Physical meaning and derivation of Schrodinger and Dirac equations

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We derive the Schrodinger and Dirac equations from basic principles. First we determine that each eigenfunction of a bound particle is a specific superposition of plane wave states that fulfills the averaged energy relation. The Schrodinger equation is derived to be the condition the particle eigenfunction must satisfy, at each space-time point, in order to fulfill the averaged energy relation. The same approach is applied to derive the Dirac equation involving electromagnetic potentials. Effectively, the Schrodinger and Dirac equations are space-time versions of the respective averaged energy relations.

1   Introduction

Erwin Schrodinger obtained in 1926 an equation that described and explained adequately atomic phenomena and which became the dynamical centerpiece of quantum wave mechanics. The Schrodinger equation yields the eigenfunctions of a particle in an energy potential. Despite its fundamental role in physics, the dynamical status and justification of the Schrodinger equation have become vague, varied and discordant.

Quantum mechanics textbooks axiomatize, justify or derive the Schrodinger equation in a variety of ways. This constitutes a unique anomaly since the fundamental equations in physics arise from first principles.

In most texts, the Schrodinger equation is termed to be "an axiom" or "a physical law analogous to Newton's second law of motion in classical physics" or a phenomenological equation that "just works" [1−5].

Other texts share the belief that the Schrodinger equation cannot be derived but proceed to obtain it "heuristically" as an extension of the free particle wave equation, either by inserting the potential energy term by hand or by introducing this term into the free particle Hamiltonian [6−12].

I find that the above statements and derivations are faulty. To begin with, the Schrodinger equation does not seem to be an independent dynamical principle since it has the form of the non-relativistic energy relation. Furthermore, the Dirac equation has the form of the relativistic energy relation. These correspondences indicate that these equations originate, not just formally, from the respective energy relations.

On the other hand, the heuristic derivations do not only involve a "leap of faith" but actually have inappropriate logic. In particular, the free particle wave equation does not contain any dynamics itself to serve as a dynamical basis that can be extended. The free particle equation

yields back what we have already put in: a plane wave of wavelength $\lambda = h/p$ and period $T = h/E$, where the momentum (p) and energy (E) are interconnected through the free particle energy relation. Bearing in mind the uncertainty principle, we realize that the insertion of the potential term (depending on position and time) into the free particle energy relation is inappropriate.

Finally, there exist a series of derivations [13−16], including the original derivation by Erwin Schrodinger [9] and that of Richard Feynman [14], but none of these arises from basic physical principles and none has been generally accepted. As a result, the physical justification of the Schrodinger equation has been cloudy and controversial.

The origin of all this confusion is the improper use of the energy relation which contains mutually exclusive dynamical variables. In quantum mechanics, the energy relation must be used in its averaged form from which we can derive the Schrodinger equation [17]. We will show that the Schrodinger and Dirac equations are space-time versions of the averaged energy relations.

2 Analysis

Below we use basic principles to grasp the structure of the eigenfunction of a bound particle and the physical meaning of the Schrodinger equation. First we reflect on how the eigenfunction of a bound particle is formed.

We start by considering the simple case of a particle inside a one dimensional box of size L. The wave properties of the particle and the boundary conditions determine that each eigenfunction is a standing wave arising from the interference of two plane waves having wavelength $\lambda_n = 2L/n$ and opposite momenta $\mathbf{p}_n = \pm h/\lambda_n$. A measurement of the momentum of the particle in the box would yield, with equal probability, either $+\mathbf{p}_n$ or $-\mathbf{p}_n$. In conclusion, each eigenfunction arises from the superposition of two plane wave states having specific momenta and equal, in magnitude, amplitudes.

Next, let us consider the ground state of the electron in a Hydrogen atom. Since there are no boundaries, the electron can have any wavelength (momentum). Therefore, the electron eigenfunction is a superposition of waves with momenta from $-\infty$ to $+\infty$ with the constraint that it fulfills the averaged energy relation.

