Derivation of the Schrödinger equation

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Abstract

It is shown that the heuristic "derivation" of the Schrödinger equation in quantum mechanics textbooks can be turned into a real derivation by resorting to spacetime translation invariance and relativistic invariance.

1 Introduction

Many quantum mechanics textbooks provide a heuristic "derivation" of the Schrödinger equation (e.g. [1-4]). It begins with the assumption that the state of a free microscopic particle has the form of a plane wave $e^{i(kx-\omega t)}$. When combining with the de Broglie relations for momentum and energy $p = \hbar k$ and $E = \hbar\omega$, this state becomes $e^{i(px-Et)/\hbar}$. Then it uses the nonrelativistic energy-momentum relation $E = p^2/2m$ to obtain the free particle Schrödinger equation. Lastly, this equation is generalized to include an external potential, and the end result is the Schrödinger equation.

In this paper, we will show that this heuristic "derivation" of the Schrödinger equation can be turned into a real derivation by resorting to spacetime translation invariance and relativistic invariance. Spacetime translation gives the definitions of momentum and energy, and spacetime translation invariance entails that the state of a free microscopic particle with definite momentum and energy assumes the plane wave form $e^{i(px-Et)/\hbar}$. Besides, the relativistic invariance of the free state further determines the relativistic energy-momentum relation, which nonrelativistic approximation is $E = p^2/2m$. This analysis may be helpful for students to undertsand the physical origin of the Schrödinger equation.

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2 Spacetime translation and its invariance

It is well known in quantum theory that the definitions of energy and momentum originate from spacetime translation, and the momentum operator P and energy opertaor H are defined as the generators of space translation and time translation, respectively[1]. A space translation operator can be defined as

$$T(a)\psi(x,t) = \psi(x-a,t). \tag{1}$$

It means translating (without distortion) the state of a system, $\psi(x,t)$, by an amount a in the positive x direction. The operator preserves the norm of the state because $\int_{-\infty}^{\infty} \psi^*(x,t)\psi(x,t)dx = \int_{-\infty}^{\infty} \psi^*(x-a,t)\psi(x-a,t)dx$. This implies that $T(a)$ is unitary, satisfying $T^\dagger(a)T(a) = I$. As a unitary operator, $T(a)$ can be further expressed as

$$T(a) = e^{-iaP}, \tag{2}$$

where P is called the generator of space translation, and it is Hermitian and its eigenvalues are real. By expanding $\psi(x-a,t)$ in order of a, we can further get

$$P = -i\frac{\partial}{\partial x}. \tag{3}$$

Similarly, a time translation operator can be defined as

$$U(t)\psi(x,0) = \psi(x,t). \tag{4}$$

Let the evolution equation of state be the following form:

$$i\frac{\partial \psi(x,t)}{\partial t} = H\psi(x,t). \tag{5}$$

where H is a to-be-determined linear operator that depends on the properties of the system[2]. Then the time translation operator $U(t)$ can be expressed as $U(t) = e^{-itH}$, and H is the generator of time translation. Note that we cannot determine whether $U(t)$ is unitary and H is Hermitian here.

[1] There are in general two different pictures of translation: active transformation and passive transformation. The active transformation corresponds to displacing the studied system, and the passive transformation corresponds to moving the environment (the coordinate system etc). Physically, the equivalence of the active and passive pictures is due to the fact that moving the particle one way is equivalent to moving the environment the other way by an equal amount. In the following we will mainly analyze spacetime translations in terms of active transformations.

[2] Note that the linearity of H is an important presupposition in our derivation of the Schrödinger equation. It can be reasonably assumed that the linear evolution and nonlinear evolution both exist, and moreover, they satisfy spacetime translation invariance respectively because they cannot counteract each other in general. Then our derivation shows that the linear evolution part, if exists, must assume the same form as the Schrödinger equation in nonrelativistic domain. But spacetime translation invariance cannot determine the concrete form of nonlinear evolution, if it exists. Certainly, our derivation cannot exclude the existence of possible nonlinear evolution either.

