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Hilbert space in quantum mechanics

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Abstract: Quantum mechanics is often considered as a relatively obscure physics course, which not only subverts beginners' cognition for Newton's motion laws in classical mechanics but also makes learners afraid, because of its complicated and profound mathematical theories in quantum mechanics. Thus, this article will, from the perspective of quantum mechanics, discuss the fundamental differences between the connotation of Hilbert space and spaces in classical mechanics. The application of Hilbert space in quantum mechanics will be expounded then. Finally, based on learners' difficulties existing in learning process, several teaching suggestions will be presented for future teaching reference.
Key words: quantum mechanics; Hilbert space; physics; mathematics

1 Introduction

Throughout the development of physics, an interesting phenomenon appears: the development of physics has never completely separated from the development of mathematical science, and even the development of physics and mathematics complemented each other and achieved each other. Such relationships exist between calculus and classical mechanics, modern physics, Riemannian geometry, general relativity, linear algebra, analytic geometry and quantum mechanics. In addition, the inseparable relationship between mathematics and physics is also reflected in the fact that many of the greatest scientists in history were both physicists and mathematicians such as Newton, Maxwell, von Neumann, Hilbert, etc. Therefore, the close integration of mathematics and physics has always been the mainstream form of scientific development [1].

It is known to all that physics, as a rigorous, precise and quantitative natural science, contains basic laws and theorems commonly expressed by mathematical formulas, which exactly reflects "the regular reaction of the functional relationship between physical quantities under certain conditions" [2] and further reflects the close relationship between physics and mathematics. In the 17th century, calculus was invented by physicist Newton in the process of studying classical mechanics. With the help of calculus, Newton unified the mechanical laws in the sky and on the ground in his Mathematical Principles of Natural Philosophy, and built a perfect classical mechanical system, which made the entire starry sky of physics and mathematics more dazzling and opened up a broader space for the further development of physics and mathematics. Quantum mechanics, developed in the early 20th century, was not divorced from the development of mathematics. Among the three equivalent expressions of quantum mechanics: Schrodinger's wave mechanics [3-5], Heisenberg's matrix mechanics [4, 5], and Feynman's path integral [6], a large number of mathematical languages are used to elaborate the basic principles and theories of quantum mechanics. Furthermore, quantum phase space theory, with its unique charm and advantages, has also been applied as a form of expression in quantum optics, statistical physics and other fields [7, 8]. This theory is very difficult for beginners, not only because quantum mechanics itself subverts people's cognition of the traditional motion laws of classical mechanics, but also because the boring and obscure mathematical formulas and operations increase the difficulty of learning and understanding. Thus, in the face of quantum mechanics, as a physics major, many learners always feel overwhelmed.

In response to this, this paper tries to start from Hilbert space and the mathematical foundation of quantum phase space theory. The author expounds the birth of Hilbert space firstly and the connotation of state vector and operator in quantum mechanics and representation transformation in Hilbert space are discussed. Finally, inspired by the connotation of Hilbert space and its application in quantum mechanics, this paper puts forward some teaching suggestions, aiming at promoting the beginners to deeply understand and learn this part of knowledge from the perspective of mathematical thinking and methods, and providing references for teachers in the future course teaching process simultaneously.

2 Hilbert space

2.1 Birth of Hilbert space

The idea of Hilbert space originated from Hilbert's research on integral equations, and its development is shown in Figure 1. In 1900, Fredholm discovered the similarity between integral equations and linear equations, and applied the research results of infinite-dimensional linear equations to the solution of integral equations [9]. Hilbert began to study integral equations as soon as he learned of Fredholm's work, and published six articles on integral equations between 1904 and 1910 [10]. The eigenvalue theory of the symmetric kernel integral equation embodies the germ of Hilbert's space thought, but it does not put forward the concept of "space". Meanwhile, Hilbert's definition of complete orthogonal system shows that there exists the idea of Hilbert space at this time. Later, under the efforts of Hilbert's followers, such as Schmidt (Hilbert's doctoral student), Riess, von Neumann, and others, they ultimately led to the establishment of the core content of functional analysis and quantum mechanics-Hilbert space.

