Quantum Mechanics Without Wavefunctions

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Quantum Mechanics Without Wavefunctions

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Abstract

We present a self-contained formulation of spin-free nonrelativistic quantum mechanics that *makes no use of wavefunctions or complex amplitudes of any kind.* Quantum states are represented as ensembles of real-valued quantum trajectories, obtained by extremizing an action and satisfying energy conservation. The theory applies for arbitrary configuration spaces and system dimensionalities. Various beneficial ramifications—theoretical, computational, and interpretational—are discussed.

I. INTRODUCTION

For nearly a century, quantum mechanics has presented philosophical and interpretational conundrums that remain as controversial as ever. Far from disappearing into the realm of esoteric academic debate, recent experimental advances, e.g. in entanglement, decoherence, and quantum computing, have brought such questions to the forefront of topical interest. The various competing viewpoints—Copenhagen,[1] Bohmian,[2–4] Many Worlds,[5] etc.—differ substantially in terms of their ontological interpretation of Ψ and its collapse, yet are all alike in their reliance upon a complex-valued wavefunction, and its propagation via the time-independent/dependent Schrödinger equation (TI/DSE). Evidently, a completely self-contained, classical-like, and real-valued formulation of quantum theory *without* wavefunctions—if such a thing were possible—would necessarily present novel and potentially very important interpretational and computational ramifications.

The aim of this paper is to show that for non-relativistic spin-free quantum mechanics, the above *can* be realized (A different approach is described in Ref. 6.) In particular, a quantum state can be represented as an ensemble of real-valued quantum trajectories, satisfying a self-contained partial differential equation (PDE). This was shown in a recent paper[7] by one of the authors (Poirier) for both the one-dimensional (1D) TISE and TDSE. It transpired that similar work had already been done for the TISE in 1D,[8] the TDSE in 3D,[9] and in greater generality.[10] In the current paper, we simplify, unify, and generalize these previous constructions, presenting quantum trajectory PDEs for arbitrary configuration spaces and system dimensionalities. The goal here is to present an alternative, standalone *reformulation* of quantum mechanics, that neither relies on the TDSE nor makes any mention of any external constructs such as Ψ, and which, in addition, is likely to provide far-reaching benefits for numerical calculations, e.g. of accurate quantum scattering dynamics for chemically reactive molecular systems.

The relevant PDEs can be derived from an action principle. We discuss symmetries of the action principle, associated conserved quantities, and other properties, such as a heretofore unexpected Hamiltonian structure in the case of 1D time-independent quantum mechanics (TIQM), which also serves as the basis of an accurate many-D numerical scheme. We single out a specific choice of Lagrangian or gauge, and show why this choice may be regarded as physically preferred. Likewise, we single out a specific choice of trajectory-labeling coordi-

nate(s), in terms of which the resultant PDE exhibits no explicit coordinate dependences. We present simple analytical solutions, and discuss some initial numerical results that appear very promising for molecular and chemical physics applications. The reformulation of quantum mechanics in terms of trajectory ensembles, in addition to shedding light on complex theoretical issues, evidently also provides important practical benefits.

II.   THE 1D TIME-INDEPENDENT CASE

As shown in Ref. 7, 1D TIQM states can be represented uniquely with a single trajectory, $x(t)$. The theory is one of a broad class of dynamical laws, for which the Lagrangian and energy are of the form

$$L(x, \dot{x}, \ddot{x}, \ldots) \; = \; \frac{1}{2}m\dot{x}^2 - V(x) - Q(\dot{x}, \ddot{x}, \ldots) \;, \tag{1}$$

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

Equations (1) and (2) are natural generalizations of the well-known classical forms. The quantum correction, Q, is similar to the potential, in that it appears with opposite signs in L and E, but is actually related to the TISE kinetic energy operator.[4] It has a universal "kinematic" form, i.e. no explicit x dependence.

