficulty, as x' can *never* be zero, and so caustics never arise; if they did, it would require that $\rho(x,t) \to \infty$, which is precluded by the laws of quantum propagation. Indeed, as a node is approached, x' approaches *infinity*, which tends to cause the inverse terms in Eq. (28) to approach *zero*. A more careful analysis reveals that it is only the last three terms that give rise to singular quantum forces at nodes, and that this is by virtue of higher-order (Taylor series) corrections associated with the higher-order spatial derivatives in the numerators.

Computationally speaking, though quantum trajectories are directed away from the nodes, and therefore never encounter singular quantum potentials directly, the proximity to nodes and even near-nodes will cause some numerical difficulty. However, since structured grids are used to compute all field quantities, these

node difficulties are anticipated to be quite minor, in comparison with other synthetic QTM calculations that use unstructured grids – i.e., along the lines of requiring small time-step sizes to handle the large quantum forces, which should be easily accommodated using adaptive algorithms. On the other hand, it should be stated that the somewhat related algorithm of Wyatt, Kouri, and Hoffman [63] does appear to face more substantial node-related difficulties.

4. Conclusions

The primary goal of this paper has been to demonstrate how the theory of time-dependent quantum mechanics can be mathematically reformulated solely in terms of the real-valued trajectory field, $\vec{x}(\vec{x}^0,t)$, and the trajectory density weighting, $\rho_0(\vec{x}^0)$. The traditional, complex-valued wavefunction, $\Psi(\vec{x},t)$, plays no fundamental role in this trajectories-only formulation, and is, in fact, logically unnecessary. This would appear to be a very far cry from the strong Copenhagen interpretation, whose completeness assumption, i.e., that "the wavefunction... provides the most complete description of the system that is, in principle, possible," [12] is a *necessary*, let alone sufficient, postulate for interpreting quantum theory. Of course, Bohm's theory – by introducing trajectories as an additional fundamental descriptive element – is already regarded as a compelling counterexample to the necessity of the completeness assumption, though it, too, requires Ψ as an essential component. In the present formulation, we push things a bit further, by demonstrating that the wavefunction *itself* can be disposed of – mathematically speaking, at least.

Our main purpose in this first publication has not been to develop a new interpretation of quantum mechanics *per se*, but rather, a new mathematical *formulation*. Like all formulations of nonrelativistic quantum mechanics, ours is mathematically consistent with the TDSE, and with all other quantum formulations (including Bohmian mechanics), but is distinguished by its own unique equations and mathematical framework. Neither have we sought here to develop or evaluate numerical codes for multidimensional molecular applications. Both are noteworthy goals, for which the present approach evidently provides important suggestions for further development – suggestions that will be explored in future publications. However, in both arenas, the starting point for progress must be an *equation* – and it is this that the present work seeks to provide, e.g., in Eq. (28).

In the present formulation, a quantum mechanical system is represented mathematically as an *ensemble* of dynamical trajectories, with each trajectory corresponding to a single possible initial value, x_0, and vice-versa. The particular state of the system is uniquely specified by the trajectory ensemble itself, together with the trajectory density weighting, $\rho_0(x_0)$. This leads to an *entirely different interpretation than Bohmian mechanics*, for which there is only *one* quantum trajectory (not an ensemble), guided by an independent wavefunction, Ψ, whose existence is also presumed as a necessary component of the system state. In particular, the $\rho_0(x_0)$ of our approach can *not* be regarded as a wavefunction; it is never complex-valued, and more importantly, it has no time (or even x-space) dependence. Instead, $\rho_0(x_0)$ is the *trajectory density weighting* – a quantity that must naturally be invoked as soon as continuously-parametrized trajectory ensembles are introduced, particularly if covariance is presumed. The fact that this interpretation applies across *all* time, rather than simply at fixed t values, might be useful, e.g., in developing a Lorentz-invariant version of the formulation. On the other hand, as in Bohmian mechanics, the physical interpretation of the individual trajectories themselves – as representing classical-like particle entities, with definite position and velocity values at all t – is clear, compelling, and immediate.

Unlike the trajectories in classical ensembles or fields, the trajectories in a given quantum ensemble can *influence* each other (in a manner that depends on $\rho_0(x_0)$), and it is this intertrajectory interaction that introduces all quantum effects. This situation provides a natural means of distinguishing derived field quantities into "classical" and "quantum" categories. Specifically, those fields derived only from $x,\dot{x},\ddot{x},\ldots,\rho_0$ can be associated with individual trajectories, and are therefore classical, whereas those that also involve spatial derivatives of x and ρ_0 are inherently quantum mechanical. In particular, a generalized quantum potential, or "quantum dynamical law," might be defined as *any* quantity $Q\left[x',x'',\ldots,\rho_0',\rho_0'',\ldots\right]$ – with the specific TDSE form of Eq. (25), as discussed, one of an *extremely* limited number of special cases for which the dynamical trajectory field extremizes the resultant Eq. (29) action. This result is perhaps the most compelling aspect of all the work presented here.

