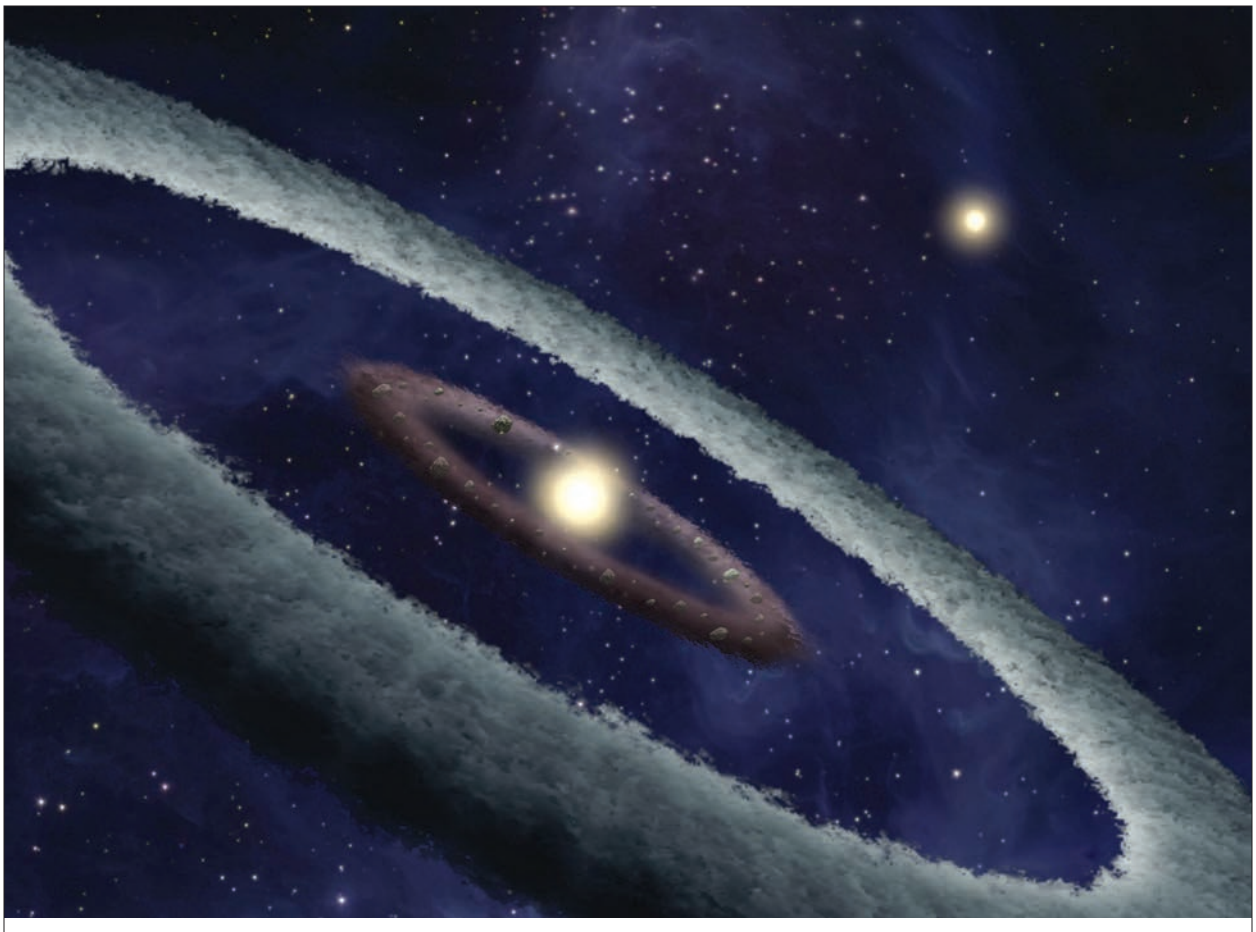

Research Journal of Physics

ISSN 1819-3463

Academic Journals Inc.

www.academicjournals.com

Research Journal of Physics 4 (2): 74-81, 2010
ISSN 1819-3463 / DOI: 10.3923/rjp.2007.19.26

Rigorous Solution of Quantum Scattering Theory*

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Abstract: In this study, the equation needed for the formal treatment of the scattering problems in the light of the Dyson's equation, which is a reduced form of the more complex Lippmann-Schwinger equation written in terms of the total Green function has been developed. This was achieved by the combination of the boundary conditions and scattering potentials and the combination of non-overlapping scattering potentials within the context of the scattering theory to obtain the transition matrix, which is the most important parameter in scattering problems due to its direct relation with the scattering cross section.

