A variational principle, wave-particle duality, and the Schrödinger equation

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Abstract. A principle is proposed according to which the dynamics of a quantum particle in a one-dimensional configuration space (OCS) is determined by a variational problem for two functionals: one is based on the mean value of the Hamilton operator, while the second one is based on the mean value of the total energy of the particle, which is determined through the phase of the wave function with help of the generalized Planck-Einstein relation. The first functional contains information about the corpuscular properties of a quantum particle, and the second one comprises its wave properties. The true dynamics is described by a wave function for which the variations of these two functionals are equal. This variational principle, which can also be viewed as a mathematical formulation of wave-particle duality, leads to the Schrödinger equation.

1. Introduction: the Schrödinger equation and the principle of least action

As is known, the Schrodinger equation cannot be derived on the basis of the axioms of standard quantum mechanics and, therefore, is considered by most researchers as its independent postulate. However, such a state of affairs, when one of the main postulates of a physical theory is formulated in the form of a (albeit brilliantly guessed) mathematical equation that does not have a generally accepted physical interpretation, is unacceptable for a physical theory. In this regard, many attempts were made to formulate a physical principle that, on the one hand, would make it possible to derive this equation and fill it with physical content, and, on the other hand, would not contradict the already known principles of quantum mechanics.

Among the most well-known directions in solving this problem are the "hydrodynamic formulation" of Madelung-de Broglie-Bohm, based on the concept of "quantum fluid" (here we mention only the recent work [1]), as well as the "quantum-field" approach (see, for example, [2, 3, 4]), where the Schrödinger equation is treated as a classical field subject to quantization. In the "quantum-field" approach, this equation is derived from the principle of least action, and it is important to understand to what extent this principle, which plays a fundamental role in classical mechanics, respects the quantum mechanical principles.
As is known (see [2, 3]), in the quantum-field approach the Schrödinger equation (for simplicity we restrict ourselves to the one-dimensional case) appears as the Euler equation
\[
\frac{\partial L}{\partial \psi} - \frac{\partial}{\partial x} \left( \frac{\partial L}{\partial \psi_x} \right) - \frac{\partial}{\partial t} \left( \frac{\partial L}{\partial \psi_t} \right) = 0
\] (1)
in the variational problem for the Lagrangian density
\[
L = \frac{i\hbar}{2} (\psi^* \psi_t - \psi \psi_t^*) - \frac{\hbar^2}{2m} \psi_x^* \psi_x - V(x) \psi^* \psi;
\] (2)
here \( \psi(x, t) \) is the wave function, and \( \psi_x \) and \( \psi_t \) are its \( x \)- and \( t \)-derivatives, respectively; \( V(x) \) is the potential of the external field in which the particle moves.

As we can see, the derivatives \( \psi_x \) and \( \psi_t \) enter this equation in the same way, and, as shown in [4], in this problem one can construct a consistent mathematical model of canonical quantization, where the time \( t \) is equipped with the corresponding operator. However, what is acceptable for canonical quantization is unacceptable for nonrelativistic quantum mechanics, where \( t \) is a parameter. Thus, it is impossible to introduce Hamilton’s principle (instead of postulating the Schrödinger equation) into standard quantum mechanics without affecting its axioms.

In this article, we will show that it is possible to formulate a modified variational principle that not only leads to the Schrödinger equation (without violating other principles of quantum mechanics), but also allows us to deepen the concept of wave-particle duality. As is known, this concept reflects one of the fundamental properties of a quantum particle. But at present, this property is formulated as a general philosophical idea that allows mathematical formulation – in the form of the de Broglie relation and the Planck-Einstein relation - only in the case of single de Broglie waves. In this article, we propose a mathematical formulation of wave-particle duality for an arbitrary (pure) quantum mechanical state. It is this formulation that will form the basis of the modified variational principle, from which the Schrödinger equation will be derived.

2. Generalized Planck-Einstein relation

Let the state of a particle moving in a one-dimensional configuration space (OCS) under an external field \( V(x, t) \) be described by the wave function
\[
\psi(x, t) = R(x, t) e^{i\phi(x, t)},
\] (3)
where \( R(x, t) \) and \( \phi(x, t) \) are the amplitude and phase of the wave function; \( \int_{-\infty}^{\infty} R^2(x, t) dx = 1 \). It is assumed that \( \psi(x, t) \) belongs to the Schwartz space, the space of infinitely differentiable functions equal to zero at infinity together with their derivatives.

