Phenomenological Derivation of the Schrödinger Equation

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The Schrödinger equation is derived classically assuming that particles present local random spatial fluctuations compatible with the presence of the zero-point field. Without specifying the forces arising from this permanent matter-field interaction but exploring its fundamental properties (homogeneity, isotropy and random aspect) to justify the emergence of the continuity equation in one-particle context, these fluctuations are described in terms of the probability density. Specifically, the starting point is the assumption that the local activities, which turn the path followed by the particle totally unpredictable, must be associated with an energy proportional to $\partial P/\partial t$. The polar form of the wave function, which connects the obtained classical equations with the corresponding quantum equation, emerges as a by-product of the approach.

1 Introduction

The evolution of the wave function in single-particle quantum systems is described by the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial\psi}{\partial t}, \tag{1}$$

where m is the mass and V is a potential. The complex wave function is generally presented in its polar form

$$\psi = \sqrt{P}\exp(iS/\hbar), \tag{2}$$

where $P=|\psi|^2$ is the probability density, and $S/\hbar$ is a phase. Substituting (2) into (1) results in two equations

$$\frac{\partial P}{\partial t} + \nabla\cdot\left(P\frac{\nabla S}{m}\right) = 0, \tag{3}$$

and

$$\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + V + Q = 0, \tag{4}$$

where

$$Q = -\frac{\hbar^2}{4m}\left[\frac{\nabla^2 P}{P} - \frac{1}{2}\frac{(\nabla P)^2}{P^2}\right] \tag{5}$$

is known as quantum potential. At the classical limit ($\hbar \to 0$) Q vanishes and (4) reduces to the Hamilton-Jacobi equation. For this reason, Bohm [1] suggested that S is the classical action function, which relates to the actual velocity, $\mathbf{v} = \nabla S/m$, of the particle. In this way (3) simply expresses the conservation of probability.

This alternative way of writing the Schrödinger equation presents advantages as regards its interpretation in terms of classical variables. However, the problem of ignoring the path followed by the particle persists. And more, we have an obvious increase in complexity: The Schrödinger equation is a single function and quite simple, on the other hand, the equation (4) is somewhat complicated - and still requires the continuity equation to account local activities. And above all, thinking that the quantum revolution, highly non-classical, has its origin in a classical equation with an additional potential is not very easy. In reality, Q is not a traditional potential, but part of the description of the motion, that is, P is playing the role of a dynamical variable at the same footing as S. Thus S and P can be said to codetermine each other. However, in approximate schemes to get information about quantum systems it can be used as a potential [2].

Equation (4) is referred as stochastic Hamilton-Jacobi-Bohm equation. Despite the fact that P is unique for a given quantum system, it is interpreted as a differential equation describing an ensemble of trajectories. This is grounded in the fact that the action S was originally defined as a field variable related with a set of potential trajectories [3].

It is paid much attention to equation (4) and less concern about (3). From a dynamical point of view, the emergence of the continuity equation is the most remarkable result: It highlights the local loss of determinism ($\partial P/\partial t \neq 0$), is valid for one-particle systems (it was obtained in this way), and contains inherently the multiple path aspect of quantum systems [4], exactly how is assigned to equation (4).

Fundamentally, to have $\partial P/\partial t \neq 0$ (change of probability at a given position), and thus to justify the emergence of the equation (3), it is necessary that the particle runs local random spatial fluctuations. Otherwise, there are local preferences, and these combined with the dynamics that emanates from the potential V (deterministic) results in a classical trajectory. Therefore these fluctuations require the presence of external forces with special features. Indeed, these forces exist and are related with the zero-point field (ZPF). They are formally treated in the context of the stochastic electrodynamics [5, 6], and under certain conditions they may be measured [7, 8]. However, their definition is outside the scope of this work; just let's enumerate its indispensable characteristics to justify

the continuity equation in the context of one-particle dynamics.

The above rewriting of the Schrödinger equation starts from propositions valid within the quantum formalism and arrives at seemingly classical equations. What will be done in the present paper is to follow an inverse path. The starting point is the fact that the local changes of the probability density — associated with isotropic random spatial fluctuations impressed by the ZPF — must be related with an energy.

