

The Physical Origin of Schrödinger Equation

Xiao-Bo Yan*

College of Electronic Science, Northeast Petroleum University, Daqing 163318, China

(Dated: November 16, 2020)

Quantum mechanics is one of the basic theories of modern physics. Here, the famous Schrödinger equation and the differential operators representing mechanical quantities in quantum mechanics are derived, just based on the principle that the translation invariance (symmetry) of a system in Hamiltonian mechanics should be preserved in quantum mechanics. Moreover, according to the form of the differential operators, the commutation relation in quantum mechanics between the generalized coordinate and the generalized momentum can be easily obtained.

After about one century of development, quantum mechanics has become a fundamental theory in physics that provides a description of the physical properties at the scale of atoms and subatomic particles. It is the foundation of all quantum physics including quantum chemistry, quantum field theory, quantum technology and quantum information science. Nevertheless, as a fundamental equation in quantum mechanics, the Schrödinger equation is given as a hypothesis in any quantum mechanics textbook, as well as the differential operators representing physical quantities. In fact, they are closely related to the translation invariance (symmetry) in Hamiltonian mechanics where the equations of motion of a system are given as

$$\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q}. \quad (1)$$

Here, q and p are respectively the generalized coordinate and generalized momentum of the system (for simplicity, we assume that the system has only one generalized coordinate q and the corresponding generalized momentum p), and $H(q, p, t)$ is the Hamiltonian function of the system. In Hamiltonian mechanics, the conserved quantities in a system are closely related to the translation invariance of the system. For instance, the generalized momentum p in Eq. (1) will be a constant if the Hamiltonian $H(q, p, t)$ is invariant under the translation transformation with respect to the generalized coordinate q .

In the 1920s, Quantum mechanics was founded by Schrödinger [1], Heisenberg [2], Born [3, 4] and others based on some hypotheses including the hypothesis of wave-particle duality proposed by de Broglie [5]. Wave-particle duality is the concept in quantum mechanics that every particle or quantum entity may be described as either a particle or a wave. It expresses that the classical concepts “particle” or “wave” cannot fully describe the behavior of quantum-scale objects. Actually, any matter will not disappear in space and time, will only be converted from one form into another. Both “particle” and “wave” are the forms of matter. In 1927, the hypothesis of de Broglie wave was first conformed in Davisson-

Germer experiment [6] which was an experimental milestone in the development of quantum mechanics. In fact, de Broglie wave can be viewed as a field of the corresponding particle just like the electromagnetic wave is the field of photons.

Although, in microscopic systems, the quantum entity behaves sometimes like a particle and sometimes like a wave, the translation invariance (symmetry) of the system should be consistent no matter from the “particle” or the “wave” viewpoint. According to this principle, the differential operators representing physical quantities and the Schrödinger equation in quantum mechanics can be easily obtained. In order to see that, let's assume that there is a particle whose motion in classical mechanics is dominated by the canonical equation in Eq. (1), and the corresponding wave can be denoted as $\psi(q, t)$ where q is the generalized coordinate of the particle in Hamiltonian mechanics. (It is conceivable that the wave function $\psi(q, t)$ must be related to the distribution of matter in the generalized coordinate space.) Now suppose that the particle system has a translation invariance with respect to the generalized coordinate q , as mentioned above, the corresponding wave $\psi(q, t)$ should have the same translation invariance, which means that the wave $\psi(q, t)$ and the shifted wave $\psi(q+a, t)$ should correspond to the same observables, here a denotes the translational value of the system.

We will see that the translation invariance (symmetry) of the system will impose severe constraints on the wave function $\psi(q, t)$. First, the wave $\psi(q, t)$ cannot be a constant in the whole coordinate space because no interference fringes can be generated by such a wave. Secondly, the quantity $\psi^*(q, t)\psi(q, t)$ should be an observable (analogy with the observable light intensity in an electromagnetic field, i.e., $E^*(r, t)E(r, t)$, here $E(r, t)$ is just the electromagnetic wave at coordinate r and time t) which will be invariant under the translation transformation. Hence, the only possible situation of the wave function $\psi(q, t)$ under the translation transformation is that

$$\psi(q+a, t) = e^{iaf(q)}\psi(q, t) \quad (2)$$

with a real function $f(q)$.

