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The principle of minimal quantum fluctuations for the time-dependent Schrödinger equation

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Abstract. It is shown that the optics–mechanics analogy which originally led Schrödinger to his famous equation stops at the time-independent level. For potentials involving time explicitly, the time-dependent Schrödinger equation cannot be deduced in a similar manner. Instead, a variational principle for the time-dependent Schrödinger equation is established. It minimizes the total quantum fluctuations of a newly defined Hamilton–Jacobi function about its limiting classical value over space–time, thereby demonstrating the existence of a deeper relationship between classical and quantum mechanics beyond the simple optics–mechanics analogy. This principle is similar in spirit to Feynman's space–time approach to quantum mechanics.

It is often useful to express the same physics in different mathematical forms such as a differential equation, or a variational principle, etc, since each may provide a different way of thinking about the physics, or of embarking on a new discovery. The Feynman path-integral formulation of quantum mechanics is a familiar example. In what follows we shall derive a variational principle for the time-dependent Schrödinger equation (TDSE) which seems to show a more intimate connection between classical mechanics and wave mechanics than hitherto anticipated. It should provide another way of thinking about processes in space–time quantum mechanically.

It is well known that in the original derivation of the time-independent Schrödinger equation (TISE), Schrödinger first wanted merely to find a suitable partial differential equation for the hydrogen atom whose solutions were required to be everywhere real, single-valued, finite and twice differentiable. He commenced with the time-independent Hamilton–Jacobi equation (TIHJE)

$$(\nabla S)^2 - 2m\big(E - V(x)\big) = 0. \tag{1}$$

An equation of the desired type could not be obtained directly from (1). So, he replaced S by $K \log \psi$, thus transforming (1) into

$$(\nabla\psi)^2 - \frac{2m}{K^2}(E - V(x))\psi^2 = 0 \tag{2}$$

where K is treated as a constant.

A differential equation of the required form could now be derived by assuming that the variation of the integral of the left-hand side of (2), taken over all space, should vanish [1, 2]. On applying the Euler–Lagrange conditions, Schrödinger arrived at his TISE:

$$H\psi - E\psi = 0 \qquad \text{or} \qquad \frac{K^2}{2m}\nabla^2\psi + (E - V(x))\psi = 0 \tag{3}$$

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provided he took K to be $\bar{h}$ in order to yield the Balmer series [3]. Note, however, that since the function S of the classical HJ equation is real, the corresponding ψ must also be understood as real, rendering ψ less general than it should be. Furthermore, the transformation of S to ψ is purely mathematical and the substitution of (2) by the variational principle is just to produce a formally suitable differential equation which, by itself, did not seem to have any justification. It was in his second communication on wave mechanics [4] that he supplied the justification by introducing the optics–mechanics analogy.

This analogy was based on an ingenious observation of the parallel between the geometric or 'ray' limit of optics, equation (4), and the Hamilton–Jacobi (HJ) form of classical dynamics, equation (5):

$$(\nabla L)^2 = n^2(x) \tag{4}$$

$$(\nabla W)^2 = 2m(E - V(x)). \tag{5}$$

In (4), the eikonal $L(x)$ is the spatial part of the phase associated with the electromagnetic potential wave, $\phi(x,t)$:

$$\begin{aligned}\phi(x,t) &= \phi(x)\exp(-\mathrm{i}2\pi\nu t)\\ &= A(x)\exp\left(\mathrm{i}2\pi\left(\frac{L(x)}{\lambda_0} - \nu t\right)\right)\end{aligned} \tag{6}$$

where both $A(x)$ and $L(x)$ are real. The spatial part $\phi(x) = A(x)\exp(\mathrm{i}2\pi L(x))$ generally obeys the Helmholtz equation

$$\nabla^2\phi(x) - k_0^2 n^2(x)\phi(x) = 0 \tag{7}$$

whose ray limit is just (4). On the other hand, the characteristic function $W(x)$ in (5) is the spatial portion of the principal function $S(x,t)$ of particle mechanics of (1):

$$S(x,t) = W(x) - Et. \tag{8}$$

Comparisons between equations (4) and (5) and between the total phases in the EM wave of (6) and in the advancing particle wavefront with constant S according to (8) enabled Schrödinger to make the mechanics–optics analogy that

$$W(x) - Et = \frac{hL(x)}{\lambda_0} - h\nu t \tag{9}$$

or separately,

$$W(x) = \frac{hL(x)}{\lambda_0} \tag{9a}$$

and

$$E = h\nu \tag{9b}$$

where the same constant of proportionality h is inserted in both equations. This constant is identified as being the Planck constant.