Some additional comments are in order. First, as in classical Lagrangian mechanics, the quantum action extremization procedure is invariant under coordinate transformations of configuration space – because $\mathscr{L}/\rho_0$ is invariant, and ρ_0 transforms as a probability density, i.e., $\rho_0\,dx_0=\rho_y\,dy$. Second, according to the definition provided in the preceding paragraph, one might presume the 1D TISE quantum potential of Eq. (11) to be a "classical" quantity. This is erroneous; in fact, Eq. (25), which is more fundamental, applies equally well to TDSE *and* TISE situations. In both cases, there is an *ensemble* of interacting trajectories, whose mutual interactions give rise to the quantum potential. The fact that only *one* trajectory need be explicitly considered in Section 2 is a consequence of the special time-delay property of the TISE ensemble, which in turn enables a mathematical substitution of space with time derivatives. The third comment pertains to locality/nonlocality, which, as in Bohm's theory, enters via the quantum potential. Since Eq. (25) involves only low-order spatial derivatives, trajectories influence each other only *locally* in configuration space – though in *physical space*, of course, this can correspond to nonlocal interactions between widely separated particles [2–5].

Another comment concerns the manner in which the action principle – one of the most universal ideas in all of physics – is generalized from classical Lagrangian mechanics. In the present approach, the quantum generalization involves replacing the classical Lagrangian with a quantum Lagrangian density. This is the *minimum* change that can be expected, given the switch from a single trajectory to a trajectory ensemble; indeed, the fundamental idea of extremizing the action itself survives completely unscathed. In contrast, the traditional route for introducing an action principle into quantum mechanics is via the path integral formalism, in which a *sum over all paths* is invoked, rather than a path optimization. Moreover, the path integrand is a complex-valued amplitude, rather than a real-valued classical-like action or Lagrangian. It is interesting that two different action principles seem to exist simultaneously in quantum mechanics, and it might be fruitful to explore the connection between the two. For the moment, however, the present approach seems to offer a decidedly more classical route for introducing the action principle into quantum mechanics.

As a final comment on the mathematical formulation, we acknowledge some parallels with the work of Faraggi and Matone (FM) [65,66], building on earlier work of Floyd [67,68]. In the FM approach, the quantum potential for 1D TISE states is *derived* to within a scaling factor, based solely on certain invariance properties under coordinate transformations, which they term the "quantum equivalence principle." As is also the case here, only well-behaved invertible transformations are allowed, as a consequence of which $\dot{x}\neq 0$. Trajectory orbits (in phase space) thus agree with those of the present work, and of Bohm, for 1D TISE stationary scattering states. However, FM also extend their analysis to the 1D TISE

bound states, for which their two-parameter family of $\dot{x} \neq 0$ trajectories, or "microstates," [67] correspond to the non-physical, non-square-integrable solution Ψ's. A detailed comparison with the present approach may help shed light in both directions, particular vis-à-vis extending the quantum equivalence principle to multidimensional systems.

The latter represents the final, crucial step in enabling the present approach to be regarded as a general reformulation of time-dependent quantum mechanics. Insofar as developing a multidimensional, completely trajectory-based propagation method is concerned, we have already demonstrated (not here) that this goal can in fact be achieved. Moreover, we have also developed a scheme for doing so, along the lines of the first type of derivation considered in the previous sections; this work will be presented in a separate publication. Here, we simply state that all of the numerical advantages discussed in Section 3.3 will also carry over to the multidimensional case – in particular, an initially narrow wavepacket remains narrow in the $\bar{x}^0$ representation for all time (thus dramatically reducing the number of grid points that might otherwise be needed), and all multidimensional spatial derivatives are performed on fixed structured grids.

We conclude with a brief discussion of some of the potential *interpretive* ramifications of the new formulation. In Bohmian mechanics, there is only one system trajectory, whereas the present approach offers an entire ensemble of trajectories. If one presumes objective existence for a single trajectory only, then the remaining trajectories in the ensemble must be regarded as "virtual," in some sense. On the other hand, one might prefer to regard *all* trajectories in the quantum ensemble as equally valid and real. It is hard to imagine how this could be achieved, without positing that each trajectory inhabits a separate world. It must be emphasized, however, that this version of the many worlds interpretation would be *very* different from the standard form [19–21]. In a nutshell, the latter associates different worlds with individual *paths*, whereas the present formulation suggests such an association for individual *trajectories* – i.e., more of a "not-so-many worlds" interpretation. Perhaps the most natural association between the present formulation and existing interpretations of quantum mechanics would be with the *statistical* or *ensemble* interpretation [16–18], whose most famous proponent was Einstein himself. Indeed, the trajectory density weighting function, $\rho_0(x_0)$, may be regarded as a classical statistical probability distribution, e.g., in Eq. (30).

In any event, much work remains to be done, if the present "trajectories-only" formulation is to be developed into a full-fledged interpretation of quantum mechanics, and regarded as a competitor, or compelling alternative, to the other existing interpretations. As for the author's view, at present I adopt an attitude similar to that held by Bohm himself, and shared by Holland, who describes it as follows [12]: "this theory of motion is not presented as a conceptually closed edifice offering the final word on quantum mechanics... Rather, it is a view worth developing for the insight it provides, and as a clue for possible future avenues of enquiry."

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