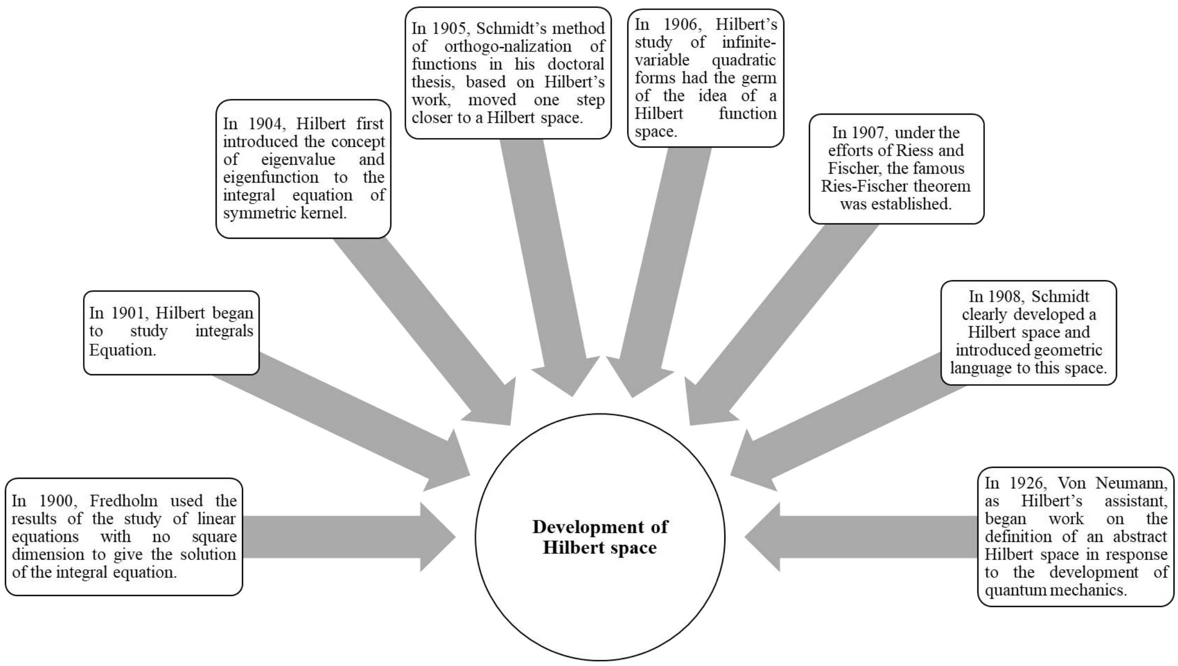

Fig. 1. Development of Hilbert space

2.2 Hilbert space and Euclidean space

One may wonder: if we build a theory of quantum mechanics in Hilbert space, what are the differences between Hilbert space and Euclidean space?

Addition satisfies the existence of commutative and associative laws, zero and negative elements, and identity elements while number multiplication satisfies the associative law and the distributive law of multiplication, which constitute the basic characteristics of a linear space. The linear space, defining the inner product, is called Euclidean space, which is a real space with the characteristics of flatness, uniformity, isotropy and so on. Euclidean space defines the length of vector, the angle between two non-zero vectors, the vertical vector, the distance between two vectors and other concepts, which promotes the introduction of the concept of inner product in the linear space over the field of real numbers, and lays a foundation for the study of real inner product space.

Hilbert space, which is no longer limited to finite dimension but extended to infinite dimensional space, can be regarded as a generalization of Euclidean space. Thus, the coordinate base vector of Hilbert space can be infinite. At the same time, on the basis of Euclidean space, Hilbert space realizes the transformation from real space to complex space. Hilbert space, therefore, is an abstract, complete complex inner product space.