In the Lagrangian formulation of classical mechanics, the Lagrange function for a particle in a one-dimensional space with a generalized coordinate \( q \) is defined as the difference between the particle’s kinetic energy \( K \) and its potential energy \( V \):
\[
L = K - V \equiv 2K - E,
\] (4)
where \( E = K + V \) is the total energy of the particle. For a quantum particle, we define

the Lagrange function \( L_c(t) \) as the difference of the average values of its kinetic and

potential energies: \( L_c(t) = \langle \hat{\psi}|\hat{K}|\psi \rangle - \langle \psi|V|\psi \rangle \), where \( \hat{K} = \hat{p}^2/2m; \hat{p} = -\imath\hbar\partial_{\!x} \) — particle

momentum operator. Thus, the action \( S_c \), which describes the quantum dynamics of a

particle between times \( t_1 \) and \( t_2 \), is

\[
S_c = \int_{t_1}^{t_2} L_c(t)dt \equiv K_c - V_c, \quad K_c = \int_{t_1}^{t_2} \langle \psi|\hat{K}|\psi \rangle dt, \quad V_c = \int_{t_1}^{t_2} \langle \psi|V|\psi \rangle dt. \tag{5}
\]

In turn, the average values of \( \langle \psi|\hat{K}|\psi \rangle \) and \( \langle \psi|V|\psi \rangle \) are associated with the kinetic

energy density

\[
\mathcal{K}_c(x,t) = -\frac{\hbar^2}{2m}\psi^* \frac{\partial^2 \psi}{\partial x^2} = \frac{\hbar^2}{2m} \left[ \frac{\partial \psi^*}{\partial x} \frac{\partial \psi}{\partial x} - \frac{\partial}{\partial x} \left( \psi^* \frac{\partial \psi}{\partial x} \right) \right] = \frac{\hbar^2}{2m} R^2 \left( \frac{\partial \phi}{\partial x} \right)^2 + \left( \frac{\partial R}{\partial x} \right)^2 - \frac{\partial}{\partial x} \left( R \frac{\partial R}{\partial x} \right) \tag{6}
\]

and potential energy density

\[
\mathcal{V}_c(x,t) = V(x,t)\psi^*(x,t)\psi(x,t) = V(x,t)R^2(x,t). \tag{7}
\]

The sum of these two functions gives the density of the particle’s total energy \( \mathcal{H}_c(x,t) \):

\[
\mathcal{H}_c = \mathcal{K}_c + \mathcal{V}_c = -\frac{\hbar^2}{2m}\psi^* \frac{\partial^2 \psi}{\partial x^2} + V\psi^*\psi. \tag{8}
\]

Now the terms \( K_c \) and \( V_c \) in the action \( S_c \) (see (5)) can be written as

\[
K_c = \int_{t_1}^{t_2} dt \int_{-\infty}^{\infty} dx \mathcal{K}_c(x,t); \quad V_c = \int_{t_1}^{t_2} dt \int_{-\infty}^{\infty} dx \mathcal{V}_c(x,t).
\]

And if we take into account the boundary conditions for the wave function and the fact

that at times \( t_1 \) and \( t_2 \) the (independent) variations of \( \delta \psi \) and \( \delta \psi^* \) are equal to zero,

then it is easy to show that

\[
\delta K_c = \int_{t_1}^{t_2} dt \int_{-\infty}^{\infty} dx \left[ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \right] \delta \psi^* + c.c. \tag{9}
\]

\[
\delta V_c = \int_{t_1}^{t_2} dt \int_{-\infty}^{\infty} dx V \psi \delta \psi^* + c.c. \tag{10}
\]

Consequently,

\[
\delta \mathcal{H}_c = \delta K_c + \delta V_c = \int_{t_1}^{t_2} dt \int_{-\infty}^{\infty} dx \left[ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi \right] \delta \psi^* + c.c. \tag{11}
\]

\[
\delta S_c = \delta K_c - \delta V_c = \int_{t_1}^{t_2} dt \int_{-\infty}^{\infty} dx \left[ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} - V\psi \right] \delta \psi^* + c.c. \tag{12}
\]

And, at this point we come to the key point of the present approach. According to

the principle of least action, in order to determine the equation for the wave function,

the variation \( \delta S_c \) would have to be equated to zero. However, based on Exp. (12),

it is obviously impossible to obtain an equation describing the dynamics of the state
of a quantum particle, since this expression does not contain time derivatives. One more important argument against using this principle of classical physics to derive the quantum mechanical equation is the fact that the variations (12) obtained on the basis of the operators of one-particle observables describe, in fact, only the corpuscular properties of a quantum particle. To take into account its wave properties, it is necessary to turn to wave-particle duality, which implies, in addition to $\mathcal{L}$, another definition of the Lagrangian for a quantum particle.