Let's now see the implications of spacetime translation invariance. The evolution law of an isolated system satisfies spacetime translation invariance due to the homogeneity of space and time. The homogeneity of space ensures that the same experiment performed at two different places gives the same result, and the homogeneity in time ensures that the same experiment repeated at two different times gives the same result. First, time translational invariance requires that H have no time dependence, namely $dH/dt = 0$[3]. This can be demonstrated as follows (see also [5], p.295). Suppose an isolated system is in state ψ_0 at time t_1 and evolves for an infinitesimal time δt. The state of the system at time $t_1 + \delta t$, to first order in δt, will be

$$\psi(x, t_1 + \delta t) = [I - i\delta t H(t_1)]\psi_0 \tag{6}$$

If the evolution is repeated at time t_2, beginning with the same initial state, the state at $t_2 + \delta t$ will be

$$\psi(x, t_2 + \delta t) = [I - i\delta t H(t_2)]\psi_0 \tag{7}$$

Time translational invariance requires the outcome state should be the same:

$$\psi(x, t_2 + \delta t) - \psi(x, t_1 + \delta t) = i\delta t[H(t_1) - H(t_2)]\psi_0 = 0 \tag{8}$$

Since the initial state ψ_0 is arbitrary, it follows that $H(t_1) = H(t_2)$. Moreover, since t_1 and t_2 are also arbitrary, it follows that H is time-independent, namely $dH/dt = 0$.

Secondly, space translational invariance requires $[T(a), U(t)] = 0$, which further leads to $[P, H] = 0$[4]. This can be demonstrated as follows (see also [5], p.293). Suppose at $t = 0$ two observers A and B prepare identical isolated systems at $x = 0$ and $x = a$, respectively. Let $\psi(x, 0)$ be the state of the system prepared by A. Then $T(a)\psi(x, 0)$ is the state of the system prepared by B, which is obtained by translating (without distortion) the state $\psi(x, 0)$ by an amount a to the right. The two systems look identical to the observers who prepared them. After time t, the states evolve into $U(t)\psi(x, 0)$ and $U(t)T(a)\psi(x, 0)$. Since the time evolution of each identical system at different places should appear the same to the local observers, the above two systems, which differed only by a spatial translation at $t = 0$, should differ only by the same spatial translation at future times. Thus the state $U(t)T(a)\psi(x, 0)$ should be the translated version of A's system at time t, namely we have $U(t)T(a)\psi(x, 0) = T(a)U(t)\psi(x, 0)$. This relation holds true for any initial state $\psi(x, 0)$, and thus we have $[T(a), U(t)] = 0$, which says that space translation operator and time translation operator are commutative.

When $dH/dt = 0$, the solutions of the evolution equation Eq.(5) assume the following form

$$\psi(x, t) = \varphi_E(x)e^{-iEt}, \tag{9}$$

[3]By Ehrenfest's theorem this leads to the law of conservaiton of energy.

[4]By Ehrenfest's theorem this leads to the law of conservaiton of momentum.

where E is a constant, and $\varphi_E(x)$ is the eigenstate of H and satisfies the time-independent equation:

$$H\varphi_E(x) = E\varphi_E(x). \tag{10}$$

The commutative relation $[P, H] = 0$ further implies that P and H have common eigenstates. This means that $\varphi_E(x)$ is also the eigenstate of P. Since the eigenstate of $P = -i\frac{\partial}{\partial x}$ is e^{ipx}, where p is the real eigenvalue, the solution of the evolution equation Eq.(5) for an isolated system will be $e^{i(px-Et)}$, where p and E are defined as the momentum and energy of the system, respectively. In other words, the state $e^{i(px-Et)}$ describes an isolated system (e.g. a free microscopic particle) with definite momentum p and energy E.

3 Relativistic invariance

The relation between momentum p and energy E can be determined by the relativistic invariance of the free state $e^{i(px-Et)}$, and it turns out to be $E^2 = p^2c^2 + m^2c^4$, where m is the rest mass of the system, and c is the speed of light[5]. In nonrelativistic domain, the energy-momentum relation reduces to $E = p^2/2m$.

Now we will derive the relation between momentum p and energy E in relativistic domain. Consider two inertial frames S_0 and S with coordinates x_0, t_0 and x, t. S_0 is moving with velocity v relative to S. Then x, t and x_0, t_0 satisfy the Lorentz transformations:

$$x_0 = \frac{x - vt}{\sqrt{1 - v^2/c^2}} \tag{11}$$

$$t_0 = \frac{t - xv/c^2}{\sqrt{1 - v^2/c^2}} \tag{12}$$

Suppose the state of a free particle is $\psi = e^{i(p_0x_0 - E_0t_0)}$, an eigenstate of P, in S_0, where p_0, E_0 is the momentum and energy of the particle in S_0, respectively. When described in S by coordinates x, t, the state is

$$\psi = e^{i(p_0\frac{x-vt}{\sqrt{1-v^2/c^2}} - E_0\frac{t-xv/c^2}{\sqrt{1-v^2/c^2}})} = e^{i(\frac{p_0+E_0v/c^2}{\sqrt{1-v^2/c^2}}x - \frac{E_0+p_0v}{\sqrt{1-v^2/c^2}}t)} \tag{13}$$

