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A Physical Perspective on Fourier Transform Underlying Its Application in Quantum Scattering

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Abstract: This paper adopts an alternative approach to explore the application of Fourier transform in quantum scattering based on the physical nature of the Fourier transform. Compared with the traditional research method which is mainly based on mathematical derivation, an innovative analysis perspective based on the physical nature is proposed. It is found that the inner product projection nature of the Fourier transform enables it to realize the screening of specific energy eigenstates at the physical level through the inner product operation of complex exponential functions, and complete the frequency screening by the resonance mechanism. In the quantum system, the frequency domain corresponds to the particle energy eigenstates one by one, successfully transforming the differential operator in the Hamiltonian operator into an algebraic operator, greatly simplifying the calculation. Meanwhile, the wave function orthogonality facilitates the independent study of wave function states at each frequency, eliminating the complex spatial coupling in the time domain. This research not only constructs a new analytical framework for quantum scattering problems, but also opens up a new path for teaching and research of quantum scattering theory, which has potential application value to quantum optics, condensed matter physics and other fields.

Keywords: Fourier Transform, Mathematical Physics, Physical Interpretation, Quantum Scattering, Quantum Mechanical Computation.

1. Introduction

The Fourier transform has always been an indispensable tool in the development of modern physics, especially in the field of quantum mechanics, and its application has run through several important research directions. In traditional research, Fourier transform is regarded as a purely mathematical tool, mainly used for the conversion between coordinate space and momentum space, or the frequency domain decomposition of complex wave functions[1,2]. For example, when dealing with the wave function of a quantum system, the Fourier transform is often used to convert it from the coordinate representation to the momentum representation in order to solve the Schrödinger equation . However, this over-reliance on the mathematical form of the application has led to the long-term neglect of the profound physical mechanisms embedded in the Fourier transform itself.

In terms of physical nature, the Fourier transform sifts the frequency components of a signal by operating on the inner product of complex exponential functions, a process that essentially

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corresponds to a resonant response to a specific frequency[3]. In classical physics, this resonance response can be intuitively understood as the selective response of a system to external excitation at a specific frequency; while in quantum mechanical systems, its significance is more far-reaching. In quantum systems, the frequency domain not only corresponds to the representation of the wave function in momentum space, but is also directly related to the energy eigenstates of the particles. This correspondence is crucial because it allows the transformation of differential operators in Hamiltonian operators into algebraic operators in the frequency domain. Taking a particle in a one-dimensional infinite deep potential well as an example, solving the Schrödinger equation corresponding to its Hamiltonian operator in the coordinate representation requires dealing with complex second-order differential equations; whereas, when converted to the frequency domain, based on the correspondence between the frequency and the energy eigenstates, the operations of the differential operators are simplified to algebraic operations, and the difficulty of solving the equations is reduced dramatically.

In addition, in the frequency domain, the orthogonality of the energy eigenstates allows the state of the wave function at each frequency to be studied independently, which contrasts with the presence of complex spatial coupling of the wave function in the time domain. In the traditional time-domain analysis, the quantum scattering problem is often due to the mutual coupling of wave functions at various points in space, which leads to a cumbersome computational process and a blurred physical image. The advantage of frequency domain analysis brought by Fourier transform provides a brand new possibility for the solution of quantum scattering problems. Unfortunately, the traditional quantum scattering research method, which is mainly based on mathematical derivation, fails to fully explore this physical connotation of the Fourier transform, which makes the research of quantum scattering problems bottle necked to a certain extent. Therefore, revisiting the application of Fourier transform in quantum scattering from the perspective of physical nature and constructing a brand-new framework of understanding have become the key to promote the development of quantum scattering theory.

2. Analysis of fourier transform expressions

Simple harmonic vibration, as the most basic form of periodic motion in nature, has wide universality and thus becomes a universal model for describing linear systems. Due to its orthogonality in the time domain, any complex signal can be uniquely represented as a linear superposition of a set of simple harmonic components, and the Fourier transform is built on this foundation. Simple harmonic motion is essentially a one-dimensional projection of circular motion, which is expressed in the complex plane as a complex exponential function, which can be regarded as a basis function in the frequency domain, and is used to realize the mapping of time-domain signals to the frequency domain[4].

2.1. Mathematical essence: inner product operation

The mathematical nature of the Fourier transform is the inner product of two continuous functions.

$$< \mathrm{f}, \mathrm{g} >= \int_a^b f(x) \bullet g * \left(\mathrm{x}\right) \mathrm{dx} \tag{1}$$

The inner product operation expressed in (1) is essentially a projection of one function into the direction of the other, the result of which measures the correlation between the two functions[1][4].

