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Incompleteness of trajectory-based interpretations of quantum mechanics

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Abstract

Trajectory-based approaches to quantum mechanics include the de Broglie–Bohm interpretation and Nelson's stochastic interpretation. It is shown that the usual route to establishing the validity of such interpretations, via a decomposition of the Schrödinger equation into a continuity equation and a modified Hamilton–Jacobi equation, fails for some quantum states. A very simple example is provided by a quantum particle in a box, described by a wavefunction that is initially uniform over the interior of the box. For this example, there is no corresponding continuity or modified Hamilton–Jacobi equation, and the space-time dependence of the wavefunction has a known fractal structure. Examples with finite average energies are also constructed.

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1. Introduction

The formalism of standard quantum mechanics is very different from that of classical mechanics, as are the generic phenomena described by each theory. This gives rise to a number of well-known interpretational issues when one tries to integrate classical and quantum aspects of the world. The Copenhagen interpretation of quantum mechanics remains foremost for most physicists in resolving such issues, and adequately explains the empirical content of the standard formalism. However, a number of alternative interpretations exist, and can be valuable in providing (i) reasonably coherent pictures for thinking about fundamental quantum phenomena such as interference and entanglement; (ii) means for marrying the microscopic with the macroscopic (in contrast to the enforced separation specified by the Copenhagen interpretation); and (iii) a variety of starting points for extending or modifying the standard quantum formalism.

One class of alternative interpretations is distinguished by retaining the classical concept of space-time trajectories for quantum particles. Thus, for example, in the de Broglie–Bohm interpretation particles follow trajectories in configuration space determined by a guiding wave, providing an underlying deterministic (but nonlocal) picture of quantum evolution [1, 2].

A second example is Nelson's stochastic interpretation, in which particles follow non-differentiable trajectories in configuration space determined by a stochastic generalization of Newton's second law [3, 4].

An important claim made by proponents of such trajectory-based interpretations is that they reproduce *all* predictions of standard quantum mechanics, at least for the case of nonrelativistic particles moving under velocity-independent potentials [1–4]. This general reproducibility is a necessary feature of any *complete* interpretation of the quantum formalism. Indeed, the de Broglie–Bohm and stochastic interpretations appear capable of going beyond the standard formalism, as they have even been applied to non-normalizable wavefunctions lying outside the Hilbert space of possible quantum states (e.g., sections 4.10, 4.11 of [2], and p 88 of [4]).

However, the aim of this note is to show that such trajectory-based interpretations, in fact, do *not* apply to all quantum states and, hence, are formally incomplete. Moreover, since some of the states in question have finite average energies, it is suggested that such interpretations may also be *physically* incomplete. Similar difficulties arise for any interpretation based on continuity and modified Hamilton–Jacobi equations, including the hydrodynamic and exact uncertainty approaches to quantum mechanics [2, 5, 6].

The results are based on a subtle property of the Schrödinger equation in the position representation, discussed in section 2. In particular, for certain states of quantum particles, this equation cannot be partitioned into separate terms involving spatial and temporal derivatives of the wavefunction, respectively. A simple example is provided by a wavefunction initially uniform over the interior of some region and vanishing elsewhere (e.g., a plane wave incident on a slit, or a particle confined to a box with maximal position entropy).

The existence of such states formally arises as a consequence of the unboundedness of the corresponding Hamiltonian operator—this operator cannot in fact be directly applied to a large class of wavefunctions, even though, paradoxically, these wavefunctions and their evolution are themselves perfectly well defined. Furthermore, as shown in section 3, such wavefunctions can have finite average energies, and hence can, in principle, be physically prepared from finite resources.

An important consequence of unboundedness is that the Schrödinger equation cannot always be decomposed into a continuity equation and a modified Hamilton–Jacobi equation. As discussed in section 4, the nonexistence of such a decomposition for certain states leads to an incompleteness of trajectory-based interpretations for these states.

