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The Green function approach to scattering amplitude

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Abstract. Scattering is discussed in classical mechanics, quantum mechanics, and quantum field theory, which shows it is an important part of physics subject. From the Rutherford scattering in classical mechanics to the simple case of a potential barrier impeding the propagating wave in quantum mechanics, scattering problems seem trivial initially but get much more complicated with the study. The scattering theory developed along with the improvement and discovery in physics, and it brings lots of benefits and techniques for researchers from different science fields. To understand the scattering, finding the scattering is a good way to build up the connection between the fundamental theory and intuitive understanding. Specifically, the author wants to emphasize the scattering amplitude in the passage, which repeals the fundamental things of scattering, and the article would include some discussion of the properties of the Green function, which is a powerful mathematical tool for physicists. The author tries to show the scattering amplitude's beauty through the discussion. Then, link them with the quantum field theory of scattering.

Keywords: Green function, scattering, scattering amplitude, partial wave.

1. Introduction

The scattering is mentioned hundreds of times in the textbook, and all the classical mechanics, quantum mechanics, and quantum field theory talk about it. The interaction between the potential and the incident propagating radiations like particles and electron magnetic waves. The trajectory of scattered radiation would change from the original one. From the classical experiment by E. Rutherford, the differential cross-section is involved [1]. Scattering has wide applications related to people's daily life. For example, the CV Raman's study on Raman spectroscopy [2]. It allows people to study molecules' vibrational and rotational modes and is widely applied in chemistry to identify and analyze chemical substances. J.J. Thomason discovered the nucleus by scattering [3]. Bragg's law, found by Lawrence Bragg and Henry William Bragg based on Laue condition, opens the door for analyzing the crystal structures for Crystallography using X-ray diffraction [4]. Scattering plays a critical role in modern science development, and it provides various methods for different subjects like physics, chemistry, astronomy, biology, engineering, etc.

To understand the scattering, the cross-section reflected by $d\sigma$ doing integral with solid angle $d\Omega$, and $d\sigma$ is the number of particles scattered into $d\Omega$ per unit time divided by the flux of incident particles (number of particles per area per time). Then, there is the relation between differential cross section and scattering amplitude: the differential cross section $d\sigma$ per solid angle $d\Omega$ is the scattering probability, which is the modulo square of the scattering amplitude people are interested in. After receiving the scattering amplitude, people can do many meaningful things with it. Ghosh S and Chandra V calculate the vacuum cross-section of a propagator [5]. Z Haba studies wave propagation in inhomogeneous medium [6].

During this paper, the author would first find the meaning and definition of the scattering amplitude. Then, two methods, partial wave analysis, and Green's function, are discussed to find the representations of scattering amplitude. Next, by discussing the scattering amplitude, the author finally finds the Green function he used and tries to show how it relates to the quantum field theory. To be more specific, the whole derivation of scattering amplitude would be based on the elastic scattering (the magnitude of momentum is invariant).

2. Calculation of scattering amplitude

For the scattering, first focus on the simple case, the central hard-sphere potential ideally. This means the incident wave acts like a plane wave or say particle if it is very far away from the potential. Then, people can represent the incident wave as $\psi_{in}(r) = e^{ikz}$ if people define the plane propagating in z-direction. Also, for the scattering, the scattered wave could go in an arbitrary direction, so the wave would go like a spherical wave. $\psi_{sc}(r) = e^{ikr}$, but the format needs to use the $\frac{e^{ikr}}{r}$, to represent the density of the probability of transmitting spherically. Also, needs to multiply with a factor $f(\theta, \varphi)$in front of it, which means the measuring angle of scattering wave with a solid angle. Thus, the total wave function would look like

$$\psi(r) = \psi_{in}(r)+\psi_{sc}(r) = e^{ikz} + f(\theta,\varphi)\frac{e^{ikr}}{r} = e^{ikz} + f(\theta)\frac{e^{ikr}}{r} \quad (1)$$

Here, the factor f is called scattered amplitude. There are two ways to access the scattering amplitude, and this paper will discuss them separately in detail.