For Schrödinger, identifying the left-hand side of (9) as the phase of the particle wavefront in its corresponding ray limit furnished the important first step. Recognizing that the classical particle trajectories are merely rays normal to such wavefronts, he now went beyond the ray limit by attaching a crucial time-independent amplitude to that phase factor, thereby rounding it up to a complete wavefunction:

$$\begin{aligned}\psi(x,t) &= A(x)\exp\left(\mathrm{i}\frac{W(x) - Et}{\bar{h}}\right)\\ &= \psi(x)\exp\left(-\mathrm{i}\frac{Et}{\bar{h}}\right)\end{aligned} \tag{10}$$

On the basis of the optics–mechanics analogy embodied in equations (4), (5) and (9*a*), (9*b*), it was then natural to assert [4] that the spatial part $\psi(x)$, just like $\phi(x)$ of (7), should indeed be governed by another Helmholtz-type equation, i.e. the TISE (3). The role of the spatially varying refractive index $n(x)$ in ray optics of (4) is seen to be played by the square root of the local kinetic energy, $\sqrt{E - V(x)}$, in the HJ mechanics of (5).

We now switch our focus to the time-dependent Schrödinger equation (TDSE), the subject of the present investigation.

Schrödinger himself generalized his wave equation to a time-dependent one by simply differentiating the time-dependent factor $\exp(-\mathrm{i}\frac{Et}{\hbar})$ of (10) which, together with (3), are then turned into

$$\begin{aligned} H\psi(x,t) &= \left(-\frac{\hbar^2}{2m}\nabla^2 + V(x)\right)\psi(x,t) \\ &= \mathrm{i}\hbar\frac{\partial\psi(x,t)}{\partial t}. \end{aligned} \tag{11}$$

It was in this somewhat cavalier manner that the TDSE was originally derived. It is obvious that this procedure works when the system possesses a definite energy. It can easily be shown that it is still valid for a wave packet comprised of states of several different energies, as long as the potential V does not depend on time explicitly, as has been assumed from (1) and up to this point. This procedure breaks down completely, however, when the potential depends explictly on time. There is no *a priori* reason to expect equation (11) to be valid when $V = V(x,t)$. Aside from claiming agreement with experiment, we want to look for a more natural way of arriving at the TDSE, imagining ourselves to be back in the days of Schrödinger again.

One possible way is to return again to the variational principle which led Schrödinger to his TISE (3) in the first place.

We first observe that the optics–mechanics analogy has its limits. When an optical medium is characterized by a refractive index not only varying in space but also in time, the wave equation becomes

$$\left(\nabla^2 - \frac{n^2(x,t)}{c^2}\frac{\partial^2}{\partial t^2}\right)\phi(x,t) = 0. \tag{12}$$

A substitution of $\phi(x,t) = \phi(x)\exp(-\mathrm{i}\omega t)$ would no longer work; it will not produce a time-independent part of the wave equation such as equation (7), since no definite frequency ω could adequately describe the time evolution. We are thus left with a rather inflexible second-order differential equation, quite unlike the first-order, time-dependent Hamilton–Jacobi equation (TDHJE):

$$(\nabla S)^2 + 2m\left(V(x,t) + \frac{\partial S}{\partial t}\right) = 0. \tag{13}$$

Unlike the close resemblance between equations (4) and (5), no easy anology between equations (12) and (13) can be drawn to establish a wave version of the HJ mechanics such as (10) in the presence of time-dependent potentials. We seem to have reached the end of the road as far as the analogy goes.

Citing the success of the optics–mechanics analogy in deriving the TISE (3) as the justification for the use of the time-independent variational principle, we now boldly adapt this principle to time-dependent situations.

Naturally, we proceed with (13) rather than (1). Recognizing that the function $S(x,t)$ is proportional to the phase of the advancing wavefronts with constant S, as was clear from its

previous time-independent version, equation (8), we construct our fully-fledged wavefunction $\psi(x,t)$ as

$$\psi(x,t) = A(x,t)\exp\left(\mathrm{i}\frac{S(x,t)}{\hbar}\right) \tag{14}$$

where $A(x,t)$ is a real amplitude dependent on both x and t. Thus ψ is a genuine complex function, distinct from its complex conjugate, ψ^*. We now define a new function of ψ and ψ^*, called the HJ function, by

$$F(\psi,\psi^*;t) \equiv \frac{\hbar^2}{2m}\frac{\partial\psi}{\partial x}\frac{\partial\psi^*}{\partial x} + V(x,t)\psi\psi^* + \frac{\hbar}{2\mathrm{i}}\left(\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t}\right). \tag{15a}$$

The classical HJ mechanics, equation (13), is described in terms of ψ and ψ^* by

$$F(\psi,\psi^*;t) = 0 \tag{15b}$$

because the amplitude $A(x,t)$ becomes simply a constant in the classical limit, as it was similarly for equation (2).