The lack of continuity and modified Hamilton–Jacobi equations, for the particular case of a particle in a box described by an initially uniform wavefunction, is connected with the known fractal structure of this wavefunction in almost all spatial and temporal directions [7]. In section 5 it is conjectured that, more generally, the nonexistence of these equations corresponds to either the wavefunction or its spatial derivative having a fractal structure (where the latter case corresponds to examples having finite average energies).

Conclusions are given in section 6.

2. A subtlety of the Schrödinger equation

Attention will primarily be restricted to quantum systems comprising a single nonrelativistic spin-zero particle. The corresponding Hilbert space is then given by the set of square-integrable complex functions on the configuration space of the particle. It is typically assumed, in what follows, that the configuration space is one-dimensional (results can easily be generalized to higher dimensions).

Consider first a system that has a Hamiltonian operator $\hat{H}$ with a discrete spectrum $\{E_n\}$, and corresponding normalized eigenfunctions $\{\psi_n(x)\}$ satisfying

$$\hat{H}\psi_n = E_n\psi_n, \qquad \int \mathrm{d}x\, \psi_m^*(x)\psi_n(x) = \delta_{mn}. \tag{1}$$

A general state of the system at any time t is then specified by

$$\psi(x,t) = \sum_n c_n \mathrm{e}^{-\mathrm{i}E_n t/\hbar}\psi_n(x) = \mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar}\psi(x,0), \tag{2}$$

where the coefficients c_n are any set of complex numbers satisfying the normalization condition

$$\sum_n |c_n|^2 = 1. \tag{3}$$

It follows immediately from equations (1) and (2) that one has the identity

$$[\hat{H} - \mathrm{i}\hbar(\partial/\partial t)]\psi(x,t) = 0 \tag{4}$$

for all states of the system (in particular, one may apply the operator in square brackets to each term of the summation to obtain the result). This equation is, of course, the Schrödinger equation for the system. However, one *cannot* in general rewrite equation (4) in the more familiar form

$$\mathrm{i}\hbar(\partial/\partial t)\psi(x,t) = \hat{H}\psi(x,t). \tag{5}$$

It is this somewhat subtle point, the inequivalence of equations (4) and (5) for certain states, that underlies the main results of this paper.

As a simple example, consider the case of a particle of mass m confined to a one-dimensional box. If the particle is confined to the interval $[0, L]$, with $\hat{H} = -\hbar^2/(2m)(\mathrm{d}/\mathrm{d}x)^2$ and the usual (Dirichlet) boundary conditions $\psi(x,t) = 0$ at $x = 0$ and $x = L$, then the energy eigenfunctions and eigenvalues are well known to be given by

$$\psi_n(x) = (2/L)^{1/2}\sin n\pi x/L, \qquad E_n = (n\pi\hbar)^2/(2mL^2), \quad n = 1, 2, 3, \ldots . \tag{6}$$

For the particular case where the wavefunction is initially uniform over the interior of the box, one then has

$$c_n = \int_0^L \mathrm{d}x\, \psi_n^*(x)\psi(x,0) = \frac{2\sqrt{2}}{\pi n}, \quad n = 1, 3, 5, \ldots, \tag{7}$$

with $c_n = 0$ for $n = 2, 4, 6, \ldots$. Hence, at time $t = 0$,

$$\hat{H}\psi(x,0) = \sum_n c_n E_n \psi_n(x) = \frac{2\pi\hbar^2}{mL^{5/2}} \sum_{k=0}^{\infty}(2k+1)\sin\frac{(2k+1)\pi x}{L},$$

which diverges for all $x \in (0, L)$. Thus, equation (5) is meaningless for this example: the operator $\hat{H}$ acts not only to kick the wavefunction out of the Hilbert space, but to knock it right out of the set of functions altogether.