2.1. *Partial wave analysis method*

The wave function can be separated by variables and written as $\psi(r) = R(r)Y_l^0(\theta)$ due to the spherical symmetry. In the general case, $\psi(r) = R(r)Y_l^m(\theta,\phi)$. The general spherical harmonic term has the representation of $Y_l^m(\theta,\phi) = (-1)^m\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}P_l^m(cos\theta)e^{im\phi}$, associated Legendre part is $P_l^m(cos\theta) = (-1)^m(1-cos\theta^2)^{\frac{m}{2}}\left(\frac{d}{dcos\theta}\right)^m P_l(cos\theta)$, and Legendre polynomial would be $P_l(cos\theta) = \frac{1}{2^l l!}\left(\frac{d}{dcos\theta}\right)^l[(cos\theta)^2-1]$. Noticed that, for the spherical case, the $m = 0$ is independent from ϕ, so the $Y_l^m(\theta,\phi) = Y_l^0(\theta) = \sqrt{\frac{2l+1}{4\pi}}P_l^0(cos\theta)$ and P_l^0 is just P_l. Now, move the attention to the radial function. Choose some u(r) that $rR(r) = u(r)$, and people can write down the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu \quad (2)$$

For the incident part, considered the r is very large so that no potential acts on plane wave which behaves like a free particle with energy $\frac{\hbar^2k^2}{2m}$. Now

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = -\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + 0u = Eu = \frac{\hbar^2k^2}{2m}u. \quad (3)$$

Canceled the $\frac{\hbar^2}{2m}$ term to get $\frac{d^2u}{dr^2} = -k^2u$, and people have an exact solution of $u(r) = Ae^{ikr} + Be^{-ikr}$. The B is zero if it is able to define the k is the propagating direction of incident wave alone z axis, $u(r) = Ae^{ikr}$. If the distance r is not so far from potential (V(r) is still about 0), the Schrödinger equation would take consideration of r term. Namely,

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$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2}+\left[V(r)+\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u=-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2}+\left[\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u=\frac{\hbar^2k^2}{2m}u \tag{4}$$

and

$$-\frac{d^2u}{dr^2}+\left[\frac{l(l+1)}{r^2}\right]u=k^2u. \tag{5}$$

Let $\rho = kr$, the above equation would have $-\frac{d^2u}{d\rho^2}+\left[\frac{l(l+1)}{\rho^2}\right]u=u$. For the upper type of equation, the solution would be $u(\rho)=A\rho j_l(\rho)+B\rho n_l(\rho)$, where n_l (spherical Neumann) and j_l (spherical Bessel). Putting it back to r, it is found that $u(r)=Arj_l(kr)+Brn_l(kr)$. Taking the limit for r approaching to zero, it is found that j_l is nonsingular but n_l is singular, so one can just discard the Neumann part since it doesn't have physical meaning [7]. Then, for r approaching infinity, $j_l(kr)\approx \frac{1}{kr}sin\left(kr-\frac{l\pi}{2}\right)$. For the incident wave,

$$e^{ikz}=e^{ikr\cos\theta}=\sum_{l=0}^{\infty}(2l+1)i^l P_l^0 j_l=\sum_{l=0}^{\infty}\sqrt{4\pi(2l+1)}i^l j_l(kr)\,Y_l^0(\theta) \tag{6}$$

Therefore, for far away incident wave, one has

$$\psi_{in}(r)=e^{ikz}=\sum_{l=0}^{\infty}\sqrt{4\pi(2l+1)}i^l\,Y_l^0(\theta)\frac{1}{2ik}\left[\frac{e^{i\left(kr-\frac{l\pi}{2}\right)}}{r}-\frac{e^{-i\left(kr-\frac{l\pi}{2}\right)}}{r}\right]. \tag{7}$$

Conventionally, one calls $+k$ outgoing and $-k$ incoming. Next, remember the scattering in the 1D case, the wave function has incident wave and reflect back due to a step potential barrier. $\psi(r)=A(e^{ikz}-e^{-ikz})$ for V(z)=0, and $\psi(r)=A(e^{ikz}-e^{i(2\delta-kz)})$ for potential is not equal to zero. The δ is the phase shift. Then, rewrite the scattering process with the phase shift delta. Since the probability density must be identical, then