3 Hilbert spaces in quantum mechanics

3.1 Why Hilbert space

At the beginning of the 20th century, with the efforts of a group of outstanding physicists such as Born, Schrodinger, Pauly, Heisenberg and de Broglie, quantum mechanics, one of the two pillars of modern physics, finally came into being. Matrix mechanics raised by Heisenberg and wave mechanics proposed by Schrodinger became the two major theories of quantum mechanics. Nevertheless, these two theories did not merge into one unified theory. Hilbert, a mathematician, tried to establish a unified axiomatic formulation from the two theories, but failed. Later, in response to the development of quantum mechanics, von Neumann expressed Hilbert's theory in a more abstract form, and for the first time defined the abstract Hilbert space as a complete and divisible complex vector space with inner product, which promoted Hilbert theory to meet the development needs of quantum mechanics and laid the foundation for the integration and unification of the two theories. Thus, it is inevitable for quantum mechanics to choose Hilbert space theory as its mathematical foundation.

3.2 State vectors in Hilbert space

State vectors in quantum mechanics are represented by points in Hilbert space, which describe the quantum states of microscopic particles in Hilbert space (vector space). Learners are often faced such a puzzle: what is the relationship between wave functions, which are used to describe quantum states of microscopic particles, and state vectors, which are also used to describe quantum states?

One of Hilbert's most remarkable achievements was to show the complete formal consistency of functions and vectors. Both satisfy the same axioms, as shown in Table 1. As can be seen from Table 1, vectors and functions have something in common in terms of concept, operation and geometric meaning. Therefore, both wave function and state vector in Hilbert space can be used to describe the process of microscopic particle state, and their description of quantum state is equivalent.

Table 1. Similarities between functions and vectors

Similarities	Vectors	Functions
Concept	N-dimensional vector $\vec{a}\,\{x_1, x_2, \ldots, x_n\} = x_1\{1,0,..,0\} + \ldots + x_n\{0,0,\ldots,1\}$	Function$\Psi(x) = \sum_n c_n\,\varphi_n(x) = c_1\varphi_1(x) + c_2\varphi_2(x) + \ldots + c_n\varphi_n(x)$
Addition Operation	Two vectors are added to create a new vector: $\vec{c} = \vec{a} + \vec{b}$, and arbitrary component $c_i = a_i + b_i$	Two vectors are added to create a new vector:$h(x) = f(x) + g(x)$, and arbitrary component$h(x_1) = f(x_1) + g(x_1)$

Similarities	Vectors	Functions
Inner Product	$(\vec{a},\vec{b}) = \sum_i a_i b_i$	$(f(x),g(x)) \equiv \int f^*(x)g(x)dx$
Length or Modulus	$\lvert\vec{a}\rvert = \sqrt{\vec{a}\cdot\vec{a}}$	$\lvert f(x)\rvert = \sqrt{f^*(x)f(x)}$
Included Angle	$\cos\varphi = \frac{(\vec{a},\vec{b})}{\lvert\vec{a}\rvert + \lvert\vec{b}\rvert}$	$\cos\varphi = \frac{(f(x),g(x))}{\lvert f(x)\rvert + \lvert g(x)\rvert}$
Orthogonal/Vertical	$\vec{a}\perp\vec{b} \Leftrightarrow (\vec{a},\vec{b}) = 0$	$f(x)\perp g(x) \Leftrightarrow (f(x),g(x)) = 0$
Parallel/Linear Correlation	$\vec{a}\parallel\vec{b} \Leftrightarrow \vec{a} = k\vec{b}$	$f(x)\parallel g(x) \Leftrightarrow f(x) = kg(x)$

3.3 Mechanical quantities in Hilbert space

Mechanical quantities in quantum mechanics are often expressed in terms of operators in Hilbert Spaces. Therefore, operators are an important concept of vector space. However, people often wonder why mechanical quantities in quantum mechanics are represented by operators.