An analogous example of the inequivalence of equations (4) and (5), for the case of a *continuous* energy spectrum, is provided by a one-dimensional free particle of mass m initially confined to some interval, i.e., with Hamiltonian operator $\hat{H} = -\hbar^2(\mathrm{d}/\mathrm{d}x)^2/(2m)$ and initial wavefunction

$$\psi(x,0) = L^{-1/2}\mathrm{e}^{\mathrm{i}p_0 x/\hbar}, \quad -L/2 < x < L/2 \tag{8}$$

(corresponding, for example, to a plane wave incident on a one-dimensional slit). It follows that the wavefunction at any later time has the Fourier decomposition

$$\psi(x,t) = \left(\frac{2\hbar}{\pi L}\right)^{1/2} \int \mathrm{d}p \, \frac{\sin(p-p_0)L/2\hbar}{p-p_0} \mathrm{e}^{\mathrm{i}px/\hbar - \mathrm{i}p^2 t/(2\hbar m)},$$

and hence that $\hat{H}\psi(x,t)$ is not well-defined (in particular, the Fourier integrand of this quantity scales as $|p|$ for large $|p|$).

Thus, for some states, equations (4) and (5) are not equivalent—indeed, the latter equation has no meaning for these states. It is this fact that lies behind the incompleteness of trajectory-based interpretations, as will be seen in section 4. First, however, this subtlety of the Schrödinger equation will be investigated a little further, in the following section.

Finally, it is of interest to note that the above examples of inequivalence arise with respect to the *position* representation of the quantum state, which is of course the representation having fundamental physical significance in trajectory-based interpretations. In contrast, no analogous inequivalence arises for the Schrödinger equation in the energy and the momentum representations, for either of the examples given above. Moreover, it may be noted from equation (2) that, even in the position representation, the action of the unitary evolution operator $\hat{U}(t) = \mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar}$ is always well defined, even though the action of the Hamiltonian $\hat{H}$ is not. Thus, in accord with Wigner's theorem [8] (and forming a basic element in most axiomatic approaches to quantum mechanics), it is unitary evolution which is fundamental to describing evolution on Hilbert space, with the Schrödinger equation following as a secondary consequence.

3. Energy considerations

It is not difficult to see that the average energy $\langle H \rangle$ of the above two examples is infinite. Thus, while these examples are perfectly valid quantum states, it is difficult to conceive of any method for their physical preparation. Any interpretation that fails to explain them therefore suffers from a formal rather than a physical incompleteness. Hence, it is important to explore the issue of energy requirements further and, in particular, to determine whether examples having *finite* average energies exist.

It is convenient for this purpose to return to the case of a discrete energy spectrum (similar considerations apply to the continuous case), and suppose that the amplitudes, energy eigenvalues and eigenfunctions scale, respectively, as

$$|c_n| \sim n^{-\alpha}, \qquad E_n \sim n^{\beta}, \qquad |\psi_n| \sim n^{\gamma} \tag{9}$$

for large n, with $\alpha > 1/2$ (to ensure that the state is square-integrable). For the examples in section 2 one has $\alpha = 1$, $\beta = 2$ and $\gamma = 0$.

It follows that (ignoring unimportant phase factors)

$$\hat{H}\psi = \sum_n c_n E_n \psi_n \sim \sum_n n^{\beta-\alpha+\gamma}, \qquad \langle H \rangle = \sum_n |c_n|^2 E_n \sim \sum_n n^{\beta-2\alpha}.$$

Hence, one can arrange for $\hat{H}\psi$ diverge almost everywhere, while keeping the average energy $\langle H \rangle$ finite, by choosing $\beta - \alpha + \gamma > 0$ and $\beta - 2\alpha < -1$, respectively. This is equivalent to the condition

$$(1+\beta)/2 < \alpha < \beta + \gamma \tag{10}$$

on α (where for consistency one requires that $\beta > 1 - 2\gamma$). Equations (9) and (10) provide a large parameter range corresponding to examples of particles with finite average energies for which equation (5) is generally invalid.

Note that the form of the Schrödinger equation in equation (5) must necessarily be valid whenever $\hat{H}\psi$ happens to be a member of the Hilbert space in question (and hence is well defined), i.e. whenever

$$\langle H^2 \rangle = \int \mathrm{d}x \, |\hat{H}\psi|^2 < \infty.$$

Thus, all counterexamples must have an infinite expectation value for the *square* of the energy of the system. It follows immediately from equations (9) that $\beta - \alpha < -1/2$, leading via equation (10) to the condition $\gamma < 1/2$ for the asymptotic scaling of discrete energy eigenfunctions for any counterexample.