$$\psi(r)=\frac{1}{k}\sum_{l=0}^{\infty}\sqrt{4\pi(2l+1)}i^l\,Y_l^0(\theta)\frac{1}{2i}\left[\frac{e^{i\left(kr-\frac{l\pi}{2}+\delta\right)}}{r}-\frac{e^{-i\left(kr-\frac{l\pi}{2}\right)}}{r}\right] \tag{8}$$

and

$$\psi(r)=e^{ikz}+f(\theta)\frac{e^{ikr}}{r}=\sum_{l=0}^{\infty}\sqrt{4\pi(2l+1)}i^l\,Y_l^0(\theta)\frac{1}{2ik}\left[\frac{e^{i\left(kr-\frac{l\pi}{2}\right)}}{r}-\frac{e^{-i\left(kr-\frac{l\pi}{2}\right)}}{r}\right]+f(\theta)\frac{e^{ikr}}{r}. \tag{9}$$

After canceling the same incoming part, the author has the outgoing part equation of $\psi_{sc}(r)=\frac{1}{k}\sum_{l=0}^{\infty}\sqrt{4\pi(2l+1)}i^l\,Y_l^0(\theta)\frac{1}{2i}(e^{2i\delta}-1)\frac{e^{i\left(kr-\frac{l\pi}{2}\right)}}{r}=f(\theta)\frac{e^{ikr}}{r}$. Finally, the scattering amplitude can be written as $f(\theta)=\frac{1}{k}\sum_{l=0}^{\infty}\sqrt{4\pi(2l+1)}i^l\,Y_l^0(\theta)e^{i\delta}sin\,(\delta)$. Also, noticed that the scattering amplitude is the summation of individual scattering amplitudes $f(\theta)=\sum_l f_l(\theta)$ for $f_l(\theta)$ with $\sqrt{4\pi(2l+1)}i^l j_l(kr)Y_l^0(\theta)$.

2.2. Born approximation method

The other method to access the scattering amplitude would be the Born approximation. Go back to the time independent Schrödinger equation $-\frac{\hbar^2}{2m}\nabla^2\psi(r)+V(r)\psi(r)=E\psi(r)$. For free particle, $\frac{\hbar^2k^2}{2m}=E$, rewrite $(\nabla^2+k^2)\psi(r)=\frac{2m}{\hbar^2}V(r)\psi(r)\equiv Q$. Now, the time independent Schrödinger equation becomes a linear operator acting with wave function and gets some source function about the potential. The format of the equation is a type of inhomogeneous Helmholtz equation, which can be solved by introducing the Green function. The Green function has the properties $LG=\delta$, for L as a linear operator and right-hand side is the delta function. $L\varphi=Q$, the φ can be written as $\psi\delta=GQ$, or in integral format $\psi(\vec{r})=$

$\frac{2m}{\hbar^2}\int V(\overrightarrow{r_0})G(\vec{r}-\overrightarrow{r_0})d^3r_0$, also use the properties of $L\psi_0 = 0$ won't affect the final result after applying the operator is

$$(\nabla^2+k^2)\psi(r) = (\nabla^2+k^2)\psi_0(r) + \frac{2m}{\hbar^2}\int V(\overrightarrow{r_0})\left[(\nabla^2+k^2)G(\vec{r}-\overrightarrow{r_0})\right]d^3r_0\,\psi(\overrightarrow{r_0}), \tag{10}$$

which can be simplified as

$$(\nabla^2+k^2)\psi(r) = \frac{2m}{\hbar^2}\int V(\overrightarrow{r_0})\delta(r-r_0)d^3r_0\psi(\overrightarrow{r_0}) = \frac{2m}{\hbar^2}V(r)\psi(r) = Q. \tag{11}$$

Therefore, for upper free particle plane wave behavior problems can lead to the $\psi_0(r) = e^{ikr}$ since $e^{ikz} + f(\theta)\frac{e^{ikr}}{r}$. Obviously, $(\nabla^2+k^2)e^{ikz} = 0$, and it is safe to let ψ_0 as an incident wave. Next, consider the delta function doing Fourier transform $\delta(\vec{r}-\overrightarrow{r_0}) = \frac{1}{(2\pi)^3}\int d^3q e^{i[\vec{q}\cdot(\vec{r}-\overrightarrow{r_0})]}$, and $G(\vec{r}-\overrightarrow{r_0}) = \int d^3q e^{i[\vec{q}\cdot(\vec{r}-\overrightarrow{r_0})]}\,\widetilde{G(\vec{q})}$ for transform Green from position space to momentum space. Put those two into the LG and delta $(-q^2+k^2)\,\widetilde{G}(\vec{q}) = \frac{1}{(2\pi)^3}$. Thus, the Green function can be represented by a transformed one,

