

An introduction to quantum scattering theory

Abstract

Quantum scattering, a fundamental phenomenon in quantum mechanics, is very important in understanding the interactions between particles at the microscopic level.^{1,2} Quantum scattering plays a pivotal role in various fields of physics, chemistry, and even beyond, influencing areas such as materials science, quantum computing, and nuclear physics among others.^{3,4} Theoretical concepts such as the Schrödinger equation, scattering amplitude, and scattering cross-section are highlighted in this, along with their significance in describing particle interactions with potential energy fields.^{5,6}

Keywords: Quantum scattering, quantum mechanics, elementary particles, scattering of light, Schrödinger equation

Volume 8 Issue 2 - 2024

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Received: May 06, 2024 | Published: June 03, 2024

Introduction

In Quantum mechanics, scattering involves alterations in particle trajectories or states during interaction essential for understanding phenomena like particle accelerations and light scattering by atoms.^{7,8} At the core of this theory is the scattering amplitude, depicting the transition probability from an initial to a final state. Various theoretical frameworks and mathematical tools like the Born approximation and partial wave analysis facilitate the study of quantum scattering.^{9,10} Recent advancements have enabled sophisticated investigations into multi-particle interactions and resonant scattering, enhancing our understanding of quantum systems. Quantum Scattering Theory is fundamental, empowering us to predict experimental outcomes and delve deeper into the microscopic realm.^{11,12} Its applications extend to cutting-edge technologies like quantum computing and sensing, underscoring its significance in shaping our understanding of quantum phenomena. The objectives of the study.

Quantum scattering principles

The two key principles of quantum scattering theory are the wave-particle duality and the Schrödinger equation. A particle with momentum p has an associated wavelength λ given by the de Broglie wavelength equation

$$\lambda = \frac{h}{p} \quad (1)$$

Where h is Planck's constant.

The Schrödinger equation is given by:

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \hat{H} \Psi(\mathbf{r}, t) \quad (2)$$

Quantum scattering formalism

An incident particle in state $|\psi_0\rangle$ is scattered by a potential V , resulting in a scattered state $|\psi_s\rangle$. The incident state $|\psi_0\rangle$ now becomes the eigenstate of the background Hamiltonian H_0 with eigenvalue E expressed mathematically as

$$(E - H_0)|\psi_0\rangle = 0 \quad (3)$$

unless otherwise stated, the background Hamiltonian H_0 should be taken as that of a free particle

$$H_0 = \frac{p^2}{2m} \quad (4)$$

and the incident state taken as a plane wave

$$\langle \vec{r} | \psi_0 \rangle = \psi_0(\vec{r}) = e^{i\mathbf{k}\cdot\vec{r}} \quad (5)$$

Scattering theory therefore aims to solve the full energy-eigenstate problem

$$(E - H_0 - V)|\psi\rangle = 0 \quad (6)$$

where $E > 0$, and $|\psi\rangle$ is the eigenstate of the full $H = H_0 + V$ with energy E .

The Lippmann-Schwinger equation

The Lippmann-Schwinger equation provides a formal solution for the scattering problem in terms of the scattering potential.

The scattered state $|\psi_s\rangle$ is defined as

$$|\psi_s\rangle = |\psi\rangle - |\psi_0\rangle \quad (7)$$

With the above, the full Schrodinger equation in [eqn \(1\)](#) can now be written as

$$E - H_0|\psi\rangle = V|\psi\rangle \quad (8)$$

considering $E - H_0|\psi\rangle = 0$, we have

$$|\psi\rangle = |\psi_0\rangle + \frac{1}{E - H_0} V|\psi\rangle \quad (9)$$

which is Lippmann-Schwinger equation.

Scattering amplitudes

Scattering amplitudes are defined as the probability amplitudes for a particle to scatter from an initial state to a final state due to interactions with other particles or potentials.¹³⁻¹⁵ Mathematically, the scattering amplitude $f(\theta)$ describes the scattering of a particle by a potential $V(\mathbf{r})$. In the Born approximation, $f(\theta)$ can be expressed as:

$$f(\theta) = -\frac{2\mu}{\hbar^2} \int V(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} d\mathbf{r} \quad (10)$$

where μ is the reduced mass of the scattering system, \hbar is the reduced Planck constant, \mathbf{k} is the wave vector of the incident particle, and \mathbf{r} represents the spatial coordinates.

Since the Born approximation assumes that the scattering potential $V(\mathbf{r})$ is weak, it allows us to expand the exponential term in the integrand as a power series. Thus, we have:

$$e^{i\mathbf{k}\cdot\mathbf{r}} \approx 1 + i\mathbf{k}\cdot\mathbf{r} - \frac{(\mathbf{k}\cdot\mathbf{r})^2}{2} + \dots \quad (11)$$

Substituting the approximation for $e^{i\mathbf{k}\cdot\mathbf{r}}$ into the integral, we obtain:

$$f(\theta) \approx -\frac{2\mu}{\hbar^2} \int V(\mathbf{r}) d\mathbf{r} \quad (12)$$

Scattering cross-section area

The differential scattering cross-section area ($d\sigma / d\Omega$) in quantum scattering describes the probability per unit solid angle of scattering into a particular direction. It is given by:

$$\frac{d\sigma}{d\Omega} = \frac{dN / d\Omega}{F} \quad (13)$$

H image

The incident flux (F) is defined as

$$F = \frac{nv}{A} \quad (14)$$

where n is the number density of incident particles, v is the velocity of incident particles, and A is the area of the target. In terms of scattering amplitude, it is expressed as:

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 \quad (15)$$

Scattering from a one-dimensional delta function potential

A one-dimensional delta function potential, often denoted as $V(x) = g\delta(x)$, is a simplified model used in quantum mechanics to describe a potential energy profile that consists of a single point-like potential located at $x = 0$. The delta function, denoted as $\delta(x)$,

is a mathematical function that is zero everywhere except at $x = 0$, where it is infinitely tall and integrates to unity over an infinitesimal interval around $x = 0$. The parameter g represents the strength of the potential.^{16,17}

Mathematically, the Schrödinger equation is given by:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + g\delta(x)\psi(x) = E\psi(x) \quad (16)$$

Let's denote this infinitesimal range as $[-\varepsilon, \varepsilon]$. Integrating this gives:

$$-\frac{\hbar^2}{2m} \int_{-\varepsilon}^{\varepsilon} \frac{d^2\psi(x)}{dx^2} dx + g \int_{-\varepsilon}^{\varepsilon} \delta(x)\psi(x) dx = E \int_{-\varepsilon}^{\varepsilon} \psi(x) dx \quad (17)$$

The integrals involving the second derivative of $\psi(x)$ can be evaluated as:

$$-\frac{\hbar^2}{2m} \left(\frac{d\psi}{dx} \Big|_{\varepsilon} - \frac{d\psi}{dx} \Big|_{-\varepsilon} \right) \quad (18)$$

Applying the boundary conditions, where $\psi(-\varepsilon) = \psi(\varepsilon)$ and $\frac{d\psi}{dx}(-\varepsilon) = \frac{d\psi}{dx}(\varepsilon)$ for a symmetric potential, we can simplify the integrals. The integral of the wavefunction over the range $[-\varepsilon, \varepsilon]$ approaches $2\varepsilon\psi(0)$ as ε tends to zero. Therefore, we have:

$$-\frac{\hbar^2}{m} \frac{d\psi}{dx}(0) + g\psi(0) = 2\varepsilon E\psi(0) \quad (19)$$

Taking the limit as $\varepsilon \rightarrow 0$, we obtain the following equation known

$$\text{as } t \rightarrow -\frac{\hbar^2}{m} \frac{d\psi}{dx}(0) + g\psi(0) = 0 \quad (20)$$

This boundary condition plays a crucial role in determining the behaviour of the wavefunction at $x = 0$ in the presence of a delta function potential.

Scattering in two and three-dimensions

To solve a two-dimensional Helmholtz equation in polar coordinates, we start with the general form of the Helmholtz equation in Cartesian coordinates:

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V(x, y) \right) \psi(x, y) = E\psi(x, y) \quad (21)$$

where ∇^2 is the Laplacian operator in two dimensions in polar form given by

$$\nabla^2 = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} \quad (22)$$

where r is the radial distance and θ is the azimuthal angle.

Now, let's express the wavefunction $\psi(x, y)$ in terms of polar coordinates r and θ :

$$\psi(x, y) = R(r)\Theta(\theta) \quad (23)$$

Substituting this into the Helmholtz equation, we get:

$$\left(-\frac{\hbar^2}{2m} \left(\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} \right) + V(r, \theta) \right) R(r)\Theta(\theta) = ER(r)\Theta(\theta) \quad (24)$$

Dividing both sides by $R(r)\Theta(\theta)$, we can separate the equation into two parts, one depending only on r and the other depending only on θ :

$$-\frac{\hbar^2}{2m} \left(\frac{1}{R(r)} \frac{1}{r} \frac{d}{dr} \left(r \frac{dR}{dr} \right) + \frac{1}{\Theta(\theta)} \frac{1}{r^2} \frac{d^2\Theta}{d\theta^2} \right) + V(r, \theta) = E$$

Both r and θ sides must be equal to a constant, which we'll denote as k^2 :

$$\frac{1}{R(r)} \frac{1}{r} \frac{d}{dr} \left(r \frac{dR}{dr} \right) + \frac{1}{\Theta(\theta)} \frac{1}{r^2} \frac{d^2\Theta}{d\theta^2} + \frac{2m}{\hbar^2} (V(r, \theta) - E) = -k^2$$

We can solve these equations separately to find the radial and angular parts of the wavefunction, $R(r)$ and $\Theta(\theta)$, respectively. The overall solution for the wavefunction in polar coordinates is then given by the product of these solutions:

$$\psi(r, \theta) = R(r)\Theta(\theta).$$

Conclusion

In conclusion, this article has delved into the intricate realm of quantum scattering theory within the framework of quantum mechanics. Through a comprehensive review of the fundamental principles and mathematical formalism involved, we have explored how particles interact with potential energy fields, leading to phenomena such as scattering and tunneling.

By considering various scattering scenarios, including one-dimensional delta function potentials, two-dimensional Helmholtz equations in polar coordinates, Scattering from a central potential, and 2D and 3D scattering, we have gained insights into the probabilistic nature of particle interactions and the wave-particle duality inherent in quantum systems.

This article underscores the importance of quantum scattering theory as a cornerstone of quantum mechanics. By continuing to explore and refine our understanding of quantum scattering phenomena, we can unlock new frontiers in technology and deepen our comprehension of the fundamental laws governing the universe.

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