Lagrangian Approach to Quantum Mechanics

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Abstract

The Lagrangian approach of Dirac is presented in a complete form. This suggests to identify the Schrödinger equation as the Euler-Lagrange equation rather than the Hamiltonian operator equation.

Planck found the relation of frequency to energy and de Broglie the relation of wavelength to momentum. In the wave-particle duality, the phase of matter waves could be written as

\[ \frac{i}{\hbar}(px - Et) \quad \text{from} \quad i(kx - \omega t). \]  

(1)

Schrödinger deduced the wave equation for a particle from the Hamiltonian of a classical system. The Schrödinger equation led to the formulation of quantum mechanics and the Hamiltonian came to be the argument of correspondence [1].

Dirac took up the question of what corresponds in the quantum theory to the Lagrangian method of classical theory [2]. Dirac tried to take over the idea rather than the equation, provided by the Lagrangian. But the action principle involves the Euler-Lagrange equation, which is identical with the Schrödinger equation. In this paper, I have tried to complete the Lagrangian approach of Dirac in relation to the Schrödinger equation. For the continuity of discussion, arguments are restricted to one-dimensional cases.

The Lagrangian approach begins by writing the phase of matter waves in the integral form

\[ \frac{i}{\hbar}(pdx - Edt), \quad \text{so} \quad \frac{i}{\hbar}L(x, \dot{x})dt. \]  

(2)

In the quantum theory of canonical coordinate and momentum, however, we cannot take over the classical notion of coordinate and velocity. Therefore, we must consider the Lagrangian as a function of \( x \) at time \( t \) and \( x + dx \) at time \( t + dt \) rather than \( x \) and \( \dot{x} \). Dirac has used the action function \( S \) for the time integral of the Lagrangian and the action principle. But the integral is called Hamilton’s principal function and Hamilton’s principle in classical mechanics [3].
In the theory of representations, the transformation function connects two observables for the state vectors \[4\]. The notation \[x' \mid x\] is given for the function when observations are made of coordinates. Dirac showed that

\[< x \mid x' \rangle \quad \text{corresponds to} \quad \exp\{iS(x, x')/\hbar\}. \quad (3)\]

We may divide up the interval into a number of small sections by the introduction of a sequence of intermediate times \(t_i\). Then we have for \(S\)

\[S(x_n, x_1) = S(x_n, x_{n-1}) + \cdots + S(x_2, x_1). \quad (4)\]

The corresponding function becomes

\[< x_n \mid x_1 > = \int \cdots \int < x_n \mid x_{n-1} > dx_{n-1} \cdots < x_3 \mid x_2 > dx_2 < x_2 \mid x_1 >. \quad (5)\]

We must integrate over the intermediate \(x_i\) between transformations, which follows from the property of state vectors. The composition law (5) can equally be expressed in the form of a recursive relation

\[< x_{i+1} | = \int < x_{i+1} \mid x_i > dx_i < x_i | \quad \text{for} \quad i = 2, 3, \ldots, n - 1. \quad (6)\]

They describe the development of a wave function with time in the general form

\[< x | = \int < x \mid x' > dx' < x' | \quad \text{or} \quad \psi(x) = \int < x \mid x' > dx' \psi(x'). \quad (7)\]

In the form of integral equation, \(< x \mid x' \rangle\) is the development of a wave function given at \(x'\) at an earlier time \(t'\) into a wave function at any other point \(x\) at a time \(t\). Dirac explained, \(< x \mid x' \rangle\) is that solution of the Schrödinger equation. Feynman remarked, it is a kind of Greens function for the Schrödinger equation. Feynman developed the path integral formulation based on equation (7) \[5\].

In the classical theory, the motion of a system from time \(t'\) to time \(t\) is such that the action function is stationary for the path of motion. The action principle is a statement that the variation of \(S\) from time \(t'\) to time \(t\) is zero:

\[\delta S = 0.\]

The classical requirement that the values of the intermediate \(x_i\) shall make \(S\) stationary corresponds to the condition in the quantum theory that all values of the intermediate \(x_i\) are important in proportion to their contribution to the integral. This shows the way in which the action principle is absorbed in the composition law. We can summarize Dirac’s remark on the action principle by requiring the variation of \(< x \mid x' >\) to be zero in (3):

\[\delta < x \mid x' > = 0 \quad \text{corresponds to} \quad \delta S = 0 \quad \text{from} \quad \delta e^{iS/\hbar} = (i\delta S/\hbar)e^{iS/\hbar}. \quad (8)\]