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When the two functions are orthogonal, the inner product is zero, indicating complete uncorrelation. For continuous-time signals, the similarity needs to be evaluated in the full time domain: the product of the function values at each time point reflects the local correspondence, and the integral realizes the global superposition. Since the Fourier transform involves complex exponential functions, in order to maintain the conjugate symmetry of the mathematical structure and to ensure physical measurability, one side of the inner product needs to be taken as the conjugate, so that the final result has a clear real-number meaning, and to avoid the imaginary part interfering with the physical interpretation[5].

$$F(\omega) = dt \tag{2}$$

The interpretation in (2) is to do the inner product operation with the target signal f(t) and the simple harmonic vibration to determine the degree of correlation between the two, when the two ω are the same, the projection amount is not 0, the integration result is not 0, then the frequency that exists in f(t) can be judged. The integral result is obtained directly from the projection coefficients of the signal projected onto each frequency basis function, which can reflect the weight of the corresponding frequency components, and all the coefficients combined are the frequency domain representation of the signal.

2.2. Physical nature: resonance

The essence of Fourier transform is frequency screening, and its physical mechanism can be regarded as the resonance response generated when two signals are matched in phase[3][6]. The complex exponential function plays the role of “detector”, which can identify whether the signal contains specific frequency components and realize the point-by-point extraction of the spectrum. According to Parseval's theorem, the energy of the signal in the time domain and the frequency domain is conserved, and the projection coefficients obtained by the Fourier transform are complex numbers, but their modulus squares reflect the energy distribution of each frequency component. When the frequency is consistent, the local oscillation superposition forms energy enhancement, and the integration result is significant; if the frequency does not match, it is canceled out in the whole time domain due to the phase difference, and the integration tends to zero. With the continuous change of the frequency of the complex exponential function, the Fourier transform realizes the scanning and analysis of the full frequency band of the signal.

2.3. Fourier inverse transformation

$$\mathrm{f}(\mathrm{t}) = \frac{1}{2\pi} \int F(\omega) e^{i\omega t} d\omega \tag{3}$$

Equation (3) is an expression for the Fourier inverse transform, which is expressed as a weighted summation of each frequency according to the corresponding weights, calculating the sum of the contributions of each frequency at the moment t, and converting the signal from the frequency domain back to the time domain. At this point it cannot be understood as an inner product operation.

3. Applications of the fourier transform to quantum scattering

Quantum scattering refers to the changes in the states of momentum, energy and direction of motion of microscopic particles caused by quantum mechanical effects when they interact with a potential

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field. The wave-particle duality of the particle determines this process, described by the wave function, and the scattering manifests itself as diffraction, interference, and redistribution of the probability amplitude of the wave function under the action of the potential field. When a particle approaches the potential field, the wave function couples with the energy gradient and spatial distribution of the potential field, leading to an exchange of momentum and energy. This exchange is not a classical "collision", but is realized by quantum state jumps and probability amplitude superposition. The angular and energetic information of the scattered signals contains details of the potential field structure, which is useful for inferring microscopic interactions, resolving the dynamics of chemical reactions, and characterizing the electronic and lattice structures of materials. Quantum scattering is an important tool for unraveling the microscopic world and physical mechanisms, from theory to applications[7].

In the framework of quantum mechanics, the central expression for the scattering process of microscopic particles is the time-containing Schrödinger equation.

$$i\hbar\frac{\partial\psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\left(r\right)\right)\psi \tag{4}$$

Equation (4) expresses that the variation of the wave function over time is driven by energy. Where the Laplace operator is the second-order derivative of the wave function to space, which represents the rate of change of the wave function with respect to the rate of change of position, reflecting the intensity of the fluctuations. The larger it is, the more violent the particle fluctuations and the more energy. The right hand side of the equation can be simplified to the Hamiltonian operator acting on the wave function.

3.1. Computational complexity of the schrödinger equation in the time domain

In the time domain, the Schrödinger equation is embodied as a partial differential equation containing higher order partial derivatives. When it is applied to the wave function, it is necessary to calculate the relationship between the variation of the wave function at neighboring points in space, and this calculation will couple the wave function values at different points in space. At the same time, the equation contains two variables, time and space, and the solution has to deal with a four-dimensional coupling problem at the same time: three-dimensional space plus one-dimensional time. The solution of this equation requires discretization of space and time, leading to an exponential growth of the computational effort with dimension. For complex potential field changes, its analytical solution is almost non-existent[1,8].

3.2. Physical eigenstates and simplifying mechanisms in the frequency domain perspective

However, the problem is simplified when treated in the frequency domain. In quantum mechanics, the time and frequency domains are associated with physical quantities in different ways. The time domain describes the change of the wave function over time, which means that all the actions on the wave function will be coupled together and cannot be separated. The frequency domain, on the other hand, corresponds to the energy eigenstates of a quantum system. By the De Broglie relation,the wave number k directly determines the momentum, which is a manifestation of wave-particle duality. Therefore, the plane wave function is the eigenstate of the momentum operator, for a plane wave, the direction and magnitude of its wave vector determine the direction and magnitude of the momentum of the particle. When a particle is in a plane wave state, its momentum has a definite

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value. In addition, it is also known from the relationship between energy and frequency that the frequency can directly determine the energy[4]. So the frequency domain corresponds to the energy eigenstate of the quantum system.