2 The multi path aspect of the motion

Suppose a particle of mass m performing a motion with velocity $\mathbf{v}$. If the associated probability density P is a continuous function of the coordinates and time, then its dynamical evolution along the trajectory is given by

$$\frac{dP}{dt} = \frac{\partial P}{\partial t} + \mathbf{v} \cdot \nabla P, \tag{6}$$

where $\partial P/\partial t$ refers to the change of probability at a given position, and the second term accounts for the spatial changes. As P is a probability, then we cannot precise the angle between ∇P and $\mathbf{v}$. Moreover, in principle, ∇P can show an isotropic distribution around each position. Indeed, as P is a conserved quantity, then the change of the probability density inside a given volume Ω (arbitrary), containing the instantaneous position of the particle, must be equal to the probability flux through a surface A surrounding this volume. Formally, we have

$$\frac{\partial}{\partial t}\int_{\Omega} P d\Omega = -\int_{A} P\dot{\mathbf{r}} \cdot d\mathbf{A}, \tag{7}$$

where $\dot{\mathbf{r}}$ is a velocity, and the vector field $P\dot{\mathbf{r}}$ represents all possible probability currents that cross the surface A. Obviously, if the particle is inside this volume, it emerges following one of these possibilities. In accordance with the properties of the ZPF, the field $P\dot{\mathbf{r}}$ must present an isotropic distribution, however, as the velocity of the particle is dictated by the dynamics of the system as a whole, then there are some privileged probability currents (the resulting motion is not a random walk). According to Green's theorem and equation (7), each one of the possible currents obeys

$$\frac{\partial P}{\partial t} + \nabla \cdot (P\dot{\mathbf{r}}) = 0. \tag{8}$$

As this process is repeated at all positions where the particle can be found, linking the successive probability currents, according to which the particle emerges from each volume Ω, is defined a path described by the velocity

$$\mathbf{v} = \frac{\nabla S}{m}, \tag{9}$$

where S is the Hamilton-Jacobi function of one possible path [3, see p. 36]. Therefore equation (8) must be written as (3).

If the local activities are ignored (classical limit), then the function S is defined on a single trajectory. This also can be easily inferred making $\partial P/\partial t = 0$ in equation (7). In this case the probability flux that enters the volume Ω equals the one that emerges from it. This means that the particle has only one possibility (probability current) to leave each successive volume Ω.

If the external field acts on the particle everywhere (homogeneously), without preferred directions (isotropic) and in a totally unpredictable (random) way, that is, like the ZPF, then we will have a local motion compatible with the continuity equation. Therefore, as the particle has several possibilities to leave each position (following one possible current $P\dot{\mathbf{r}}$), this assigns a multi path aspect to the motion. This means that the particle can travel on each one of them indiscriminately; there is no preferred path. Note, not having a preferred path means that all are equally probable. We realize that this fact is consistent with the formulation of quantum mechanics in terms of path integrals, where Feynman and Hibbs [4, see p. 28] begin with the following statement: "Now we can give the quantum-mechanical rule. We must say how much each trajectory contributes to the total amplitude to go from a to b. It is not that just the particular path of extreme action contributes; rather, it is that all the paths contribute. They contribute in equal amounts to the total amplitude, but contribute as different phases. The phase of the contribution from a given path is the action S for that path in units of the quantum of action $\hbar$". Coincidently, this is a description of the evolution operator $\exp(iS/\hbar)$ (unitary), present in (2), which is the core of the path integrals.

3 The main proposition

In a classical system, the particles are actuated by forces in such a way that they move along single predictable trajectories, and this leads to $\partial P/\partial t = 0$ everywhere (the local activities are ignored). By other side, if particles are being actuated by a field, with the characteristics pointed above, local exchange of energy between them occurs in such a way that $\partial P/\partial t \neq 0$. Admitting that this is a fact, let's write an effective stationary action function S_{eff} that, in addition to describing a path through the function S, also takes into account the local activities described in terms of probability density, that is,

$$S_{eff} = S + S_l, \tag{10}$$

where S_l is a local action that depends only on P. Following the same formalism obeyed by the stationary Hamilton's function, the energy and momentum of the particle over a possible path are, respectively, written as

$$H = -\frac{\partial S_{eff}}{\partial t} = -\frac{\partial S}{\partial t} - F\frac{\partial P}{\partial t}, \tag{11}$$

and

$$\mathbf{p} = \nabla S_{eff} = \nabla S + F\nabla P, \tag{12}$$

where $F = \partial S_l/\partial P$ should be a function of P which must comply the dynamics of the system. Specifically, this function must obey the conservation of probability and the local conservation of energy (the particle cannot extract energy from the field indefinitely).