Finally, to give an optical example, consider a single-mode field of frequency ω in a nonlinear Kerr medium, with photon annihilation operator $\hat{a}$, number operator $\hat{N} = \hat{a}^\dagger \hat{a}$, and Hamiltonian operator

$$\hat{H} = \hbar\omega\hat{N} + \kappa\hat{N}^2.$$

The energy eigenfunctions $\psi_n(x)$, in the usual quadrature representation defined by $\hat{X} = (\hat{a} + \hat{a}^\dagger)/2$, are Hermite–Gaussians, and for large photon numbers scale as $n^{-1/4}$ on any finite interval [9]. Furthermore, for this case, one has $E_n \sim n^2$. Thus $\beta = 2$ and $\gamma = -1/4$. It then follows from equation (10) that amplitudes scaling as

$$|c_n| \sim n^{-\alpha}, \quad 3/2 < \alpha < 7/4, \tag{11}$$

yield states with finite average energy, for which the form of the Schrödinger equation in equation (5) is not valid. As a particular example, one may choose the initial state of the field to have the number state expansion

$$|\psi_0\rangle := [\zeta(13/4)]^{-1/2} \sum_{n=0}^{\infty} (n+1)^{-13/8} |n\rangle, \tag{12}$$

corresponding to $\alpha = 13/8$, where $\zeta(z)$ denotes the Riemann zeta-function and $|n\rangle$ denotes the nth photon number eigenstate. It would be of interest to find a scheme for the physical generation of such states.

4. Incompleteness

Given any wavefunction $\psi(x,t)$ associated with some quantum system, one can define quantities $P(x,t)$ and $S(x,t)$ via the polar decomposition

$$\psi = P^{1/2} \mathrm{e}^{\mathrm{i}S/\hbar} \tag{13}$$

of the wavefunction. Note that $P(x,t) = |\psi(x,t)|^2$ is the probability density associated with finding the system at position x in configuration space, at time t.

In trajectory-based interpretations of quantum mechanics, the position of the system is assumed to be a 'real' property at all times, and the probability density $P(x,t)$ reflects incomplete knowledge of this property (in the de Broglie–Bohm interpretation, $P(x,t)$ also has a more fundamental role as a 'real' physical degree of freedom associated with the guiding wave $\psi(x,t)$). Thus quantum mechanics is interpreted as describing an *ensemble* of systems, with each member of the ensemble following a specific trajectory in configuration space. Such a combination of trajectories and statistics provides an illuminating quasi-classical picture of quantum systems (although it should be noted that the trajectories can have rather 'surrealistic' properties that conflict with naive classical notions of position and its measurement [10]). The aim of such interpretations is to explain the evolution of the ensemble as a consequence of

the evolution of P and S. It is necessary to do this for *all possible* wavefunctions if such interpretations are to provide a *complete* explanation of quantum systems.

Now, if one assumes that the form of the Schrödinger equation in equation (5) is valid, then for the Hamiltonian operator $\hat{H} = -(\hbar^2/2m)\nabla^2 + V(x)$, one may multiply this equation on the left by ψ^*, and take real and imaginary parts, to obtain the corresponding equations of motion

$$\frac{\partial P}{\partial t} + \nabla \cdot \left(P \frac{\nabla S}{m} \right) = 0, \qquad \frac{\partial S}{\partial t} + \frac{|\nabla S|^2}{2m} + V - \frac{\hbar^2 \nabla^2 P^{1/2}}{2m P^{1/2}} = 0, \tag{14}$$

for P and S. The first equation is a continuity equation, ensuring conservation of probability, and the second equation is a modified Hamilton–Jacobi equation. Both the de Broglie–Bohm interpretation and Nelson's stochastic interpretation are based on these equations [1–4] and, hence, the consistency of these interpretations with quantum mechanics follows whenever equation (5) is valid.