$$G(\vec{r}-\overrightarrow{r_0}) = G(\vec{R}) = -\frac{1}{(2\pi)^3}\int d^3q e^{i[\vec{q}\cdot\vec{R}]}\frac{1}{q^2-k^2} = -\frac{1}{(2\pi)^2 iR}\int_{-\infty}^{\infty}\frac{e^{iqR}}{q^2-k^2}dq \tag{12}$$

The $q = +k$ and $q = -k$ would be considered as two critical points for the Green function [8,9]. Using the residue theorem to calculate the contour integral to get

$$G(\vec{R}) = -\frac{1}{4\pi^2 iR}\int_{-\infty}^{\infty}\frac{e^{iqR}}{q^2-k^2}dq = -\frac{e^{ikR}}{4\pi R} \tag{13}$$

which can be written as $G(\vec{r}-\overrightarrow{r_0}) = -\frac{e^{ik|\vec{r}-\overrightarrow{r_0}|}}{4\pi|\vec{r}-\overrightarrow{r_0}|}$ [8].

This exponential term has the same appearance as the outgoing wave, call it $G^+(\vec{r}-\overrightarrow{r_0}) = -\frac{e^{ik|\vec{r}-\overrightarrow{r_0}|}}{4\pi|\vec{r}-\overrightarrow{r_0}|}$. it is reasonable to call it an outgoing solution if author lets G=g(r)/r(means r is not zero) and apply the same operator $\frac{d^2g}{dr^r} + k^2 = 0$ (delta is zero), which has been shown before for this ordinary differential equation. In addition, the $G(r) = A\frac{e^{ikr}}{r} - B\frac{e^{-ikr}}{r}$, so $G^+ \propto \frac{e^{ikr}}{r}$ as the outgoing solution [8, 9]. The last step is put it back to wave equation (far from potential $e^{ikz} + f(\theta)\frac{e^{ikr}}{r}$),

$$\psi(\vec{r}) = e^{i\overrightarrow{k_{in}}\cdot\vec{r}} - \frac{m}{2\pi\hbar^2}\int V(\overrightarrow{r_0})\frac{e^{ik_{in}|\vec{r}-\overrightarrow{r_0}|}}{|\vec{r}-\overrightarrow{r_0}|}d^3r_0\psi(\overrightarrow{r_0}). \tag{14}$$

Then, the first order born approximation can be considered as the original function with r and to substitute r0 with another same format wave function $\psi(\vec{r}) = e^{i\overrightarrow{k_{in}}\cdot\vec{r}} - \frac{m}{2\pi\hbar^2}\int V(\overrightarrow{r_0})\frac{e^{ik_{in}|\vec{r}-\overrightarrow{r_0}|}}{|\vec{r}-\overrightarrow{r_0}|}d^3r_0\, e^{i\overrightarrow{k_{in}}\cdot\overrightarrow{r_0}} - \left[-\frac{m}{2\pi\hbar^2}\int V(\overrightarrow{r_0})\frac{e^{ik|\vec{r}-\overrightarrow{r_0}|}}{|\vec{r}-\overrightarrow{r_0}|}d^3r_0\frac{m}{2\pi\hbar^2}\right]\int V(\overrightarrow{r_{00}})\frac{e^{ik_{in}|\overrightarrow{r_0}-\overrightarrow{r_{00}}|}}{|\overrightarrow{r_0}-\overrightarrow{r_{00}}|}d^3r_{00}\psi(\overrightarrow{r_{00}})$. Thus, let $U(r) = \frac{2m}{\hbar^2}V(r)$, the pattern is clear right now,

$$\psi(\vec{r}) = e^{i\overrightarrow{k_{in}}\cdot\vec{r}} + \int GUe^{i\overrightarrow{k_{in}}\cdot\vec{r}} + \int GU\int GUe^{i\overrightarrow{k_{in}}\cdot\overrightarrow{r_0}} + \int GU\int GU\int GUe^{i\overrightarrow{k_{in}}\cdot\overrightarrow{r_{00}}} + \cdots \tag{15}$$