Accordingly, we write the eigenfunction of a spinless particle as the superposition of plane wave states of momentum (p_i) and energy (E_j) having amplitudes $a(p_i, E_j)$

$$\psi(r,t) = \sum_{i,j} a(p_i, E_j) e^{\frac{i}{\hbar}(p_i \cdot r - E_j t)} \tag{1}$$

where, for convenience, we have suppressed the eigenfunction indices in $\psi_n(r,t)$ and $a_n(p_i, E_j)$.

Using periodic boundary conditions, the normalization of $\psi(r,t)$ in (1) yields

$$\frac{1}{V_o T_o \hbar^4} \int \psi^*(r,t)\psi(r,t) d^3 r dt = \sum_{i,j} a^*(p_i, E_j) a(p_i, E_j) = 1 \tag{2}$$

where $V_0 T_0$ is the space-time quantization volume.

The energy relation provides the dynamics of a system by interrelating its dynamical variables. But, in quantum mechanics, specific values of momentum and energy cannot be related directly to specific values of position and time. For that reason, the energy relation that includes potentials should be used in its averaged form.

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The non-relativistic averaged energy relation for a particle inside a potential $V(r,t)$ is

$$\overline{\frac{p^2}{2m}} + \overline{V}(r,t) = \overline{E} \tag{3}$$

The eigenfunctions of the particle are superpositions of plane wave states with amplitudes that yield average kinetic, potential and total energy values fulfilling the above relation.

In the next section, the Schrodinger equation will be derived from (3). Below we show, in fewer steps, that a particle eigenfunction $\psi(r,t)$ that satisfies the Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(r,t)}{\partial r^2} + V(r,t)\psi(r,t) = i\hbar\frac{\partial\psi(r,t)}{\partial t} \qquad \text{at each } (r,t) \tag{4}$$

fulfills the averaged energy relation (3).

Using (1) the Schrodinger equation takes the form

$$i\hbar\frac{\partial\psi(r,t)}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2\psi(r,t)}{\partial r^2} = \sum_{i,j}\left[E_j - \frac{p_i^2}{2m}\right]a(p_i,E_j)e^{\frac{i}{\hbar}(p_i\cdot r - E_j t)} = V(r,t)\psi(r,t) \tag{5}$$

Next, we multiply the last equation by $\psi^*(r,t)$ and integrate over the quantization volume to get

$$\frac{1}{V_0 T_0 \hbar^4}\int \psi^*(r,t)\sum_{i,j}\left[E_j - \frac{p_i^2}{2m}\right]a(p_i,E_j)e^{\frac{i}{\hbar}(p_i\cdot r - E_j t)}d^3rdt = \frac{1}{V_0 T_0 \hbar^4}\int \psi^*V(r,t)\psi d^3rdt \tag{6}$$

On the left hand side, we substitute $\psi^*(r,t)$ from (1), we carry out the space-time integrations that yield δ-functions in momenta and energies, and we obtain

$$\sum_{i,j}a^*(p_i,E_j)\left[E_j - \frac{p_i^2}{2m}\right]a(p_i,E_j) = \frac{1}{V_o T_o \hbar^4}\int \psi^*(r,t)V(r,t)\psi(r,t)d^3rdt$$

$$\overline{E} - \overline{\frac{p^2}{2m}} = \overline{V}(r,t) \tag{7}$$

Thus, we have shown that a particle eigenfunction that satisfies the Schrodinger equation fulfills the averaged energy relation.

3 Derivation of the Schrodinger equation

We start by considering that the eigenfunction of a spinless particle inside a potential is a superposition of plane wave states of momentum (p_i) and energy (E_j)

$$\psi(r,t) = \sum_{i,j}a(p_i,E_j)e^{\frac{i}{\hbar}(p_i\cdot r - E_j t)}$$

where the amplitudes $a(p_i, E_j)$ are such so that $\psi(r,t)$ fulfills the averaged energy relation.