3.3. Fourier transform and simplification of schrödinger equation in frequency domain

$$\phi\left(p,t\right)=\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}\psi\left(x,t\right)e^{-\frac{ipx}{\hbar}}dx \tag{5}$$

The Fourier transform of the quantum system is expressed as shown in (5), and since plane waves of different frequencies are orthogonal to each other, the wave function in the time domain can be decomposed into a linear superposition of countless plane waves of different momentum, and thus the time-containing Schrödinger equation of the quantum system in the frequency domain is shown in (6).

$$i\hbar\frac{\partial\phi(p,t)}{\partial t}=\left[\frac{p^2}{2m}+\widetilde{V}\left(p,t\right)\right]\phi\left(p,t\right) \tag{6}$$

Each frequency corresponds to a definite energy value, and the energy does not change with time, which makes the role of Hamiltonian operators simplified from differential operations to algebraic operations, greatly reducing the complexity of equation solving[2][6]. At the same time, the wave functions of different frequencies do not interfere with each other due to their orthogonality, which makes it possible to analyze the energy properties of the system by splitting the overall problem into several sub-problems that are not coupled with each other, and to study the physical state represented by the wave function at each frequency. This property is of great significance in quantum scattering studies and enables the simplified treatment of complex scattering processes. For example, in the study of scattering of electrons and complex molecules, by analyzing the wave functions at each frequency independently, not only the computational efficiency can be improved, but also the nature of the scattering mechanism can be revealed more deeply.

4. Conclusion

In this study, a series of research results of great value have been obtained through the in-depth analysis of the physical nature of the Fourier transform and its application in quantum scattering. From the point of view of Fourier transform itself, its core is not limited to mathematical formulas, but is based on the nature of physical operations -- the time domain signal and the orthogonal basis function in the frequency domain for the inner product operation, through the projection of the signal on the basis function to determine whether the signal has the corresponding frequency, the process is essentially based on the resonance between the signal and the basis function to achieve This process is essentially based on the resonance between the signal and the basis function to realize the screening and extraction of frequency. The projection coefficient mathematically reflects the degree of correlation between the two, and in the physical sense indirectly reflects the energy superposition of the two resonances, and different integration results represent the contribution of different frequencies, while the inverse transformation completes the signal reconstruction by weighted summation.

When the Fourier transform is applied to the quantum scattering problem, by virtue of the energy eigenstates of the corresponding quantum system in the frequency domain and the orthogonality

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between the wave functions at different frequencies, the coupling between the neighboring points in the coordinate space is successfully stripped away, making it possible to study the state of the wave functions at each frequency individually in the frequency domain. This analysis provides a more concise and clearer physical image for the dynamical analysis of quantum systems. Taking the scattering of electrons and molecules as an example, the traditional method needs to solve the equations containing many coupling terms in the complex coordinate space, while based on the method proposed in this study, the scattering process in each state can be analyzed independently in the frequency domain according to the frequencies corresponding to the different energy eigenstates of the electrons, which greatly simplifies the analytical process and the computational difficulty.

The application of Fourier transform to the Schrödinger equation can clearly reveal the core law of quantum scattering. After converted to the momentum space by Fourier transform, the differential operator is transformed into an algebraic operator, which corresponds to the determination of the momentum, making the Schrödinger equation simplified to an independent evolution equation of the energy eigenstates, avoiding the complicated spatial coupling calculations in the coordinate space, and directly revealing the physical essence of quantum scattering, which is the "conservation of energy drives the particle motion". This result not only provides an efficient method for solving quantum scattering problems, but also offers a new perspective for understanding the motion laws of microscopic particles.

The "physical nature first" research framework proposed in this paper breaks through the traditional "mathematical derivation-dominated" mode of thinking, proving that the Fourier transform is not only a mathematical tool, but also an important bridge connecting abstract mathematics and intuitive physics. For quantum scattering theory, in-depth analysis of the physical mechanism can reveal the operation law of the microscopic world better than simple formula derivation. In teaching, the research results help students to get rid of the mechanical memorization of complex mathematical formulas, understand the quantum scattering phenomenon from the physical nature, and improve the teaching effect; in the field of research, it provides a new way of thinking and methodology for the research of quantum mechanics related problems.

In the future, this research framework is expected to be further expanded to other fields, such as quantum optics and condensed matter physics, to promote the in-depth integration and synergistic development between "Physical Understanding" and "Mathematical Modeling", and to provide innovative solutions for solving more complex physical problems.

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