The action principle is a statement about the integral of \(L\), from which we obtain the solution of the problem via the Euler-Lagrange equation. Here, the variational problem is to determine \(< x \mid x' >\) that will make the development of a wave function stationary. When viewed from the present point, the Schrödinger equation is the condition for a wave function to take on a stationary distribution.
In the classical theory, $S$ is the generating function of a contact transformation relating $(x, p)$ to $(x', p')$:
\[
\frac{\partial}{\partial x} S(x, x') = p, \quad -\frac{\partial}{\partial x'} S(x, x') = p'.
\] (9)

In the quantum theory, it becomes the generator of a unitary transformation connecting the two state vectors:
\[
\frac{\hbar}{i} \frac{\partial}{\partial x} \langle x | x' \rangle = p \langle x | x' \rangle, \quad -\frac{\hbar}{i} \frac{\partial}{\partial x'} \langle x | x' \rangle = p' \langle x | x' \rangle.
\] (10)

The quantum equation for $\langle x |$ or $| x' \rangle$ is given by multiplying with $\langle x' |$ or $| x \rangle$ and integrate over $x'$ or $x$. Written in terms of wave function, they are
\[
\frac{\hbar}{i} \frac{\partial \psi}{\partial x} = p \psi, \quad -\frac{\hbar}{i} \frac{\partial \psi^*}{\partial x} = p^* \psi^*.
\] (11)

We can extend the analogue of transformation to the equation of motion. This we do by applying the idea of Dirac to the Hamilton-Jacobi equation. The relation to the Schrödinger equation is the center of attention. The Hamilton-Jacobi equation is
\[
\frac{\partial S}{\partial t} + H = 0.
\] (12)

Thus, the quantum analogue has the form
\[
\frac{\hbar}{i} \frac{\partial}{\partial t} \langle x | x' \rangle + H \langle x | x' \rangle = 0.
\] (13)

From the form of the Hamiltonian, the Hamilton-Jacobi equation can be written
\[
\frac{\partial S}{\partial t} + \frac{1}{2m} \left( \frac{\partial S}{\partial x} \right)^2 + V = 0.
\] (14)

Then, the quantum analogue has the form
\[
\frac{\hbar}{i} \frac{\partial}{\partial t} \langle x | x' \rangle + \frac{1}{2m} \left( \frac{\partial S}{\partial x} \right)^2 \langle x | x' \rangle + V \langle x | x' \rangle = 0.
\] (15)

The quantum equation for $\langle x |$ follows from the form of (15), as can be seen when we multiply the equation by $\langle x' |$ and integrate with respect to $x'$. The quantum equation is essentially the same as used for the derivation of the Schrödinger equation. In putting into the Schrödinger equation, however, the momentum should be treated as a constant. In general,
\[
\left( \frac{\hbar}{i} \frac{\partial}{\partial x} \right)^2 \langle x | x' \rangle = \frac{\hbar}{i} \left( \frac{\partial S}{\partial x} \langle x | x' \rangle \right) = \frac{\hbar}{i} \left( \frac{\partial^2 S}{\partial x^2} \langle x | x' \rangle \right) = \frac{\hbar}{i} \left( \frac{\partial S}{\partial x} \right)^2 \langle x | x' \rangle.
\] (16)

In deriving the Schrödinger equation, actually, the momentum has been treated as a constant.
The potential scattering is represented by a potential energy which is appreciably different from zero only within a finite region. The Hamilton-Jacobi equation for scattering can then be written as

\[
\frac{1}{2m} \left( \frac{\partial S}{\partial x} \right)^2 - H_0 = \begin{cases} 
-V(x) & \text{if } x \to x' \\
0 & \text{otherwise}
\end{cases},
\]

(17)

where \(H_0\) is the energy of the free particle. From this form of the Hamilton-Jacobi equation we may deduce the corresponding quantum equation of the form

\[
\frac{1}{2m} \left( \frac{\partial S}{\partial x} \right)^2 <x|x'> - H_0 <x|x'> = -V(x)\delta(x - x').
\]

(18)

The inhomogeneity of potential energy is the reason for the choice of the \(\delta\) function instead of the transformation function. As the momentum of the free particle is a constant, we can put the quantum equation into the form

\[
-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} <x|x'> - H_0 <x|x'> = -V(x)\delta(x - x').
\]

(19)

The Hamilton-Jacobi equation for scattering gives the integral form of the Schrödinger equation. This is identical with the integral equation which was introduced by Born from the Schrödinger equation for scattering. Here, the quantity \(<x|x'>\) has been a link relating the two equations, differential and integral.