If $\psi(x,t)$ satisfies the above equation, a different ψ, say, with a fully space- and time-dependent $A(x,t)$, would generally not satisfy this equation. We now postulate a variational principle, not for the classical $\psi(x,t)$ that satisfies (15*b*), but for the true wavefunction which only approaches the classical $\psi(x,t)$ in the limit of slow variation for the amplitude $A(x,t)$. This principle is akin to the one originally adopted by Schrödinger for the time-independent ψ, which we now call the principle of minimal quantum fluctuations:

$$\begin{aligned} 0 &= \delta\int F(\psi,\psi^*;t)\,\mathrm{d}x\,\mathrm{d}t \\ &= \delta\int\left\{\frac{\hbar^2}{2m}\frac{\partial\psi}{\partial x}\frac{\partial\psi^*}{\partial x} + V(x,t)\psi\psi^* + \frac{\hbar}{2\mathrm{i}}\left(\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t}\right)\right\}\mathrm{d}x\,\mathrm{d}t. \end{aligned} \tag{16}$$

While the integrand in (16) is just (15*a*), the integration is not only over all space but also over time. Since the amplitude is allowed full variation, ψ and ψ^* can be varied independently. Upon integrating by parts with no variations allowed at the distant space–time boundary, equation (16) immediately leads to the correct TDSE

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x,t)\psi + \frac{\hbar}{\mathrm{i}}\frac{\partial\psi}{\partial t} = 0 \tag{17}$$

and its complex-conjugate counterpart. Since $F_{\mathrm{class}}(\psi,\psi^*;t) \equiv F(\psi_{\mathrm{cl}},\psi^*_{\mathrm{cl}};t) = 0$, the deviation of the HJ function $F(\psi,\psi^*;t)$ from its classical counterpart $F_{\mathrm{class}}(\psi,\psi^*;t)$ is

$$\Delta F \equiv F(\psi,\psi^*;t) - F_{\mathrm{class}}(\psi,\psi^*;t) = F(\psi,\psi^*;t). \tag{18}$$

This means that the fluctuation ΔF is totally quantum mechanical in nature. Our variational principle (16) states that the total fluctuations of F about F_{class} over the entire space–time domain is a minimum with respect to the changes of ψ and ψ^*:

$$\int \Delta F(\psi,\psi^*;t)\,\mathrm{d}x\,\mathrm{d}t = \text{minimum}. \tag{19}$$

Note that it is the first-order nature of the TDHJE (13) or (15*b*) which gives rise eventually to the first-order TDSE (17). In contrast, the optics–mechanics analogy stops at the time-independent level. The first-order TDSE can never be drawn from any parallel between the TDHJE (15*b*) and the second-order wave equation (12) in optics. Without guidance from any analogy there is no *a priori* reason why the TDHJE should lead us to the realm of quantum mechanics. Our success by starting from the TDHJE (13) or (15*b*) seems to say that the classical

HJ equation, in both its time-independent and time-dependent forms, is more fundamentally related to wave mechanics in its own right than the relationship implied by the simple optics–mechanics analogy as first conceived by Schrödinger. So, even without the anology, classical mechanics and wave mechanics are intimately and deeply related in that the total fluctuations over space–time of $F(\psi, \psi^*; t)$ about its classical limit must be minimized to obtain the correct wavefunction $\psi(x, t)$.

In the special case of $V = V(x)$, the time-dependent equations (17) and (16) reduce immediately, of course, to the TISE and the corresponding static variational principle, respectively. Finally, we remark that the time-dependent variational approach (19) is similar in spirit to the space–time approach of Feynman to quantum mechanics [5], in that all the different space–time paths from an initial state $\psi(x, t_i)$ $\left(= \sqrt{\delta(x - x_i)}\right.$ at $t = t_i$ in the case of the Feynman propagator $\left.K(x, t; x_i, t_i)\right)$ to the final destination x, t must all be sampled, and their contributions compared, before the true final-state wavefunction $\psi(x, t)$ (or the Feynman amplitude $K(x, t; x_i, t_i)$) can be determined in both approaches.

In conclusion, we note that while the mathematical step of changing from the static variational principle to the present time-dependent one might seem trivial once it has been pointed out, the implication of the deeper connection between classical and quantum mechanics should be significant, in addition to providing a fresh way of thinking about quantum processes in space–time.

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