[5]Most existing "derivations" of the energy-momentum relation are based on the somewhat complex analysis of an elastic collision process. Moreover, they resort to either some Newtonian limit (e.g. $p = mv$) or some less fundamental relation (e.g. $p = Eu/c^2$) or even some mathematical intuition (e.g. four-vectors) [6-11]. As we think, the logic of these "derivations" seems a little upside-down, and they are only heuristic demonstrations of the energy-momentum relation.

This means that in frame S the state is still the eigenstate of P, and the corresponding momentum p and energy E is[6]

$$p = \frac{p_0 + E_0 v/c^2}{\sqrt{1 - v^2/c^2}} \tag{14}$$

$$E = \frac{E_0 + p_0 v}{\sqrt{1 - v^2/c^2}} \tag{15}$$

We further suppose that the particle is at rest in frame S_0. Then the velocity of the particle is v in frame S[7]. Considering that the velocity of a particle in the momentum eigenstate $e^{i(px-Et)}$ or a wavepacket superposed by these eigenstates is defined as the group velocity of the wavepacket, namely

$$u = \frac{dE}{dp}, \tag{16}$$

we have

$$dE_0/dp_0 = 0 \tag{17}$$

$$dE/dp = v \tag{18}$$

Eq.(17) means that E_0 and p_0 are independent. Moreover, since the particle is at rest in S, E_0 and p_0 do not depend on v. By differentiating both sides of Eq.(14) and Eq.(15) relative to v we obtain

$$\frac{dp}{dv} = \frac{v}{c^2}\frac{p_0 + E_0 v/c^2}{(1 - v^2/c^2)^{\frac{3}{2}}} + \frac{E_0/c^2}{(1 - v^2/c^2)^{\frac{1}{2}}} \tag{19}$$

$$\frac{dE}{dv} = \frac{v}{c^2}\frac{E_0 + p_0 v}{(1 - v^2/c^2)^{\frac{3}{2}}} + \frac{p_0}{(1 - v^2/c^2)^{\frac{1}{2}}} \tag{20}$$

Dividing Eq.(20) by Eq.(19) and using Eq.(18) we obtain

$$\frac{p_0}{\sqrt{1 - v^2/c^2}} = 0 \tag{21}$$

This means that $p_0 = 0$. Inputing this important result to Eq.(15) and Eq.(14), we immediately have

$$E = \frac{E_0}{\sqrt{1 - v^2/c^2}}, \tag{22}$$

$$p = \frac{E_0 v/c^2}{\sqrt{1 - v^2/c^2}}, \tag{23}$$

[6] Alternatively we can obtain the transformations of momentum and energy by directly requiring the relativistic invariance of momentum eigenstate $e^{i(px-Et)}$, which leads to the relation $px - Et = p_0 x_0 - E_0 t_0$.

[7] Note that we can also get this result from the definition Eq. (16) by using the above transformations of momentum and energy Eq.(14) and Eq.(15).

Then the energy-momentum relation is:

$$E^2 = p^2c^2 + E_0^2 \tag{24}$$

where E_0 is the energy of the particle at rest, called rest energy of the particle, and p and E is the momemtum and energy of the particle with velocity v. By defining $m = E_0/c^2$ as the (rest) mass of the particle[8], we can further obtain the familar energy-momentum relation

$$E^2 = p^2c^2 + m^2c^4 \tag{25}$$

In nonrelativistic domain, this energy-momentum relation reduces to $E = p^2/2m$.

4 Derivation of the Schrödinger equation

The relation between energy E and momentum p in nonrelativistic domain implies that the operator relation is $H = P^2/2m$ for an isolated system, where H is usually called the free Hamiltonian of the system. Note that since the value of E is real by Eq.(24), H is Hermitian and $U(t)$ is unitary for free evolution. By inputing this operator relation to the evolution equation Eq.(5), we can obtain the free evolution equation, which assumes the same form as the free particle Schrödinger equation:

$$i\frac{\partial\psi(x,t)}{\partial t} = -\frac{1}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} \tag{26}$$

It is worth noting that, unlike the free particle Schrödinger equation, the reduced Planck constant $\hbar$ with dimension of action is missing in this equation. However, this is in fact not a problem. The reason is that the dimension of $\hbar$ can be absorbed in the dimension of the mass m. For example, we can stipulate the dimensional relations as $p = 1/L$, $E = 1/T$ and $m = T/L^2$, where L and T represents the dimensions of space and time, respectively (see [16] for more discussions). Moreover, the value of $\hbar$ can be set to the unit of number 1 in principle. Thus the above equation is essentially the free particle Schrödinger equation in quantum mechanics.