We are taught the correspondence between the Schrödinger equation and the Hamiltonian of classical systems. But their correspondence is not complete. Because the differential operator acts on everything that stands to the right, the same relation does not always hold between operators as between variables. As can be seen in (16), the second application of the momentum operator to a wave function gives rise to the differentiation of \(p\) in addition to the general effect of multiplication of the wave function by \(p^2\). If the momentum is a constant, there is no additional term. This is the case for the hydrogen atom problem where the angular momentum is the quantum number. But it is actually so in the harmonic oscillator problem, for the momentum depends linearly on its coordinate. In fact, the zero-point energy is a result of the additional term in the Schrödinger equation of harmonic oscillator. It characterizes a difference of correspondence with the Hamiltonian of classical system. The zero-point energy was also noted by Heisenberg in his quantum theoretical calculations [6]. The Schrödinger equation needs to be justified in a different way.

Their correspondence is not complete either in form. It is the expectation value in the quantum theory that corresponds to the Hamiltonian of classical theory. As shown by Ehrenfest [7], the equation for physical quantities can be supposed to be the equation for the expectation values in the quantum theory. The Hamiltonian required by the transition from classical to quantum physics should therefore have the form

\[
\int <x|\frac{\hbar}{\partial t} |x> dx + \int <x|\frac{1}{2m} \left( \frac{\partial S}{\partial x} \right)^2 |x> dx + \int <x|V|x> dx = 0. \quad (20)
\]
This follows for an arbitrary \( |x'\rangle \) from the very form of (15) when we multiply the equation by \( |x\rangle \) and integrate over \( x \). Written in terms of wave function, the quantum theoretical Hamiltonian reads

\[
\int \psi^* E \psi \, dx = \int \left\{ \frac{1}{2m} \left( -\frac{\hbar}{i} \frac{\partial \psi^*}{\partial x} \right) \left( \frac{\hbar}{i} \frac{\partial \psi}{\partial x} \right) + \psi^* V \psi \right\} \, dx.
\] (21)

This is known as an example of variational problem provided by the Schrödinger equation [8]. The variational approach is more than just a matter of academic curiosity. The form of expression is just what we should take in the quantum theory for the Hamiltonian of classical system. By the action principle, actually, it has shown how the Hamiltonian of quantum system goes over into the Schrödinger equation. Here, the action principle becomes a statement that the energy of quantum system is a constant: \( \delta <E> = 0 \).

According to Dirac, the action principle comes to be the argument of correspondence of the classical to quantum equations of motion. In fact, it is the variational expression in (21) that corresponds completely to the Hamiltonian of classical system. In the Schrödinger equation has the differentiation of \( p \) been involved unintentionally. If the momentum is not a constant, the additional term is unavoidable. It does not matter if the term is included in the equation of motion. But it does in the Hamiltonian. This is a problem of justification.

In form and content, it is reasonable to identify the Schrödinger equation as the Euler-Lagrange equation obtained from the variational principle for the energy of quantum system rather than the Hamiltonian operator equation.

**Appendix: The zero-point energy in calculation**

The linear harmonic oscillator is the one-dimensional motion of a point mass \( m \) attracted to an equilibrium position \( x = 0 \) by a force that is proportional to the displacement \( x \) from it. The restoring force can be represented by the potential energy \( V(x) = m\omega^2 x^2 / 2 \). Introducing the variable \( \xi = (m\omega/\hbar)^{1/2} x \) and the eigenvalue \( \lambda = 2E/\hbar \omega \), we can put the Schrödinger equation in the form

\[
\frac{d^2 \psi}{d\xi^2} + (\lambda - \xi^2) \psi = 0.
\] (22)

For sufficiently large \( \xi \), the dominant behavior of \( \psi \) is given by \( \exp(-\xi^2/2) \). Thus, we can assume an exact solution of the form \( H(\xi) \exp(-\xi^2/2) \). In the process of solving (21), we have used for the asymptotic part the relations

\[
\frac{d\psi}{d\xi} = -\xi \psi \quad \text{and} \quad \frac{d^2 \psi}{d\xi^2} = \xi^2 \psi - \psi.
\] (23)

The first shows a typical operator-eigenvalue relation. But the second gives an additional term, a result of differentiating \( \xi \). This corresponds formally to the differentiation of momentum itself, resulting in the zero-point energy.
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