In order to see what we can obtain from Eq. (2), we

*Electronic address: xiaoboyan@126.com

do the Taylor expansion on both sides of Eq. (2), i.e.,

$$\psi(q+a, t) = \psi(q, t) + a\psi'(q, t) + \frac{a^2}{2}\psi''(q, t) + \dots \quad (3)$$

$$e^{iaf(q)}\psi(q, t) = [1 + ia f(q) - \frac{a^2 f^2(q)}{2} + \dots]\psi(q, t). \quad (4)$$

Since Eq. (2) is true for any value a , the corresponding terms in Eqs. (3) and (4) must be equal. According to the second and third terms in Eqs. (3) and (4), we have

$$\psi'(q, t) = if(q)\psi(q, t), \quad (5)$$

$$\psi''(q, t) = -f^2(q)\psi(q, t). \quad (6)$$

According to Eqs. (5) and (6), it is easy to obtain

$$f'(q) = 0, \quad (7)$$

which means the function $f(q)$ can only be a constant, denoted by k . Then Eq. (5) becomes

$$-i\frac{\partial}{\partial q}\psi(q, t) = k\psi(q, t), \quad (8)$$

which is an eigen equation of the Hermitian operator $-i\frac{\partial}{\partial q}$ with the eigenfunction $\psi(q, t)$ and the eigenvalue k . The eigenvalue k is a real number because in mathematics, the eigenvalues of any Hermitian operator are all real numbers.

What Eq. (8) means is that when a particle system has a translation invariance with respect to a generalized coordinate q (the corresponding generalized momentum p is a constant), the corresponding wave $\psi(q, t)$ must satisfy the eigen equation of the Hermitian operator $-i\frac{\partial}{\partial q}$, vice versa. Hence, the eigenvalue k in Eq. (8) should be directly related to the generalized momentum p . Meanwhile, the important Planck constant \hbar , which can reflect the quantum properties of a microscopic system, is obviously absent in Eq. (8). However, we can always multiply both sides of Eq. (8) by the Planck constant \hbar . In fact, the number $\hbar k$ is just the momentum p of the particle, which can be directly verified by substituting the plane electromagnetic wave e^{ikq} to $\psi(q, t)$ in Eq. (8) with the Einstein's hypothesis that the photon's momentum p satisfies $p = \hbar k$. Therefore, it can be concluded that operating on the wave function $\psi(q, t)$, the Hermitian operator $-i\hbar\frac{\partial}{\partial q}$ will give out the value of momentum p of the system, hence the Hermitian operator $-i\hbar\frac{\partial}{\partial q}$ can be considered as the generalized momentum operator (denoted by \hat{p}). In fact, the momentum operator $-i\hbar\frac{\partial}{\partial q}$ is exactly the famous Born's assumption in the establishment of quantum mechanics, while here we know that the form of the momentum operator comes from the translation invariance in Hamiltonian mechanics.

If we take the complex conjugate to both sides of Eq. (8) and multiply the Planck constant \hbar , we have

$$i\hbar\frac{\partial}{\partial q}\psi^*(q, t) = p\psi^*(q, t) \quad (9)$$

with $p = \hbar k$. It means that operating on the eigenfunction $\psi^*(q, t)$, the differential operator $i\hbar\frac{\partial}{\partial q}$ can give the same momentum p of the system. Hence, we can also choose the differential operator $i\hbar\frac{\partial}{\partial q}$ as the generalized momentum operator \hat{p} of the system.

Since the physical quantities are represented by operators, the order in which they act on the wave function becomes important. The commutation relation (order relationship) between the generalized coordinate q and the generalized momentum operator $\pm i\hbar\frac{\partial}{\partial q}$ can be directly obtained as

$$[\pm i\hbar\frac{\partial}{\partial q}, q] = \pm i\hbar, \quad (10)$$

according to $[\frac{\partial}{\partial q}, q] = 1$ with definition $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$. In fact, the equation with minus sign in Eq. (10) is exactly the Dirac's canonical quantization rule which we obtain very naturally here. It can be seen from Eq. (10) that the generalized momentum p is represented by an operator \hat{p} while the coordinate q is the same as that in classical mechanics. The reason is that in the analysis above we study the wave function in generalized coordinate space (called coordinate representation). If we do that in generalized momentum space (called momentum representation), the situation is the opposite.