As in classical theory, the quantum trajectories, $x(t)$, are obtained via extremization of the action, $S = \int L\,dt$. Since L is autonomous, the resultant $x(t)$ solutions exhibit time-translation invariance and energy conservation for any choice of Q. However, for general Q, the conserved energy for Eq. (1) obtained via Noether's theorem does *not* take the form of Eq. (2). Requiring this equivalence imposes rather special conditions on Q, e.g., that Q must be invariant under time rescaling. The simplest, well-behaved, nontrivial Q giving the form of Eq. (2) is

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

Here $\hbar$ is, in principle, an arbitrary positive constant. However, with the usual identification of $\hbar$ as Planck's constant, Eq. (3) is equivalent to the quantum potential of Bohmian mechanics[2–4] for the 1D Cartesian TISE.[7] This is surprising, given that the expression Eq. (3), being universal and kinematic, is determined entirely by the trajectory, $x(t)$. In particular, no reference to the wavefunction, Ψ, or the TISE itself, is used in this derivation.

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Our quantum trajectories are nevertheless Bohmian trajectories, although our formulation and interpretation are not at all that of Bohmian mechanics, because no Ψ is involved.

Action extremization applied to Eqs. (1) and (3) yields the following fourth-order autonomous ODE, describing 1D TIQM quantum trajectories:

$$m\ddot{x} + \frac{\partial V(x)}{\partial x} + \frac{\hbar^2}{4m}\left(\frac{\ddddot{x}}{\dot{x}^4} - 8\frac{\dddot{x}\,\ddot{x}}{\dot{x}^5} + 10\frac{\ddot{x}^3}{\dot{x}^6}\right) = 0 \ . \tag{4}$$

Two of the four constants of integration correspond to time-translation invariance and energy, as in the classical case. The other two constants determine which particular TIQM state the trajectory is associated with. A one-to-one correspondence thus exists between trajectory solutions [of Eq. (4)] and (scattering) TIQM states.[7]

Any fourth-order ODE can be rewritten as a set of four coupled, first-order ODE's. Remarkably, Eq. (4) can be rewritten:

$$\dot{x} = \frac{s}{m} \ ; \ \dot{p} = -\frac{\partial V(x)}{\partial x} \ ; \ \dot{s} = \frac{4rs^4}{m\hbar^2} \ ; \ \dot{r} = \frac{p-s}{m} - \frac{8r^2s^3}{m\hbar^2} \ , \tag{5}$$

which are *Hamilton's equations for a 2D system*,

$$\dot{x} = \frac{\partial H}{\partial p} \ ; \ \dot{p} = -\frac{\partial H}{\partial x} \ ; \ \dot{r} = \frac{\partial H}{\partial s} \ ; \ \dot{s} = -\frac{\partial H}{\partial r}, \tag{6}$$

for the Hamiltonian

$$H(x,p,r,s) = \frac{s(2p-s)}{2m} + V(x) - \frac{2r^2s^4}{m\hbar^2} \ . \tag{7}$$

In the above equations, (x,p) are the "classical" dimension phase space variables, and (r,s) correspond to an additional, "quantum" dimension, essentially describing quantum interference. Note that Eq. (7) reduces to the classical Hamiltonian when $r = 0$ and $s = p$.

In terms of the time derivatives of $x(t)$,

$$s = m\dot{x} \ ; \ r = \frac{\hbar^2\ddot{x}}{4m^2\dot{x}^4} \ ; \ p = m\dot{x} + \frac{\hbar^2}{4m}\left(\frac{\dddot{x}}{\dot{x}^4} - \frac{2\ddot{x}^2}{\dot{x}^5}\right). \tag{8}$$

Substitution of Eq. (8) into Eq. (7) then reveals H to be the conserved Noether energy of Eq. (2). For the free particle case $[\partial V/\partial x = 0]$, p is a second conserved quantity, in involution with H (and also derivable from Noether's theorem). The importance of p is difficult to overstate; it represents the "particle momentum," analogous to the well-known "particle energy," $E = H$.[3,4] Yet remarkably, p has barely been considered[8] in the previous literature, which generally regards $s = m\dot{x}$ as particle momentum. Note that p is conserved for *all* free

particle TIQM states, including those exhibiting interference, whereas s is conserved *only* for plane wave states—i.e., the classical special case for which $p = s$.