In classical mechanics, the values of mechanical quantities are determined, and the physical states are directly described by mechanical quantities which are functions of states. Therefore, the numerical values of mechanical quantities and physical states in classical mechanics are unified. Different from the situation of quantum mechanics, microscopic particles have wave-particle duality, and their quantum states are described by wave functions. In general, for certain quantum states, the value of corresponding mechanical quantities cannot be determined simultaneously [11]. In other words, quantum states and mechanical quantities in quantum mechanics are not unified, but separate. As a result, the concept of sports in quantum mechanics and the description of the movement changed, and it is no longer suitable for describing the mechanical quantities of microscopic particles in the classical mechanics way.

In order to adapt to this change in quantum mechanics, the mathematical representation of mechanical quantities and motions also needs to be changed accordingly, which results in the introduction of operators to represent mechanical quantities.

This is the basic assumption recognized as one of the fundamental principles of quantum mechanics: the mechanical quantity F in quantum mechanics is represented by $\widehat{F}$. If the system is in an eigenstate ψ_n where the eigenvalue of operator $\widehat{F}$ is λ_n, the mechanical quantity F has a definite value λ_n; If the system is in an eigenstate ψ_n that is not operator $\widehat{F}$, the mechanical quantity F has no definite value, but only a series of possible values.

Furthermore, in Hilbert space, the mechanical quantities in quantum mechanics must be linear Hermitian operators. The reason is: only operators whose mean value is a real number can represent mechanical quantities in quantum mechanics. For wave function φ and ψ, if operator $\widehat{F}$ satisfy

$$\int_{-\infty}^{+\infty} \psi^* \widehat{F} \varphi d\tau = \int_{-\infty}^{+\infty} (\widehat{F}\psi)^* \varphi d\tau$$

where operator $\widehat{F}$ is an Hermitian operator. It can be shown that the average Hermitian operator is a real number:

$$\overline{F} = \int_{-\infty}^{+\infty} \psi^* \widehat{F} \psi d\tau = \int_{-\infty}^{+\infty} (\widehat{F}\psi)^* \psi d\tau = \int_{-\infty}^{+\infty} \psi (\widehat{F}\psi)^* d\tau = \int_{-\infty}^{+\infty} (\psi^* \widehat{F}\psi)^* d\tau = \overline{F^*}$$

Thus, the mechanical quantities in quantum mechanics are represented by Hermitian operators. Quantum states need to satisfy the principle of superposition of states, so the mechanical quantity operator is also a linear operator.

The concrete representation of the mechanical quantity operator in Hilbert space is related to the representation. In different quantum mechanical representations, the forms of mechanical quantity operators are completely different. For example, in coordinate representation, the position operator is the position vector itself; but in momentum representation, position operator $\hat{\vec{r}} = i\hbar\left(\frac{\partial}{\partial p_x}\vec{i} + \frac{\partial}{\partial p_y}\vec{j} + \frac{\partial}{\partial p_z}\vec{k}\right) = i\hbar\nabla_p$. Next, we illustrate the representations of position operators, coordinate operators and energy operators in the coordinate representation.

Suppose existential quantum state $\psi(\vec{r},t)$, the probability density of t particle appearing at position $\vec{r}$ at time is $\rho(\vec{r},t) = |\psi(\vec{r},t)|^2$. The mean value of the particle position vector is

$$\bar{\vec{r}} = \int \vec{r}\,\rho(\vec{r},t)d\vec{r} = \int \vec{r}\,|\psi(\vec{r},t)|^2 d\vec{r} = \int \psi^*(\vec{r},t)\vec{r}\,\psi(\vec{r},t)d\vec{r} \qquad (1)$$

In the momentum representation, the quantum state of the particle is represented as

$$C(\vec{p},t) = \frac{1}{(2\pi\hbar)^{3/2}}\int \psi(\vec{r},t)e^{-i\vec{p}\cdot\vec{r}}\,d\vec{r}$$