It is possible to find more and more precise solution if having higher order of approximation. Back to first order approximation with large r, $|\vec{r}-\overrightarrow{r_0}|^2 = (\vec{r}^2 - 2\vec{r}\cdot\overrightarrow{r_0} + \overrightarrow{r_0}^2)^{1/2} \approx r^2(1 - 2\frac{\vec{r}\cdot\overrightarrow{r_0}}{r^2})$, and $|\vec{r}-\overrightarrow{r_0}| \approx r - \hat{r}\cdot\overrightarrow{r_0}$. Thus, $e^{ik|\vec{r}-\overrightarrow{r_0}|} \approx e^{ikr}e^{-i\vec{k}\cdot\overrightarrow{r_0}}$, and $\frac{e^{ik|\vec{r}-\overrightarrow{r_0}|}}{|\vec{r}-\overrightarrow{r_0}|} \approx \frac{e^{ikr}}{r}e^{-i\vec{k}\cdot\overrightarrow{r_0}}$. Now the incident wave can be chosen as ψ_0,

$$\psi(\vec{r}) \cong e^{ikz} - \frac{m}{2\pi\hbar^2}\left[\int e^{-i\overrightarrow{k_{sc}}\cdot\overrightarrow{r_0}}\, V(\overrightarrow{r_0})\psi(\overrightarrow{r_0})d^3r_0\right]\frac{e^{ikr}}{r} \qquad (16)$$

For $\psi(\overrightarrow{r_0})$, the $\psi(\overrightarrow{r_0}) = e^{i\vec{k}\cdot\overrightarrow{r_0}} + \text{perturbation term}$, by approximate tiny perturbation and very small change from propagating direction z. Therefore, $e^{ikz} \approx e^{i\overrightarrow{k_{in}}\cdot\overrightarrow{r_0}}$ and

$$\psi(\vec{r}) \cong e^{ikz} - \frac{m}{2\pi\hbar^2}\left[\int e^{-i\overrightarrow{k_{sc}}\cdot\overrightarrow{r_0}}\, V(\overrightarrow{r_0})e^{i\overrightarrow{k_{in}}\cdot\overrightarrow{r_0}}d^3r_0\right]\frac{e^{ikr}}{r} = e^{ikz} + f(\theta,\varphi)\frac{e^{ikr}}{r} \qquad (17)$$

Here, $f_{Born}(\theta,\varphi) \approx -\frac{m}{2\pi\hbar^2}\left[\int e^{i\vec{G}\cdot\overrightarrow{r_0}}\, V(\overrightarrow{r_0})d^3r_0\right]$.

3. Application of scattering amplitude

The Scattering amplitude mainly can help people find the cross section. The Optical Theorem can be derived from f, and receive $\sigma = \frac{4\pi}{k}\mathrm{Im}[f(0)]$.

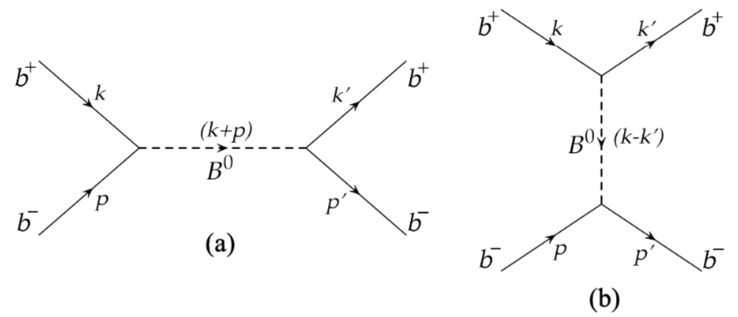

Figure 1. Illustration of scatter process. (a) as s channel and (b) as t channel [5].