The above Hamiltonian approach is proving extremely useful in numerical calculations of quantum reactive scattering phenomena.[11] For any 1D TIQM application, *exact quantum* results are obtained simply by propagating a single $x(t)$ trajectory using the *classical* Hamilton's equations of Eq. (6), until $p(t)$ flattens asymptotically to the desired level of numerical accuracy. The final p value then provides a direct measure of the quantum reaction probability. Note that Eq. (6) is amenable to efficient, symplectic numerical integrators as are used in classical simulations, and the conservation of E can be monitored as an on-the-fly measure of computed accuracy. This approach is extremely robust, accurate, and efficient, leading to 15 digits of accuracy, even in the extremely deep tunneling regime (where absorbing potentials render conventional exact quantum scattering methods intractible). For many-D TIQM applications, classical-like sampling over quantum trajectory initial conditions leads to an approximate simulation scheme that has also proven to be remarkably accurate (i.e., to two or three digits).[11]

III.   THE 1D TIME-DEPENDENT CASE

For the case of 1D time-dependent quantum mechanics (TDQM), any self-contained formulation must involve a PDE, rather than an ODE. It is no longer possible to exactly represent a quantum state as a single trajectory, $x(t)$, but rather as a one-parameter *ensemble* of trajectories, $x(C, t)$, where the real-valued, space-like coordinate C labels individual trajectories. The equation of motion should be a PDE involving C and t derivatives, preferably derived from a field-theoretic action principle.

In Refs. 7, 9, and 10, C was chosen as the initial trajectory value [$x(C,0)=x_0=C$]. The resultant PDE is complicated, exhibits explicit x_0 dependence through the initial probability density, $\rho_0(x_0)=\rho(x_0,0)$, and bears little resemblance to Eq. (4). In addition, Q is expressed in terms of C rather than t derivatives of x. The PDE can be simplified by a better choice of the trajectory parameter, C, which in general can be taken to be any monotonic function of x_0 (regardless of the initial wavefunction). A crucial idea of the current paper is that C *should be chosen so as to uniformize the probability density*. In particular, since

$\rho_C(C)\, dC = \rho(x, t)\, dx$, if we choose

$$C = \int_{-\infty}^{x_0} \rho_0(x_0')\, dx_0' \;, \tag{9}$$

then C takes values from 0 to 1 (for normalized wavepackets), and $\rho_C(C) = 1$.

Working with Eq. (9) (or any uniformizing choice of C), and writing $x' = \partial x / \partial C$, $\dot{x} = \partial x / \partial t$ etc., the PDE of Ref. 7 simplifies very substantially to

$$m\ddot{x} + \frac{\partial V(x)}{\partial x} + \frac{\hbar^2}{4m} \left(\frac{x''''}{x'^4} - 8\frac{x'''x''}{x'^5} + 10\frac{x''^3}{x'^6} \right) = 0 \;. \tag{10}$$

Equation (10) is the perturbed Newton equation for the 1D TDQM case; it has no explicit coordinate dependences. It also bears an extremely close resemblance to Eq. (4), obtained by replacing C derivatives with t derivatives in the last term on the left hand side (representing the quantum force). More formally, Eq. (4) is obtained on looking for travelling wave solutions of Eq. (10), i.e. solutions of the form $x(C, t) = x(t - \lambda C)$ where λ is a constant. In the 1D TIQM context, t thus serves as an effective uniformizing coordinate. Equation (10) also admits t-independent solutions, which correspond to the *bound* (fluxless) 1D TIQM quantum states (the previous section concerns only the scattering states).