The mean value of the particle momentum is

$$\bar{\vec{p}} = \int \vec{p}\,\rho(\vec{p},t)d\vec{p} = \int \vec{p}\,|C(\vec{p},t)|^2 d\vec{r} = \int C^*(\vec{p},t)\vec{p}\,\psi(\vec{p},t)d\vec{r} = \int \psi^*(\vec{r},t)(-i\hbar\nabla)\,\psi(\vec{r},t)d\vec{r} \quad (2)$$

In a similar way, in quantum state $\psi(\vec{r},t)$, particle kinetic energy $T = \frac{p^2}{2\mu}$ can get the average $\bar{T} = \frac{\overline{p^2}}{2\mu} = \int \psi^*(\vec{r},t)(-\frac{\hbar^2}{2\mu}\nabla^2)\,\psi(\vec{r},t)d\vec{r}$ (A is the mass of the particle)

Based on the above discussion, the operators corresponding to the position vector $\vec{r}$, momentum $\vec{p}$ and energy T can be expressed as $\vec{r}$、$-i\hbar\nabla$、$-\frac{\hbar^2}{2\mu}\nabla^2$ respectively:

$$\hat{\vec{r}} \equiv \vec{r}$$

$$\hat{\vec{p}} \equiv -i\hbar\nabla$$

$$\hat{T} \equiv -\frac{\hbar^2}{2\mu}\nabla^2$$

Therefore, in quantum mechanics, due to the wave-particle duality of the microscopic particles, the wave function description of the quantum state determines that the mechanical quantity must be represented by the corresponding linear Hermitian operator.

3.4 Representation in Hilbert space

In quantum mechanics, states and mechanical quantities are described in certain representations. You can see the importance of representation in quantum mechanics. The so-called representation refers to the concrete representation of states and mechanical quantities in quantum mechanics [4]. Generally speaking, representation refers to physical quantity that is used to express the function of the state of the physical system.

In quantum mechanics, the wave function describing a quantum state is treated as a vector and we identify a representation Q which is equivalent to a coordinate system in Euclidean space. Eigenfunction $\hat{Q}$, like $f_1(x), f_2(x), f_3(x)\cdots f_n(x)\cdots$, is the basis vector of the representation similar to the normalization of eigenfunctions unit vector $\vec{i}$、$\vec{j}$、$\vec{k}$ in Cartesian coordinate system; the normalization of eigenfunctions $\hat{Q}$ is similar to geometric coordinate system $\vec{i}\cdot\vec{i} = 1, \vec{j}\cdot\vec{j} = 1, \vec{k}\cdot\vec{k} = 1$ in Euclidean space; orthogonality of the eigenfunction accounts to $\vec{i}\cdot\vec{j} = \vec{j}\cdot\vec{k} = \vec{i}\cdot\vec{k} = 0$ as shown in Table 1. In quantum mechanics, there are infinitely many eigenfunctions of $\hat{Q}$, and the space in which the state vector resides is called Hilbert space.

Just as the background space of classical mechanics is Euclidean space, the background space of relativistic mechanics is Minkovski and Rimann space, and the background space of quantum mechanics is Hilbert space, the eigenfunction is the coordinate base vector of the space. Choosing a representation is equivalent to choosing a set of basis vectors in Hilbert space.

4 Teaching inspiration

4.1 Attach equal importance to mathematical thinking and physical thinking, and strengthen the application of mathematical thinking and methods in quantum mechanics

Physics and mathematics complement each other and achieve each other. Theorems and laws in physics can be expressed perfectly in mathematical form. Hilbert space is a mathematical concept, in which the description of the laws of quantum mechanics laid the mathematical foundation, especially in the early development of quantum mechanics to provide theoretical support for the perfect unity of matrix mechanics and wave mechanics. Mathematics increases the difficulty of physical problems, but maintains the rigor and science of quantum theory, and stimulates the enthusiasm of students to explore the unknown. Of course, this does not require teachers to develop complex arguments and calculations, but to gradually train students in basic mathematical methods.