Indeed, according to the Planck-Einstein and de Broglie relations, the wave $e^{i(kx-\omega t)}$ describes an ensemble of (free) particles with energy $E = \hbar \omega$ and momentum $p = \hbar k$. For a wave function (3) of a general form, these relations can be written for each point of the OCS in the form of local connections between corpuscular and wave characteristics:

$$E(x,t) = \hbar \omega(x,t), \quad p(x,t) = \hbar k(x,t);$$
$$\omega(x,t) = -\frac{\partial \phi(x,t)}{\partial t}, \quad k(x,t) = \frac{\partial \phi(x,t)}{\partial x}. \quad (13)$$

It remains to clarify the question of whether the physical meaning of the quantities $E$ and $p$ is preserved in the transition from the de Broglie wave to the wave function of the general form, that is, is it possible to treat the function $E(x,t)R^2(x,t)$ as the particle’s total energy density, and the function $p(x,t)R^2(x,t)$ as the particle’s momentum density.

The results obtained above allow us to unambiguously answer the second question. Indeed, if we take into account the relation (13) for the function $p(x,t)$ in Exp. (6), then it becomes clear that the function $p(x,t)R^2(x,t)$ determines only a part of the particle’s kinetic energy and therefore cannot be interpreted as the momentum density of a quantum particle. As regards the function $E(x,t)R^2(x,t)$, the results obtained above do not prohibit treating this function as the density of the total energy of the particle. On this basis, we postulate that the wave function (3) describes a one-particle quantum ensemble in which the density of the total energy of particles at the OCS points is given by the expression

$$\mathcal{H}_w(x,t) = E(x,t)R^2(x,t) = -\hbar \frac{\partial \phi(x,t)}{\partial t}R^2(x,t) \equiv \frac{i\hbar}{2} \left( \psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right). \quad (14)$$

As a consequence, for a quantum particle, with making use of the right-hand expression in (4) we can now define an $S_w$ action that incorporates the wave properties of the particle: $S_w = 2K_c - H_w$, where

$$H_w = \int_{t_1}^{t_2} dt \int_{-\infty}^{\infty} dx \mathcal{H}_w(x,t). \quad (15)$$

Since the (independent) variations of $\delta \psi$ and $\delta \psi^*$ are zero at times $t_1$ and $t_2$, it is easy to show (integrating by parts) that

$$\delta S_w = 2\delta K_c - \delta H_w, \quad (16)$$

where

$$\delta H_w = \int_{t_1}^{t_2} dt \int_{-\infty}^{\infty} dx \delta \mathcal{H}_w(x,t) = i\hbar \int_{t_1}^{t_2} dt \int_{-\infty}^{\infty} dx \left( \frac{\partial \psi}{\partial t} \delta \psi^* - \frac{\partial \psi^*}{\partial t} \delta \psi \right). \quad (17)$$
Further, since the variations $\delta S_c$ and $\delta S_w$ (see Exps. (11) and (16)) describe the same particle, they must be equal. That is, the equality $2\delta K_c - \delta H_w = \delta K_c - \delta V_c$ must hold, from which it follows that $\delta H_w = \delta K_c + \delta V_c \equiv \delta H_c$. In the last analysis, the essence of the proposed variational approach is that the variation of the functional $H_c$, which describes the corpuscular properties of a particle, must coincide with the variation of the functional $H_w$, which describes its wave properties:

$$\delta H_c = \delta H_w.$$  

(18)

Now we have here to take into account Exps. (11) and (17) for $\delta H_c$ and $\delta H_w$, and the fact that the equality (18) must hold for both independent variations of $\delta \psi$ and $\delta \psi^*$. Lastly, equating the integrands containing the $\delta \psi^*$ variation, we obtain the Schrödinger equation

$$\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi.$$

3. Conclusion

A variational principle has been developed, which, in fact, represents a mathematical formulation of wave-particle duality for the wave function of a general form:

$$\int_{t_1}^{t_2} dt \int_{-\infty}^{\infty} dx \delta (\psi^* \hat{H} \psi) = \frac{i\hbar}{2} \int_{t_1}^{t_2} dt \int_{-\infty}^{\infty} dx \delta \left( \psi^* \frac{\partial \psi}{\partial t} - \psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right).$$

This principle does not conflict with the well-known postulates of standard quantum mechanics.

References

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