As in the 1D TIQM case, Eq. (10) is a variational equation, obtained by extremizing the action

$$\iint dC\, dt \left[\frac{1}{2} m\dot{x}^2 - V(x) - \frac{\hbar^2}{4m} \left(\frac{x'''}{x'^3} - \frac{5}{2} \frac{x''^2}{x'^4} \right) \right], \tag{11}$$

c.f. Eqs. (1) and (3). This action is invariant under translations of both coordinates t and C. By Noether's theorem this gives rise to two conservation laws, which are easily found to be, respectively,

$$\frac{\partial}{\partial t} \left[\frac{1}{2} m\dot{x}^2 + V(x) + \frac{\hbar^2}{4m} \left(\frac{x'''}{x'^3} - \frac{5}{2} \frac{x''^2}{x'^4} \right) \right] \tag{12}$$
$$+ \frac{\hbar^2}{4m} \frac{\partial}{\partial C} \left[\left(\frac{x'''}{x'^4} - \frac{2x''^2}{x'^5} \right) \dot{x} + 2\frac{x''\dot{x}'}{x'^4} - \frac{\dot{x}''}{x'^3} \right] = 0 \;,$$

$$\frac{\partial}{\partial t} \left[m\dot{x}x' \right] + \frac{\partial}{\partial C} \left[-\frac{1}{2} m\dot{x}^2 + V(x) + \frac{\hbar^2}{4m} \left(\frac{x'''}{x'^3} - \frac{5}{2} \frac{x''^2}{x'^4} \right) \right] = 0. \tag{13}$$

The first corresponds to conservation of energy. In the free particle case, there is also a momentum conservation law, arising from x-translation symmetry:

$$\frac{\partial}{\partial t} \left[m\dot{x} \right] + \frac{\hbar^2}{4m} \frac{\partial}{\partial C} \left[\frac{x'''}{x'^4} - \frac{2x''^2}{x'^5} \right] = 0 \tag{14}$$

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Interpreted as hydrodynamical balance equations of the general form $\partial A/\partial t + \partial B/\partial C = 0$, the first square bracket in Eq. (12) [Eq. (14)] represents the energy [momentum] density, and the second term the corresponding flux. This designation is only determined up to addition of a C-derivative to the density A and subtraction of the corresponding t-derivative from the flux B. Consequently, the energy density need not conform to the standard TDQM "field" form,[3] but instead may be chosen to be the particle energy, $T+V+Q$, as in Eq. (12). This choice is appropriate for the Lagrangian $T-V-Q$ [cf. Eqs. (1) and (2)], and has the great advantage of being conserved along individual trajectories in the TIQM limiting case (in general, only the total ensemble energy is conserved). However, in the momentum conservation law Eq. (14), it does not seem to be possible to use a density that reduces to the particle momentum p in Eq. (8).

Also of note is the balance equation, Eq. (13). For any autonomous Euler-Lagrange PDE, the Lagrangian density L is determined only up to the addition of a divergence (i.e., the sum of C- and t-derivatives). We have chosen forms of the action [Eq. (11)] and the conservation laws such that L appears as (minus) the flux in Eq. (13). Via gauge transformations, it is possible to eliminate the third-order derivative from the Lagrangian and energy densities, but not from the flux of Eq. (13). The choice of L we have made has the advantage that the trajectory action, $S(C,t) = \int_0^t L(C,t')dt'$, expressed in units of $\hbar$, can be identified with the change in phase of Ψ.