The successful application of advanced mathematical language is the profound and perfect expression of quantum mechanics. For students who are beginning to learn quantum mechanics, they can focus on the analysis of physical concepts, replace or avoid mathematical difficulties with physical thinking, and complete the teaching objectives by simplifying models and concept extension and comparison. For example, in the teaching of Hilbert space, Euclidean space in classical mechanics can be used as the introduction to complete the extension and contrast teaching of concepts.

On this basis, students are gradually guided to strengthen the application of mathematical thinking and methods through the establishment of mathematical models, and then extend it to the specific application of quantum mechanics, so as to truly realize the teaching process of completing the concept analysis and theoretical deduction of quantum mechanics from the surface to the inside, deep and simple.

4.2 Use analogy teaching to give full play to the positive role of classical physics in quantum mechanics teaching

Although quantum mechanics describes the laws of motion of microscopic particles, which are not unrelated to the macroscopic world, "the laws of quantum mechanics govern not only the microscopic world, but also the macroscopic world" [6]. Bohr's reciprocity principle states that at quantum number $n\to\infty$, the behavior of quantum systems should gradually transition to classical mechanics. For example, Newton's second Law and Schrodinger's equation can be used to complete the teaching process by analogy.

According to the Schrodinger equation, the momentum of particles moving in the potential field $V(\vec{r})$ satisfies the Schrodinger picture $\frac{d<\hat{p}>}{dt}=\frac{1}{i\hbar}<[\hat{p},H]>=-\overline{\nabla U(r)}$. The Newtonian mechanical equations of motion with the average value of physical quantities $\frac{d\overline{P}}{dt}=-\nabla U(\overline{r})$ [12] can be obtained by further derivation.

Therefore, it is necessary to grasp the difference and connection between classical mechanics and quantum mechanics, look for the analogies of different physical concepts in classical physics and quantum mechanics, and grasp the rich logical correspondence among them, so as to give full play to the positive role of classical physics in the teaching of quantum mechanics, and then make the difficult content of quantum mechanics simple and easy to learn, thereby, eliminating students' resistance to quantum mechanics in learning.

4.3 Pay attention to the development history of quantum mechanics and stimulate students' interest in studying quantum mechanics

At the beginning of the 20th century, there were two dark clouds floating in the clear sky of classical physics, which made classical physics face unprecedented challenges. In 1900, Planck creatively introduced the concept of energy quantum, successfully explained the phenomenon of blackbody radiation, and the concept of quantum emerged. Until 1924, de Broglie made a breakthrough in proposing that microscopic particles have wave-particle duality, which gradually diverged from the classical theory. The Fifth Solvay Conference in 1927, widely regarded as the greatest gathering of natural science masters in history, included 17 Nobel Prize winners among the 29 attendees, pictured in Figure 2. Some important events in the birth of quantum mechanics from 1887 to the 1940s are shown in Figure 3. Under the efforts of a large number of outstanding physicists such as Born, Schrodinger, Pauli, Heisenberg, de Broglie, Einstein, von Neumann, Feynman and so on, quantum mechanics, known as one of the two pillars of modern physics, finally came out. The history of physics from birth to development of quantum mechanics contains innovative thinking that is incomparable to any other discipline so far. Therefore, in the teaching of quantum mechanics, we review the birth process of the history of quantum mechanics together with students, and guide the historical background of the course into the classroom teaching to edify their innovative spirit quality.

First row from left to right: Irving Langmuir、 Max Planck 、 Marie Sklodowska-Curie 、 Hendrik Lorentz 、 Albert Einstein 、 Paul·Langevin 、 Charles Goodyear 、 Charles Thomson Rees Wilson 、 Owen Willans Richardson ;
Second row from left to righ : Peter Joseph William Debye 、 Martin Knudsen 、 William Lawrence Bragg 、 H.A.Kramers 、 P.A.M.Dirac 、 A.H.Compton 、 L. de Broglie 、 M.Born 、 N.Bohr ;
Third row from left to right : A.Piccard、E.Henriot、P.Ehrenfest、Ed.Herzen、Th. de Donder、E.Schrodinger、E.Verschaffelt、W.Pauli、W.Heisenberg、R.H.Fowler、L.Brillouin .