Next we will consider the equation of motion under an external potential $V(x,t)$. When $V(x,t) = V_0$ is a constant potential, we still have the free state $e^{i(px-Et)}$ with $E = p^2/2m + V_0$. Thus the corresponding equation of motion is

$$i\frac{\partial\psi(x,t)}{\partial t} = -\frac{1}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V_0\psi(x,t) \tag{27}$$

For the general situation, the equation of motion also assumes the similar form

$$i\frac{\partial\psi(x,t)}{\partial t} = -\frac{1}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x,t)\psi(x,t) \tag{28}$$

[8] Note that we can in principle avoid talking about mass in modern physics from a more fundamental view (cf. [12-15]).

This is exactly the Schrödinger equation in quantum mechanics. Note that the potential here is classical and it has a definite (real) value in each position at every instant. The concrete form of the potential will be determined by the nonrelativistic approximation of the quantum interactions involved, which are described by the relativistic quantum field theory. Besides, the Hamiltonian $H = P^2/2m + V(x,t)$ is Hermitian because the potential $V(x,t)$ is real-valued. As a result, the time translation operator $U(t)$ is unitary.

5 Further discussions

We have derived the Schrödinger equation in quantum mechanics, mainly based on spacetime translation invariance and relativistic invariance. As we think, the derivation may not only make the Schrödinger equation more logical and understandable, but also shed some new light on the physical meaning of the state function (or wave function) $\psi(x,t)$.

The Schrödinger equation is usually "derived" in textbooks by analogy and correspondence with classical physics. There are at least two mysteries in such a heuristic "derivation". First, even if the behavior of microscopic particles likes wave and thus a wave function is needed to describe them, it is unclear why the wave function must assume a complex form. Indeed, when Schrödinger originally invented his equation, he was also very puzzled by the inevitable appearance of the imaginary unit "i" in the equation. Next, one doesn't know why there are the de Broglie relations for momentum and energy and why the nonrelativistic energy-momentum relation must be $E = p^2/2m$. Usually one can only resort to experience and classical physics to answer these questions. This is unsatisfactory in logic as quantum mechanics is a more fundamental theory, of which classical mechanics is only an approximation.

As shown above, the key to unveil these mysteries is to analyze the real origin of momentum and energy. According to our modern understanding, spacetime translation gives the definitions of momentum and energy. The momentum operator P is defined as the generator of space translation, and it is Hermitian and its eigenvalues are real. Moreover, the form of momentum operator can be uniquely determined by its definition and it is $P = -i\frac{\partial}{\partial x}$, and its eigenstate is e^{ipx} as a result, where p is the real eigenvalue. Similarly, the energy operator H is defined as the generator of time translation. But its form is determined by the concrete situation. Fortunately, for an isolated system (e.g. a free microscopic particle) the form of energy operator, which determines the evolution equation, can be fixed by the requirements of spacetime translation invariance and relativitic invariance. Concretely speaking, time translational invariance requires that $dH/dt = 0$, and the solution of the evolution equation $i\frac{\partial\psi(x,t)}{\partial t} = H\psi(x,t)$ must assume the form $\psi(x,t) = \varphi_E(x)e^{-iEt}$. Besides, space translational invariance requires $[P,H] = 0$, and this further determines that $\varphi_E(x)$ is the eigenstate of P, namely $\varphi_E(x) = e^{ipx}$. Thus spacetime translation invariance entails that the state of a free microscopic particle with definite momentum and energy assumes the plane wave form $e^{i(px-Et)}$. Furthermore, the relation between p and E or the energy-momentum relation can be determined by the relativistic invariance of the free state $e^{i(px-Et)}$, and its nonrelativistic approximation is just $E = p^2/2m$. Then we can obtain the form of energy operator for a free particle, $H = P^2/2m$, and the free particle Schrödinger equation Eq.(26). To sum up, this analysis can answer why the wave function must assume a complex form in general and why there are the de Broglie relations and why the nonrelativistic energy-momentum relation is what it is.