We now consider Gaussian wavepacket evolution under the free particle ($V = 0$) and harmonic oscillator ($V = \frac{1}{2}m\omega^2 x^2$) potentials. The respective $x(C,t)$ solutions are

$$x_0 + \frac{p_0(t-t_0)}{m} + a\,\mathrm{erfinv}(2C-1)\sqrt{1 + \frac{\hbar^2(t-t_0)^2}{m^2 a^4}} \qquad \text{and} \qquad (15)$$

$$x_0\cos\omega(t-t_0) + \frac{p_0\sin\omega(t-t_0)}{m\omega} + a\,\mathrm{erfinv}(2C-1) \times \sqrt{\cos^2\omega(t-t_0) + \frac{\hbar^2\sin^2\omega(t-t_0)}{m^2 a^4\omega^2}}, \quad (16)$$

where x_0, p_0, t_0, a are real wavefunction parameters, and $0 \le C \le 1$. Note these solutions diverge as $C \to 0$ or 1. In general, $x(C,t)$ must diverge at the C endpoints; modulo this requirement, any solution of Eq. (10) (or its arbitrary-C generalization) can be used to reconstruct a normalized solution $\Psi(x,t)$ of the 1D TDSE.

We have successfully numerically integrated Eq. (10) for an Eckart potential and initial Gaussian wavepacket, using the Stormer-Verlet and other methods. Initial results compare favorably with those obtained using standard Ψ-based methods, but further improvements in efficiency and accuracy are planned. In any case, these calculations represent a milestone

achievement, as the *first successful synthetic Bohmian quantum trajectory calculations ever achieved for a system with substantial reflection interference*—a much-sought goal eluding chemical dynamics researchers for over a decade, and a major hurdle preventing exact quantum wavepacket calculations for large molecular systems with few reaction pathways.[4,12]

IV.   THE MANY-D TIME-DEPENDENT CASE

The 1D analysis generalizes to many-D. The single variable x is replaced with the n-dimensional configuration space vector $\mathbf{x}$, with C likewise replaced with $\mathbf{C}$, so that $\mathbf{x}(\mathbf{C}, t)$ represents an n-parameter family of trajectories. One option[9] is to take $\mathbf{C} = \mathbf{x}_0$, though we wish to consider more general choices for which $\mathbf{C}$ and $\mathbf{x}_0$ are related via any invertible coordinate transformation.

In analogy with the 1D case, it can be shown that for an arbitrary choice of the parametrization $\mathbf{C}$,

$$\rho(\mathbf{x}, t) = \frac{\rho_{\mathbf{C}}(\mathbf{C})}{\det J}, \tag{17}$$

where J is the Jacobi matrix, $J^i{}_j = \partial x^i / \partial C^j$. As in the 1D case, we mostly work with a uniformizing $\mathbf{C}$ for which $\rho_{\mathbf{C}}(\mathbf{C}) = 1$. The resulting perturbed Newton equation, i.e. the many-D generalization of Eq. (10), can be written in various different forms, the most compact being

$$m\, \ddot{x}^i + \frac{\partial V(\mathbf{x})}{\partial x^i} - \frac{\hbar^2}{4m} \frac{\partial}{\partial C^m} \left(K^k{}_i K^m{}_j \frac{\partial^2 K^l{}_j}{\partial C^k \partial C^l} \right) = 0 \; . \tag{18}$$

Here $K = J^{-1}$ denotes the inverse Jacobi matrix. The Einstein summation convention is used, albeit with some mismatched indices as we are currently assuming the Euclidean metric on $\mathbf{x}$ space.

Equation (18) is the variational PDE for the action

$$\iint d^n C \, dt \left[\frac{1}{2} m\, \dot{\mathbf{x}} \cdot \dot{\mathbf{x}} - V(\mathbf{x}) - Q \right] , \qquad \text{where} \tag{19}$$

$$Q = -\frac{\hbar^2}{4m} \left(K^k{}_j \frac{\partial^2 K^l{}_j}{\partial C^l \partial C^k} + \frac{1}{2} \frac{\partial K^l{}_j}{\partial C^l} \frac{\partial K^k{}_j}{\partial C^k} \right) \; . \tag{20}$$

Equation (19) is the many-D generalization of Eq. (11), which preserves the $L = T - V - Q$ and Ψ phase properties. Like Eq. (11), Eq. (19) has associated laws of conservation of energy and momentum. Invariance under C translation is replaced by invariance under the infinite-dimensional group of volume preserving diffeomorphisms.