However, as was demonstrated by explicit example in the previous sections, there are perfectly well-defined quantum states for which equation (5) is *not* valid. For these states, one *cannot* follow the above procedure to derive corresponding continuity and modified Hamilton–Jacobi equations. It follows that interpretations relying on these equations cannot explain the evolution of such states, and so are incomplete. This result in fact applies not only to trajectory-based interpretations, but also to *any* interpretation based on equations (14), including the hydrodynamic and exact uncertainty interpretations [2, 5, 6].

Note that there seems at first to be a possible caveat on the above incompleteness result. One could argue in particular that such interpretations do not *need* a corresponding Schrödinger equation—they only need equations (14). However, such an argument is consistent if and only if equations (14) lead to the same predictions as the standard quantum formalism, for the states in question. Unfortunately, this is not the case. In particular, if the continuity and modified Hamilton–Jacobi equations are assumed to be *a priori* valid for such states, then the spatial and temporal derivatives of $P^{1/2}$ and $\mathrm{e}^{\mathrm{i}S/\hbar}$ must exist almost everywhere, and one can then *derive* equation (5) from equations (13) and (14). This contradicts the examples of the previous sections. It is therefore concluded that the continuity and modified Hamilton–Jacobi equations do *not* correctly describe the states in question.

For the first example discussed in section 2, of a particle confined to a one-dimensional box with the wavefunction initially uniform over the interior of the box, the incompleteness of trajectory-based interpretations may be seen even more directly. In particular, in such interpretations, the initial wavefunction corresponds to an ensemble of particles with initial positions uniformly spread over the interior of the box (with no particles located at the boundaries of the box). Thus, in the neighbourhood of every member of the ensemble, P and S are initally constant, implying that their spatial derivatives vanish. It then follows immediately from equations (14) that P and S must remain constant everywhere in the interior of the box, i.e. that the ensemble is *stationary*. This contradicts the quantum evolution, where the wavefunction ψ evolves according to equation (2).

The above example further provides an instance of the breakdown of the velocity equation

$$v = m^{-1}\nabla S = (\hbar/m)\,\mathrm{Im}\{\psi^{-1}\nabla\psi\}, \tag{15}$$

postulated for each trajectory in the de Broglie–Bohm interpretation [1, 2], and for the average drift velocity of the forward and backward processes in Nelson's stochastic interpretation [3, 4]. In particular, it has been shown by Berry that the space-time dependence of the wavefunction $\psi(x, t)$ for this example has a *fractal* structure [7]. Hence, $\nabla\psi$ is not defined for almost all x and t and, therefore, equation (15) cannot be used to define any corresponding trajectories or processes.

5. Fractal connections

The formal cause of the incompleteness of trajectory-based (and other) interpretations is seen to stem from the fact that the form of the Schrödinger equation in equation (5) is not valid for all states—each side of this equation can be strongly divergent in the position representation, even for states with finite average energy. Here some evidence is collected suggesting that, for quantum particles, this divergence is associated with fractal structures of the corresponding wavefunctions.

For the example of the one-dimensional particle in a box, with a wavefunction initially uniform over the box, Berry has shown that the probability distribution $P(x,t)$ has fractal dimension $3/2$ in the spatial direction for almost all fixed times t, and fractal dimension $7/4$ in the time direction for almost all fixed positions x. A simplified expression for $P(x,t)$ for this example is given in [11], and an approximate experimental realization of the fractal structure, via an optical analogue, is discussed in [12, 13]. Further fractal and near-fractal wavefunctions have been constructed by Wojcik *et al* [9] and Amanatidis *et al* [14] (all having infinite average energies in the fractal limit). For such wavefunctions, both P and S in equation (13) are typically also fractals and, hence, provide further examples where equations (14) and (15) are not well defined.