The motion equations of the system can be obtained in the following way: As S and P are taking values on a volume, then the average energy of the multi path system need to be written in the form

$$\bar{H} = \int d^3rPH = \int d^3r\mathcal{H}, \tag{13}$$

where the integral is taken over whole space. Here, $\mathcal{H}$ has the role of Hamiltonian density. With H given by (11) we have

$$\bar{H} = \int d^3rP\left(-\frac{\partial S}{\partial t} - F\frac{\partial P}{\partial t}\right). \tag{14}$$

As $\bar{H}$, written in this way, is a functional of the functions S and P, taking the functional derivatives with respect to these functions, according to the well known rules

$$\frac{\delta\bar{H}}{\delta\xi} = \frac{\partial\mathcal{H}}{\partial\xi} - \frac{\partial}{\partial x_\alpha}\left(\frac{\partial\mathcal{H}}{\partial(\partial\xi/\partial x_\alpha)}\right), \tag{15}$$

where $x_\alpha = x, y, z, t$ and $\xi = S$ or P, we obtain respectively

$$\frac{\delta\bar{H}}{\delta S} = \frac{\partial P}{\partial t} \tag{16}$$

and

$$\frac{\delta\bar{H}}{\delta P} = -\frac{\partial S}{\partial t}. \tag{17}$$

This shows that the proposition (10) preserves the shapes of the canonical equations, where S and P behave as dynamical conjugate variables of the canonically transformed Hamiltonian $\bar{H}$ [1].

Taking into account the momentum (12), the energy (11) can be expressed by

$$H = \frac{|\nabla S + F\nabla P|^2}{2m} + V, \tag{18}$$

then (13) can also be written as

$$\bar{H} = \int d^3rP\left(\frac{|\nabla S + F\nabla P|^2}{2m} + V\right), \tag{19}$$

and, consequently, the canonical equation (16) takes the form

$$\left[\frac{\partial P}{\partial t} + \nabla\cdot\left(P\frac{\nabla S}{m}\right)\right] + (F + PF')\frac{(\nabla P)^2}{m} + PF\frac{\nabla^2 P}{m} = 0, \tag{20}$$

where $F' = \partial F\,/\,\partial P$. The first term, being the continuity equation, is zero, and the trivial solution of the resulting equation gives simultaneously $F = cte/P$ and $F = 0$. However, if this trivial solution is valid, F is not defined in the field of real numbers.

Generalizing the constant to complex numbers, the non zero solution is written as $F = (S_1 + iS_0)/P$, where S_1 and S_0 are real constants (they have dimension of action). Thus, returning this complex shape of F into (19), from (16), results

$$\left[\frac{\partial P}{\partial t} + \nabla\cdot\left(P\frac{\nabla S}{m}\right)\right] + S_1\frac{\nabla^2 P}{m} = 0, \tag{21}$$

which shows that probability conservation is obeyed if F is a pure imaginary ($S_1 = 0$). As this occurs independently of the P^{-1} functionality, then it only justifies the complex aspect of the trivial solution of (20).

Another evidence that F is pure imaginary comes from the fact that the momentum (12) is apparently incompatible with the actual velocity (9); it seems that we should have

$$\mathbf{v} = \frac{\nabla S}{m} + F\frac{\nabla P}{m}. \tag{22}$$

In reality, this behavior is not entirely unexpected, since, as we saw earlier, the actual velocity is the end result of the system dynamics as a whole, that is, S is also dictated by the local activities. Therefore, to reconcile these equations, F shall be such that (9) refers to the real part of (22).

The resulting apparent complex character of the energy (11) and the momentum (12) is only a stage of the calculations. In effect, the canonical equations (16) and (17) can also be obtained even making

$$\int d^3rP\left(-F\frac{\partial P}{\partial t}\right) = 0 \tag{23}$$

in Eq. (14), which makes the average energy (14) real. However, this implies that, on average, the exchange of energy between the particle and the field is zero, meaning that the energy provided by field is promptly returned to it in equal amount. This, besides constituting the desired local energy balance — it can be related with atomic stability [9] — also puts some insight in the complex shape of the mentioned real quantities.

In fact, the local energy balance (23) is satisfied by the trivial solution of (20), expressed by

$$F = \frac{\partial S_l}{\partial P} = \imath\frac{S_o}{P}, \tag{24}$$

as can be easily verified from the normalization of P. So this proven the P^{-1} functionality, which is not achieved only from probability conservation, as pointed above.

Substituting (24) into (19), results in

$$\bar{H} = \int d^3rP\left(\frac{(\nabla S)^2}{2m} + \frac{S_o^2}{2m}\frac{(\nabla P)^2}{P^2} + V\right), \tag{25}$$

which, with the canonical equations (16) and (17), reproduces the equations (3) and (4), respectively, if S_0 is identified with

$\hbar/2$. Therefore, to complete the classical derivation of the Schrödinger equation, the anzatz (2) must also be obtained in a classical context. This is the subject of the next section.