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For a general (not necessarily uniformizing) choice of $\mathbf{C}$, and allowing a non-Euclidean metric $g_{ij}(\mathbf{x})$ on $\mathbf{x}$-space [note in this case a factor of $\sqrt{g}$ should be inserted in the denominator of the RHS of Eq. (17)], the action, in a simpler gauge involving only second derivatives, becomes

$$
\iint \rho_{\mathbf{C}}(\mathbf{C}) \, d^n C \, dt \left[\frac{1}{2} m \, g_{ij}(\mathbf{x}) \, \dot{x}^i \dot{x}^j - V(\mathbf{x}) \right.
$$
$$
\left. - \frac{\hbar^2}{8m} g^{jl}(\mathbf{x}) \left(\frac{\det J}{\rho_{\mathbf{C}}(\mathbf{C})} \right)^2 (J^{-1})^i{}_j (J^{-1})^k{}_l \frac{\partial}{\partial C^k} \left(\frac{\rho_{\mathbf{C}}(\mathbf{C})}{\det J} \right) \frac{\partial}{\partial C^i} \left(\frac{\rho_{\mathbf{C}}(\mathbf{C})}{\det J} \right) \right], \qquad (21)
$$

cf. Eq. (3.5) in Ref. 10. Note that a many-D solution of the TDSE gives rise to a solution of Eq. (18), but the converse holds only if the initial $\dot{\mathbf{x}}$ field is a gradient; this property is then preserved by the evolution Eq. (18).[10]

V. CONCLUDING REMARKS

We have developed a self-contained, trajectory-based formulation of spin-free nonrelativistic TDQM, achieving all goals as outlined in the Introduction. Further developments are underway. Theoretical progress will require a correct treatment of spin, relativity, particle indistinguishability, and second quantization—with a promising start having been made by Holland and others.[3,9,10] The invariance of Eq. (21) under volume-preserving diffeomorphisms suggests a connection with gravity, though the physical significance of $\mathbf{C}$ is not yet clear.

Numerically, the prospect of stable, synthetic quantum trajectory calculations for many-D molecular applications will be fully explored, as the benefits here could prove profound.[4,7,11] Our formalism offers flexibility for restricting action extremization to trajectory ensembles of a desired form (e.g., reduced dimensions), thereby providing useful variational approximations. Our exact TDQM equations are PDEs, not single-trajectory ODEs—the entire ensemble must be determined at once. But they provide the great advantage of making no reference to any external fields, such as densities or wavefunctions. Alternatively, the many-D Hamiltonian ODE approach is approximate, but evidently quite accurate.[11]

Regarding interpretation, we draw no definitive conclusions here. However, it is clearly of great significance that the form of Q can be expressed in terms of x and its C derivatives—implying the key idea that the interaction of nearby *trajectories*, rather than particles, is the

source of all empirically observed quantum phenomena (suggesting a kind of "many worlds" theory, albeit one very different from Ref. 5). As such, it is locality in *configuration* space, rather than in the usual position space *per se*, that is relevant. In effect, we have a hidden variable theory that is local in configuration space, but nonlocal in position space—though the latter is hardly "spooky" in the present nonrelativistic context [even classical theory is nonlocal in this sense, depending on $V(\mathbf{x})$]. Many ramifications are anticipated for a wavefunction-free interpretation of measurement, entanglement, etc. One wonders whether Bohm would have abandoned pilot waves, had he known such a formulation was possible— or, for that matter, whether the notion of quantum trajectories might have actually appealed to Einstein.

VI. ACKNOWLEDGEMENTS

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