The non-relativistic averaged energy relation can be written as

$$\overline{E} - \frac{\overline{p^2}}{2m} = \overline{V}(r,t)$$

$$\sum_{i,j} a^*(p_i, E_j)\left[E_j - \frac{p_i^2}{2m}\right]a(p_i, E_j) = \frac{1}{V_oT_o\hbar^4}\int \psi^*(r,t)V(r,t)\psi(r,t)d^3rdt \qquad (8)$$

This last equation can be put in the form

$$\frac{1}{V_oT_o\hbar^4}\int \psi^*(r,t)\left\{\sum_{i,j}\left[E_j - \frac{p_i^2}{2m}\right]a(p_i, E_j)e^{\frac{i}{\hbar}(p_i \cdot r - E_j t)} - V(r,t)\psi(r,t)\right\}d^3rdt = 0$$

$$or \qquad \frac{1}{V_oT_o\hbar^4}\int \psi^*(r,t)\{\Phi(r,t)\}d^3rdt = 0 \qquad (9)$$

The above expression states that the average value of the integrand over the space-time volume V_0T_0 is zero. One solution of this equation is to take the bracket in the integrand equal to zero at all points

$$\Phi(r,t) = 0 \quad at\ each\ (r,t) \qquad (10)$$

In other words, we take the integrand at each point to be equal to its average (zero) value. This solution is actually the Schrodinger equation.

Mathematically, there are infinite other conditions that can satisfy the averaged energy relation (9) for which the integrand is positive at some points and negative at others, averaging to zero. However, none of these solutions can be physically acceptable because there is no principle to dictate the infinite number of choices and parameters we have to impose.

Therefore, $\Phi = 0$ is the only physically acceptable solution that we write as

$$\sum_{i,j}\left[E_j - \frac{p_i^2}{2m}\right]a(p_i, E_j)e^{\frac{i}{\hbar}(p_i \cdot r - E_j t)} = V(r,t)\psi(r,t) \qquad at\ each\ (r,t) \qquad (11)$$

Next we employ (1), that $\psi(r,t)$ arises from the superposition of plane waves states, and we get

$$i\hbar\frac{\partial\psi(r,t)}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2\psi(r,t)}{\partial r^2} = \sum_{i,j}\left[E_j - \frac{p_i^2}{2m}\right]a(p_i, E_j)e^{\frac{i}{\hbar}(p_i \cdot r - E_j t)} = V(r,t)\psi(r,t) \qquad (12)$$

Rearranging terms, we obtain a space-time differential equation, the Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(r,t)}{\partial r^2} + V(r,t)\psi(r,t) = i\hbar\frac{\partial\psi(r,t)}{\partial t} \qquad at\ each\ (r,t) \qquad (13)$$

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Since $\psi(r,t)$ is the eigenfunction of a particle, we can impose normalization and single value requirement conditions to extract physically meaningful solutions.

Finally, we note that the Schrodinger equation is effectively a space-time version of the non-relativistic averaged energy relation.

4 Derivation of the Dirac equation

We will show that the Dirac equation is the condition that the eigenfunction of a charged spin-1/2 particle inside an electromagnetic potential (A_μ) must satisfy in order to fulfill the relativistic averaged energy relation.

The eigenfunction of a spin-1/2 particle arises from a superposition of plane wave states of the form

$$\psi(r,t) = \sum_{i,j} a(p_i, E_j)u(p_i, E_j)e^{\frac{i}{\hbar}(p_i \cdot r - E_j t)} \tag{14}$$

where the four-row spinor $u(p_i, E_j)$ describes the spin orientation.