4 Parameterization of the equations

Knowing any one of the solutions (one of the paths) of the motion equations resulting from (25), the energy and momentum at each position, according to the equations (13), (12) and (24), are, respectively, given by

$$H = -\frac{\partial S}{\partial t} - \frac{\imath S_o}{P}\frac{\partial P}{\partial t} \tag{26}$$

and

$$\mathbf{p} = \nabla S + \frac{\imath S_o}{P}\nabla P. \tag{27}$$

Integrating these partial differential equations (minus a possible constant), we obtain the following dimensionless equation

$$\frac{1}{2\imath S_o}\left(\sum_i \int_0^{x_i} p_i dx_i - \int_0^t H dt\right) = \frac{S}{2\imath S_o} + \ln\sqrt{P}, \tag{28}$$

as can be easily verified by following the inverse procedure. The upper limits of the integrals are the coordinates and time of the positions occupied by the particle along a possible path, therefore the left hand side of (28) is a complex function of these parameters, which will be defined in the following way:

$$\ln\psi = \frac{1}{2\imath S_o}\left(\sum_i \int_0^{q_i} p_i dq_i - \int_0^t E dt\right). \tag{29}$$

As both sides of (28) are independent of the path followed by the particle, we can write the following relation between S and P, valid for all paths:

$$\ln\psi = \frac{S}{2\imath S_o} + \ln\sqrt{P}, \tag{30}$$

or

$$\psi = \sqrt{P}\exp\left(\frac{S}{2\imath S_o}\right). \tag{31}$$

This equation with $S_0 = \hbar/2$ is in full agreement with (2). And more, for constant energy and momentum the function defined in (29) is a solution of the Schrödinger equation for a free particle.

Finally, let's re-write the equations obtained in this work in terms of ψ. From (30) and its complex conjugate we obtain the following parametric shapes for S and P:

$$S = \frac{\imath\hbar}{2}\left(\lg\psi - \ln\psi^*\right) \tag{32}$$

and

$$P = \psi^*\psi. \tag{33}$$

Consequently, the equations (25), (26) and (27) can be re-written, respectively, in the forms:

$$\bar{H} = \int d^3 r\left(\frac{\hbar^2}{2m}\nabla\psi^*\cdot\nabla\psi + \psi^* V\psi\right), \tag{34}$$

$$\imath\hbar\frac{\partial\psi}{\partial t} = H\psi, \tag{35}$$

and

$$-\imath\hbar\nabla\psi = \mathbf{p}\psi. \tag{36}$$

Applying the divergence operator on both sides of equation (36), allied to fact that $\mathbf{p}$ is coordinate independent (it is independent of the followed path), gives

$$-\imath\hbar\nabla\cdot\nabla\psi = \mathbf{p}\cdot\nabla\psi, \tag{37}$$

and expressing $\mathbf{p}$ in terms of the complex conjugate of (36), we obtain the equality

$$-\psi^*\nabla^2\psi = \nabla\psi^*\cdot\nabla\psi. \tag{38}$$

Therefore the equation (34) can be written in the well known quantum form

$$\bar{H} = \int d^3 r\psi^*\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi. \tag{39}$$

5 Conclusion

The approach shows that the Schrödinger equation and its accessory are necessary and natural equations, parameterized shapes of the complicated — not to say unsolvable — equations resulting from a classical treatment including a special field with homogeneous, isotropic and random characteristics.

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References

1. Bohm D. A suggested interpretation of the quantum theory in terms of "hidden variables" I. *Physical Review*, 1952, v. 85, no. (2), 166–179.
2. Nerukh D., Frederick J. H. Multidimensional quantum dynamics with trajectories: a novel numerical implementation of the Bohmian mechanics. *Chemical Physics Letters*, 2000, v. 332, 145–153.
3. Holland P. V. The Quantum Theory of Motion. Cambridge University. Press, Cambridge, 1993.
4. Feynman R. P., Hibbs A. R. Quantum Mechanics and Path Integrals. McGraw-Hill Book Company 1965.
5. Milonni P. W. The Quantum Vacuum: An Introduction to Quantum Electrodynamics. Academic Press, 1994.
6. de la Peña L., Cetto A. M. The Quantum Dice. An Introduction to the Stochastic Electrodynamics. Kluwer Academic, Dordrecht, 1996.
7. Casimir H. B. G. On the attraction between two perfectly conducting plates. *Proceedings of the Royal Netherlands Academy of Arts and Sciences*, 1948, v. B51 793–795.
8. Lamoraux S. K. Demonstration of the Casimir Force in the 0.6 to 6μm Range. *Physical Review Letters*, 1997, v. 78, no. 1, 5–8.
9. Puthoff H. E. Ground state of hydrogen as a zero-point-fluctuation-determined state. *Physical Review D*, 1987, v. 35, no. 10, 3266–3269.