Fig. 2. The 5th Solvay Conference participants (image from Wikipedia Solvay Conference entry)

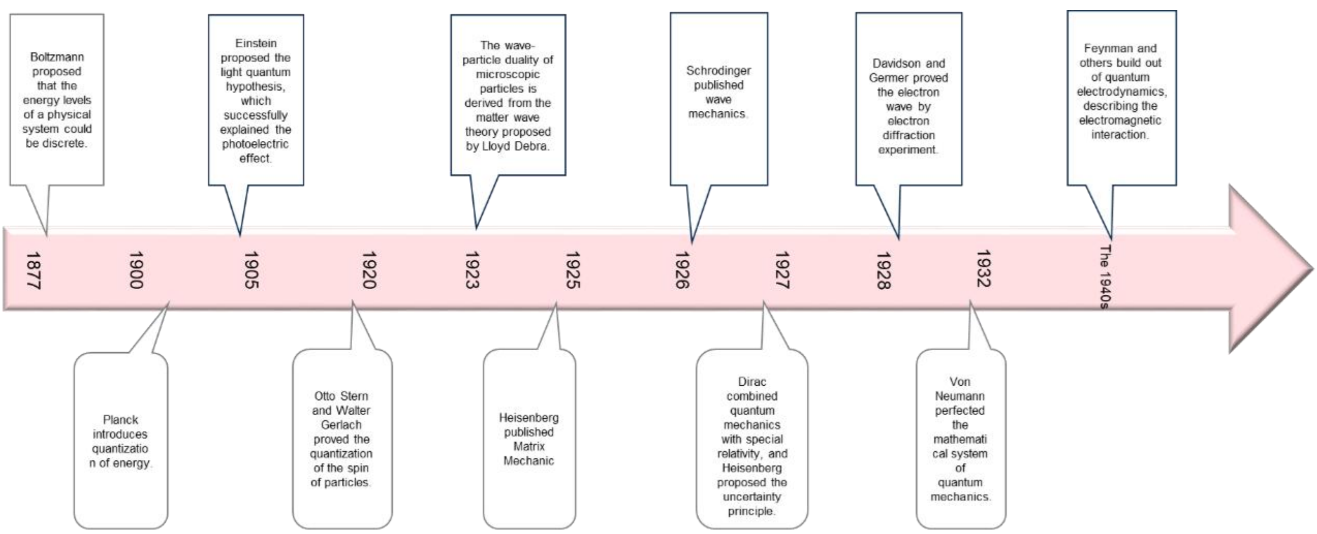

Fig. 3. A brief history of the birth of quantum mechanics

5 Conclusion

Starting from Hilbert space, the mathematical foundation of quantum theory, this paper first discusses the birth course of Hilbert space and its relation and difference with Euclidean space. Hilbert space can be regarded as the extension of Euclidean space, and Hilbert space is no longer limited to finite dimension, but extended to infinite dimension space. At the same time, Hilbert space realizes the transformation from real space to complex space on the basis of Euclidean space.

Furthermore, the connotations of state vectors and operators and representations in Hilbert space are discussed. State vectors in quantum mechanics are represented by points in Hilbert space and are used to describe the quantum states of microscopic particles. In Hilbert space, due to the wave-particle duality of microparticles, the wave function description of quantum states determines that the mechanical quantity must be represented by the corresponding linear Hermitian operator.

Finally, inspired by the connotation of Hilbert space and its application in quantum mechanics, this paper puts forward relevant teaching suggestions for quantum mechanics courses from three perspectives: the relationship between mathematics and physical thinking, the analogy between classical physics and quantum mechanics, and the history of quantum mechanics, so as to improve the teaching effect of quantum mechanics courses. It can provide reference for teachers in the teaching reform of quantum mechanics course in the future.

Conflicts of interest

The author declares no conflicts of interest regarding the publication of this paper.

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