The energy relation of a spin-1/2, charge q particle ($q = -e$ for the electron) bound in an electromagnetic potential $A_\mu(r,t)$ can be written in linear form as

$$\gamma_0(E - qA_0) - \boldsymbol{\gamma} \cdot \left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right)c - mc^2 = 0 \tag{15}$$

Multiplying the above equation by

$$\gamma_0(E - qA_0) - \boldsymbol{\gamma} \cdot \left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right)c + mc^2 \tag{16}$$

and using the anticommutation properties of the γ matrices, we get the relativistic energy-momentum relation

$$(E - qA_0)^2 = \left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right)^2 c^2 + m^2 c^4 \tag{17}$$

Now, we write the averaged form of the linear energy relation (15) as

$$\gamma_0\overline{E_j} - \boldsymbol{\gamma} \cdot \overline{\mathbf{p}_i}c - mc^2 = \gamma_0 q\overline{A_0}(r,t) - \boldsymbol{\gamma} \cdot q\overline{\mathbf{A}}(r,t)$$

$$\sum_{i,j} a^*(p_i, E_j)\overline{u}(p_i, E_j)\left[\gamma_0 E_j - \boldsymbol{\gamma} \cdot \mathbf{p}_i c - mc^2\right]u(p_i, E_j)a(p_i, E_j) \tag{18}$$

$$= \frac{1}{V_0 T_0 \hbar^4} \int \overline{\psi}(r,t)\left[\gamma_0 q A_0(r,t) - \boldsymbol{\gamma} \cdot q\mathbf{A}(r,t)\right]\psi(r,t)d^3 r dt$$

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where $\bar{u} = u^\dagger \gamma_0$ and $\bar{\psi} = \psi^\dagger \gamma_0$.

Next, we put equation (18) in the form

$$\frac{1}{V_0 T_0 \hbar^4} \int \bar{\psi}(r,t) \Theta(r,t) d^3 r dt = 0$$

$$where \quad \Theta(r,t) = \tag{19}$$

$$\sum_{i,j} \left[\gamma_0 E_j - \boldsymbol{\gamma} \cdot \mathbf{p}_i c - mc^2 \right] a(p_i, E_j) u(p_i, E_j) e^{\frac{i}{\hbar}(p_i \cdot r - E_j t)} - \left[\gamma_0 q A_0(r,t) - \boldsymbol{\gamma} \cdot q\mathbf{A}(r,t) \right] \psi(r,t)$$

The above equation states that the average value of the integrand over the space-time volume is zero. This is possible in two cases: either the integrand is zero at each space-time point or it can have arbitrary values averaging to zero. The only physically acceptable solution of (19) is to take the integrand to be equal to its average (zero) value.

So, we take $\Theta(r,t) = 0$ at each (r,t) point. Then we have

$$\sum_{p_i, E_j} \left[\gamma_0 E_j - \boldsymbol{\gamma} \cdot \mathbf{p}_i c - mc^2 \right] a(p_i, E_j) u(p_i, E_j) e^{\frac{i}{\hbar}(p_i \cdot r - E_j t)} = \left[\gamma_0 q A_0(r,t) - \boldsymbol{\gamma} \cdot q\mathbf{A}(r,t) \right] \psi(r,t) \tag{20}$$

Employing (14) – that the eigenfunction arises from a superposition of plane wave states – the above equation becomes

$$\left[\gamma_0 i\hbar \frac{\partial}{\partial t} - \boldsymbol{\gamma} \cdot (-i\hbar c) \frac{\partial}{\partial \mathbf{r}} - mc^2 \right] \psi(r,t)$$

$$= \sum_{p_i, E_j} \left[\gamma_0 E_j - \boldsymbol{\gamma} \cdot \mathbf{p}_i c - mc^2 \right] a(p_i, E_j) u(p_i, E_j) e^{\frac{i}{\hbar}(p_i \cdot r - E_j t)} = \left[\gamma_0 q A_0(r,t) - \boldsymbol{\gamma} \cdot q\mathbf{A}(r,t) \right] \psi(r,t) \tag{21}$$

Rearranging terms we get

$$\gamma_0 \left(i\hbar \frac{\partial}{\partial t} - q A_0 \right) \psi(r,t) - \boldsymbol{\gamma} \cdot \left(-i\hbar \frac{\partial}{\partial \mathbf{r}} - \frac{q}{c}\mathbf{A} \right) c\psi(r,t) = mc^2 \psi(r,t) \tag{22}$$

which is the Dirac equation for a charged spin-1/2 particle in an electromagnetic potential A_μ.