In classical mechanics, the energy will be conserved if the Hamiltonian of the system is time independent. In this case, the system is said to have time translation invariance (symmetry). As previously mentioned, if there is some translation invariance in a particle system, then the corresponding wave must also have that. Based on the time translation invariance, and through some similar calculations as those in Eqs. (2)–(8), it is easy to find that the change of the wave function $\psi(q, t)$ with time will satisfy

$$-i\hbar\frac{\partial}{\partial t}\psi(q, t) = E\psi(q, t). \quad (11)$$

Here, the constant E should be the energy of the system, which can be verified by substituting the plane electromagnetic wave $e^{i\omega t}$ to $\psi(q, t)$ in Eq. (11) with the Einstein's hypothesis that the photon's energy E satisfies $E = \hbar\omega$. Therefore, it can be concluded that operating on the wave function $\psi(q, t)$, the Hermitian operator $-i\hbar\frac{\partial}{\partial t}$ will give out the value of energy E of the system. Hence, the Hermitian operator $-i\hbar\frac{\partial}{\partial t}$ can be considered as the energy operator of the system (of course, we can also choose $i\hbar\frac{\partial}{\partial t}$ as the energy operator of the system).

Meanwhile, there exists another energy operator in the system, i.e., the Hamiltonian operator $\hat{H}(\hat{q}, \hat{p}, t)$ since the Hamiltonian function $H(q, p, t)$ is just the energy of the system in Hamiltonian mechanics. It means that the two Hermitian operators are equivalent when they operate on a wave function, i.e.,

$$\pm i\hbar\frac{\partial}{\partial t} \equiv \hat{H}(\hat{q}, \hat{p}, t). \quad (12)$$

Hence, according to Eq. (12), the time evolution of a wave function $\psi(q, t)$ will satisfy

$$\pm i\hbar \frac{\partial}{\partial t} \psi(q, t) = \hat{H}(\hat{q}, \hat{p}, t) \psi(q, t). \quad (13)$$

In fact, there are four equivalent time evolution equations in Eq. (13) because the momentum operator \hat{p} can be chosen as $i\hbar \frac{\partial}{\partial q}$ or $-i\hbar \frac{\partial}{\partial q}$ (in coordinate representation). If we choose $-i\hbar \frac{\partial}{\partial q}$ as the momentum operator \hat{p} , then the equation with plus sign in Eq. (13) is just the famous Schrödinger equation in quantum mechanics.

In summary, due to the wave-particle duality in mi-

croscopic systems, Hamiltonian mechanics describing the macroscopic properties of a system has to be replaced by quantum mechanics when we study the properties of quantum-scale objects. And the origins of the Schrödinger equation and the differential operators representing mechanical quantities in quantum mechanics all come from the translation invariance (symmetry) in Hamiltonian mechanics. We believe the results in this paper are very beneficial to understand the physical origin of quantum mechanics.

-
- [1] E. Schrödinger, “An Undulatory Theory of the Mechanics of Atoms and Molecules”, *Physical Review* **28**, 1049 (1926).
- [2] W. Heisenberg, “Über quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen”, *Zeitschrift für Physik* (in German), **33**, 879–893 (1925).
- [3] M. Born and P. Jordan, “Zur Quantenmechanik”, *Zeitschrift für Physik*, **34**, 858–888 (1925).
- [4] M. Born, W. Heisenberg, and P. Jordan, “Zur Quantenmechanik II”, *Zeitschrift für Physik*, **35**, 557–615 (1926).
- [5] L. de Broglie, “Waves and quanta”, *Nature* **112**, 540 (1923).
- [6] C. J. Davisson and L. H. Germer, “Reflection of Electrons by a Crystal of Nickel”, *Proceedings of the National Academy of Sciences of the United States of America* **14**, 317–322 (1928).