The vacuum cross section under a $b^+(k) + b^-(p) \to b^+(k') + b^-(p')$ scattering can be calculated [5]. The particle B_0, b^+, b^- are created (annihilated) by real (complex) scalar field $\Phi, \phi, \phi^\dagger$ with $\mathcal{L}_{interaction} = g\Phi\phi\phi^\dagger$, invariant amplitudes get from Feynman rules for s and t channels (see Figure 1 for illustration) are $\mathcal{M}_s = g^2\left[\frac{1}{s-M^2+i\epsilon}\right]$ and $\mathcal{M}_t = g^2[\frac{1}{t-M^2+i\epsilon}]$, and the Mandelstam variable s, t, u are defined as $s = (k+p)^2 = (k'+p')^2$ $t = (k-k')^2 = (p-p')^2$ $u = (k-p')^2 = (p-k')^2$ [5]. During the interaction, M is the mass of unstable particles, and as B_0 for this case. The total cross section is $\sigma(s) = \frac{1}{16\pi\lambda(s,m^2,m^2)}\int_{-\frac{\lambda(s,m^2,m^2)}{s}}^{0} dt|\mathcal{M}_s + \mathcal{M}_t|^2$. The total cross-section is easily received by applying

$$\sigma \equiv \frac{1}{4E_AE_B|v|}\int\frac{|\mathcal{M}|^2}{(4\pi)^2}\delta^4(p_A + p_B - p'_A - p'_B)\frac{d^3p'_A}{E'_A}\frac{d^3p'_B}{E'_B} = \frac{1}{4|p|W}\frac{1}{(4\pi)^2}\frac{|p|}{W}\int|\mathcal{M}|^2 d\Omega. \qquad (18)$$

Next, the author accesses the same thing by using optical theorem under zero external magnetic field and get the final result by adding a magnetic field (weak and strong) to solve scattering cross section numerically. The green function is a powerful tool that is called a propagator in quantum field theory. Ignore relativity, and it has the format of $G(x,t;x',t') = \frac{1}{i\hbar}\Theta(t-t')K(x,t;x',t')$, the upper derivation is $G(x,t;x',t') = K(x,t;x',t') = K(x;x')$ since time-independent potential. The relativistic case would be $G(x,y) = \frac{1}{(2\pi)^4}\int d^4p\frac{e^{-ip(x-y)}}{p^2-m^2\mp i\epsilon}$. Also, in the expression $G(\vec{R}) = -\frac{1}{(2\pi)^3}\int d^3q e^{i[\vec{q}\cdot\vec{R}]}\frac{1}{q^2-k^2}$, there should be a $i\epsilon$ term to do Cauchy integral, and this format of G satisfy the Feynman propagator (not in the same side of real axis). For non-relativistic cases, people can calculate the Feynman propagator in momentum space by Schwinger's method [10]. Haba et al. use the Green function to discuss wave propagation in an inhomogeneous medium [6]. For the case, $(B\,\partial_0{}^2 + \partial_j A\,\partial_j)G = \delta$, can finally yield the

$$G\left(x_0, x; x_0', x'\right) = \int d\omega \int d\tau\, E\left[\exp\left(-\omega^2 \int_0^\tau B\left(q_s(x)\right) ds\right)\right] \exp\left(i\omega\left(x_0 - x_0'\right)\right) \delta\left(q_\tau(x) - x'\right). \quad (19)$$

The spatial singularity and the decrease at infinity of the potential can be determined from Eq. (19).

4. Conclusion

In conclusion, scattering amplitude plays a crucial role in people's understanding of how particles interact and exchange energy, and the concepts are essential in a wide range of scientific disciplines: nuclear physics, particle physics, and material science. Scattering amplitude serves as a mathematical representation of the probability of particles scattering at different angles or momenta during a collision, which provides a way to describe the interaction involving the exchange of virtual particles. The amplitude can be calculated using various techniques, such as the Partial wave analysis, the Born approximation, or more advanced methods. These calculations develop valuable insights into the underlying forces governing the interaction, uncovering the fundamental laws of physics. In this paper, the author finishes the mathematical derivation of scattering amplitude. From the discussion, both the scattering amplitude and the green function method show the importance and power of solving the scattering problem. Then, the brief discussion of the application connects those scattering amplitude and green functions to quantum field theory, which can be much more helpful in solving practical problems. Both two methods used above are approximate scattering amplitude, and they still need to be done with it more precisely. People usually only did the first order of them since the second order would become highly complicated mathematically. In summary, these methods enable scientists to uncover the mysteries of particle physics and contribute to human's knowledge.

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