5 Amplitudes of plane waves

Our derivations have been based on the insight that a particle eigenfunction arises from the superposition of plane wave states $|p_i, E_j>$ with amplitudes $a(p_i, E_j)$. This can be tested by experimentally measuring the amplitudes $a(p_i, E_j)$.

Once we have solved, say, the Schrodinger equation and have obtained the eigenfunction of a state, we can extract the amplitude of each plane wave contributing to the eigenfunction by reversing the superposition equation.

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$$\psi(r,t) = \sum_{i,j} a(p_i, E_j) e^{\frac{i}{\hbar}(p_i \cdot r - E_j t)} \quad \rightarrow \quad a(p_i, E_j) = \frac{1}{V_o T_o \hbar^4} \int \psi(r,t) e^{-\frac{i}{\hbar}(p_i \cdot r - E_j t)} d^3 r dt \qquad (23)$$

As an example, we consider the electron ground state eigenfunction $\psi_0(r,t)$ in the Hydrogen atom. Solving the corresponding Schrodinger equation, with $V(r,t) = -ke^2/r$ and with p taking continuous values, we obtain

$$\psi_0(r,t) = \frac{1}{\sqrt{\pi r_0^3}} e^{-\frac{r}{r_0}} \times e^{-\frac{i}{\hbar}E_0 t} = \int_{-\infty}^{+\infty} a_0(p) e^{\frac{i}{\hbar}p \cdot r} d^3 p \times e^{-\frac{i}{\hbar}E_0 t} \qquad (24)$$

where $r_0 = \hbar^2/(mke^2)$ and $E_0 = -ke^2/2r_0 = -13.6 \, eV$.

Inverting (24) we get

$$a_0(p) = \frac{1}{\pi} \left(\frac{2r_0}{\hbar} \right)^{\frac{3}{2}} \frac{1}{\left[1 + \frac{r_0^2}{\hbar^2} p^2 \right]^2} \qquad (25)$$

The electron momentum distribution in (25) has been verified experimentally by measurements of photoelectrons in ionization experiments and in inelastic electron scattering experiments [6].

6 Discussion

The Schrodinger equation is the only fundamental equation in physics with controversial dynamical status. Some textbooks claim that it is an independent physical law, others derive it as a "plausible extension of the free particle wave equation" and some texts use various heuristic derivations not based on first principles.

However, the confusion surrounding the physical justification and derivation of the Schrodinger equation originates from inappropriate physical arguments.

Based on first principles we have obtained a transparent and justified dynamical picture. Each eigenfunction of a bound particle is a specific superposition of plane waves that fulfills the averaged energy relation. The Schrodinger and Dirac equations are the conditions that the particle eigenfunction must satisfy at each space-time point in order to fulfill the respective averaged energy relation. Effectively, the Schrodinger and Dirac equations are space-time versions of the respective energy relations.

The assumption that the Schrodinger equation is an independent principle prevents us from discerning that the eigenfuntion arises from a superposition of plane waves.

Furthermore, we point out that the heuristic derivations use, uncritically, the analogy of form that exists between the free energy relation and the free wave equation and extend this analogy to the energy relation with potential terms. This analogy is deceptive. The free particle wave equation and the Schrodinger equation are dynamically different. The former does not contain any dynamics and has plane wave eigenfunctions with momentum and energy related through the

free energy relation. On the other hand, the eigenfunctions of the Schrodinger equation are specific superpositions of plane wave states that fulfill the averaged energy relation.

The use of the Schrodinger and Dirac equations is most appropriate for particles bound in smoothly varying potentials. Particles hitting potential barriers or bound inside square wells should be described by using the wave properties of particles with appropriate boundary conditions, while particle scattering processes can be considered best as arising from intermediate particle exchanges.

The concepts used in this paper can be applied to provide a simpler and more justified presentation of quantum mechanics.

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