The fractal nature of the wavefunctions in [7, 9] was derived as a consequence of the result that functions of the form

$$f(x) = \sum_n a_n \mathrm{e}^{\mathrm{i}nx},$$

for which the amplitudes a_n scale asympotically as

$$|a_n| \sim |n|^{-z} \quad \text{with } 1/2 < z \leqslant 3/2,$$

are continuous but nondifferentiable, and have fractal dimension $5/2 - z$ [7]. Thus, for example, for a particle in a one-dimensional box with amplitudes $|c_n| \sim n^{-\alpha}$ in equation (2), it follows via equation (6) that the wavefunction has a fractal structure whenever $1/2 < \alpha \leqslant 3/2$ (this includes the particular case of the initially uniform wavefunction, for which $\alpha = 1$). Note, however, that since $\langle H \rangle \sim \sum_n n^{2-2\alpha}$, all such examples have infinite average energies and hence cannot be physically prepared.

It turns out that fractal structures can also be associated with states having finite average energies. In particular, consider again states of the particle in the box with coefficients $|c_n| \sim n^{-\alpha}$ in equation (2), where α is now chosen to be in the parameter range corresponding to equation (10) in section 3. Since $\beta = 2$ and $\gamma = 0$ for this case, this range is given by $3/2 < \alpha < 2$. Now, by construction, the corresponding states have finite average energy and do not satisfy the form of the Schrödinger equation in equation (5). On the other hand, they do not satisfy the fractal criterion given above. However, from equation (6) one finds that the *spatial derivative* of the corresponding wavefunctions has the form

$$(\mathrm{d}/\mathrm{d}x)\psi(x,t) = \sqrt{2}\pi L^{-3/2} \sum_n n c_n \cos n\pi x/L.$$

This quantity *does* satisfy the above fractal criterion whenever $1/2 < \alpha - 1 \leqslant 3/2$ and, hence, in particular for the range $3/2 < \alpha < 2$ of interest. The corresponding fractal dimension is $7/2 - \alpha$ and, hence, also lies between $3/2$ and 2.

Based on the above results, it is conjectured that the incompleteness of trajectory-based interpretations for quantum particles corresponds to the existence of states for which the space-time dependence of the wavefunction, or of its spatial derivative, has a fractal structure.

6. Conclusions

The incompleteness of trajectory-based interpretations arises for systems with unbounded Hamiltonian operators. It applies not only to the very simple case of a wavefunction initially uniform over the interior of a box, but also to a number of examples having finite average energies and hence which can, in principle, be physically prepared. For quantum particles, the incompleteness of such interpretations appears to be connected with associated fractal structures.

Strictly speaking, one should differentiate between the notions of formal and physical incompleteness. The results of the paper show that trajectory-based interpretations are formally incomplete, as they do not describe all possible states in the Hilbert space, even though these states and their (unitary) evolution are well defined. The results further suggest that such interpretations are *physically* incomplete, as the states in question include those having finite average energies and, hence, can plausibly be physically prepared from finite resources. However, it is open to proponents of such interpretations to argue for physical completeness on the grounds that even the finite-average-energy counterexamples are unphysical. For example, noting the discussion in section 3, it would suffice to provide a convincing argument that *all* moments of the energy of a physical system must be finite.

In the case of wavefunctions for which P and S are fractals there would appear to be little chance of overcoming incompleteness, via some supplementary rule that specifies how to generate the corresponding (presumably fractal) trajectories. In contrast, in the case of wavefunctions for which the spatial derivative is a fractal, the velocity equation in equation (15) is well defined and, hence, might be used to specify a set of associated trajectories (e.g. via $\dot{x} = v$ in the de Broglie–Bohm interpretation). However, given the nonexistence of a corresponding continuity equation according to equation (14), it is not clear that an ensemble of these trajectories can evolve in agreement with the Schrödinger equation in equation (4). It would be of interest to perform some numerical experiments in this regard.

As previously remarked, the incompleteness result applies to any interpretation that relies on the continuity and modified Hamilton–Jacobi equations in equation (14) [1–6]. Thus quantum mechanics goes where these intepretations do not follow, despite their (at least in principle) duty to do so.

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