So far so good. But how does the thus-derived Schrödinger equation, in particular, the state function $\psi(x,t)$ in the equation, relates to the actual physical situation? Without answering this question the above analysis seems vacuous in physics. This leads us to the problem of interpreting the state function. Exactly what does the state function $\psi(x,t)$ describe? According to the standard probability interpretation, the state function is a probability amplitude, and the square of its absolute value represents the probability density of finding a particle in certain locations. This can be understood from the continuity equation derived from the Schrödinger equation. Multiplying the Schrödinger equation Eq. (28) by $\psi^*(x,t)$, its conjugate by $\psi(x,t)$, and taking the difference, we get

$$i\frac{\partial[\psi^*(x,t)\psi(x,t)]}{\partial t} = -\frac{1}{2m}[\psi^*(x,t)\frac{\partial^2\psi(x,t)}{\partial x^2} - \psi(x,t)\frac{\partial^2\psi^*(x,t)}{\partial x^2}] \tag{29}$$

Note that the real-valuedness of the potential $V(x,t)$ is used here. This equation can be further written as

$$\frac{\partial[\psi^*(x,t)\psi(x,t)]}{\partial t} + \frac{1}{2mi}\frac{\partial[\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x} - \psi(x,t)\frac{\partial\psi^*(x,t)}{\partial x}]}{\partial x} = 0 \tag{30}$$

By defining

$$\rho(x,t) \equiv |\psi(x,t)|^2 \tag{31}$$

and

$$j(x,t) \equiv \frac{1}{2mi}[\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x} - \psi(x,t)\frac{\partial\psi^*(x,t)}{\partial x}], \tag{32}$$

the above equation becomes the familiar form of continuity equation:

$$\frac{\partial\rho(x,t)}{\partial t} + \frac{\partial j(x,t)}{\partial x} = 0. \tag{33}$$

According to the standard interpretation, the density $\rho(x,t) \equiv |\psi(x,t)|^2$ in the continuity equation represents the probability density of finding the particle in certain locations, and the equation represents the conservation of detection probability. We can also write the state function $\psi(x,t)$ in terms of $\rho(x,t)$ and $j(x,t)$:

$$\psi(x,t) = \sqrt{\rho(x,t)}e^{im\int_{-\infty}^{x}\frac{j(x',t)}{\rho(x',t)}dx'}. \tag{34}$$

Accordingly there exists a one-to-one relation between $\psi(x,t)$ and $\rho(x,t)$, $j(x,t)$ when omitting an absolute phase. Moreover, it seems that the latter is more physical than the former because they are real-valued and can be directly measured. For example, by measuring the position probability distribution $\rho(x,t)$ we can identify the wavelength of a standing wave composed of two momentum eigentsates with opposite momenta and further measure the value of momentum.

Notwithstanding the success of the standard interpretation, our derivation of the Schrödinger equation may have more implications on the physical meaning of the state function $\psi(x,t)$. First, it seems to suggest that the state function $\psi(x,t)$ is a description of the actual physical state of a particle, rather than the probability amplitude relating only to measurement. In our derivation we never refer to the measurement of the isolated system after all. Moreover, it seems to further imply that the state function $\psi(x,t)$ is a complete description of the physical state. Which kind of physical state then? This is still a debatable issue. But if the state function $\psi(x,t)$ is indeed a (complete) description of the state of motion for a single particle, then $|\psi(x,t)|^2dx$ will not only give the probability of the particle being *found* in an infinitesimal space interval dx near position x at instant t, but also give the objective probability of the particle *being* there. This accords with the commonsense belief that the probability distribution of the measurement outcomes of a property is the same as the actual distribution of the property in the measured state. On this tentative interpretation, the objective motion of a particle is essentially random and discontinuous, and the quantities $\rho(x,t)$ and $j(x,t)$, as well as the state function $\psi(x,t)$ being a mathematical complex composed of them, provides a complete description of the state of such motion. It has been argued that this suggested interpretation might provide a natural realistic extension to the standard view [17-18]. Certainly, the transition process from "being" to "being found", which is closely related to the notorious quantum measurement problem, needs to be further accounted for [19].

To sum up, we have shown that the heuristic "derivation" of the Schrödinger equation in quantum mechanics textbooks can actually be turned into a real derivation by resorting to spacetime translation invariance and relativistic invariance. The derivation may reveal the logic of the Schrödinger equation and thus make this important equation more understandable for students. Moreover, it might also cast some new light on the physical meaning of the state function in the equation.

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