Key words: Scattering theory, lippmann-schwinger equation, T-matrix, cross section, scattering amplitude, Dyson's equation

INTRODUCTION

Quantum scattering has been an important subject of study since the early days of quantum mechanics. It plays a vital role in broadening our perception of the forces and interactions of particles in microscopic world and provides us with a convenient framework for the solution of variety of problems. Though, we have a sound understanding and instinct for simple scattering problems, such as single channel scattering, we cannot precisely say the same for more general scattering problems. There have been many attempts to generalize scattering theory to deal with more complicated cases. However, the literature in this field, though vast, is highly implicit and not constructive (Omnes, 1994; Adam, 1998; Yoav *et al*., 1998).

In its phenomenological form, scattering can best be appreciated if we look at it as a transition process from an initial unperturbed state to perturbed state due to small interaction (Eugen, 2003).

In this study, the Lippmann-Schwinger equation will be introduced which will be recast in the more formal form of the Dyson's equation suitable for proper treatment of any scattering process with the Green function as a key parameter in solving the Schrödinger equation ideal for scattering theory.

THEORETICAL FRAMEWORK

Basic Formulation

Quantum mechanically, the collision of two (spinless) particles in the centre-of-mass coordinate system can be recast into problem of a particle of mass μ (where μ is the reduced mass) in a fixed potential V (r). The Hamiltonian describing this relative motion (in a field of single scatterer) is:

$$H = H_0 + V(r) \quad (1)$$

where, H_0 is the unperturbed Hamiltonian $= \frac{\hbar^2 K^2}{2\mu}$ and V (r) = interaction potential between the two particles ($r = r_1 - r_2$) (Leonard, 1955; Umahi and Ekuma, 2007).

Originally Published in Research Journal of Physics, 2007

The wave function for the scattered particle with energy E>0 can be obtained by solving the steady state Schrödinger equation:

$$(\nabla^2 + K^2)\ \Psi\ (k, r) = U\ (r)\ \Psi\ (k, r) \tag{2}$$

where, $U(r) = \frac{2\mu}{\hbar^2} V(r)$; $K^2 = \frac{2\mu E}{\hbar^2}$, K is the wave vector with direction parallel to the incident wave (Umahi and Ekuma, 2007; Davydov, 1965). Assuming a potential of shorter range than the Coulomb potential, then V (r) → 0 faster than 1/r as r → ∞; then a special solution of (2) has the asymptotic form:

$$\phi(r)_{r\to\infty} \to N\left[\exp ik.r + f_k(\theta,\varphi)\frac{\exp ik.r}{r}\right] \tag{3}$$

where, the first term is the incident wave vector and the second term, the outgoing spherical wave vector (Hong-Jun, 1999). Let us adopt a perturbation approach of the form:

$$\Psi\ (k, r) = \exp ik.r + \upsilon\ (r) \tag{4}$$

where, υ (r), the scattered wave is the small perturbation term. Using (4) in (2), we have that

$$(\nabla^2 + K^2)\ \upsilon\ (r) = U\ (r)\ \exp ik.r + U\ (r)\ \upsilon\ (r) \tag{5}$$

A consequence of the assumed smallness of υ (r) as compared to exp ik.r suggests that the second term on the right hand side of (5) will evidently be small enough to be neglected. Hence, we solve the inhomogeneous equation

$$(\nabla^2 + K^2)\ \upsilon\ (r) = U\ (r)\ \exp ik.r \tag{6}$$

where the right hand side is known precisely. A sufficient criterion for the validity of our solution is that:

$$|\upsilon(r)| \ll |e^{ik.r}| = 1;\quad \forall r \tag{7}$$

Hence, we write down the solution of (6) by the Green function method as:

$$\psi(k,r) = \phi(k,r) + \int G_o(k,r,r')U(r')\psi(k,r')dr' \tag{8}$$

where, G_o (k, r, r') is the free Green function satisfying the conditions:

$$(\nabla^2 + K^2)\ \phi\ (k, r) = 0 \tag{9a}$$

$$(\nabla^2 + K^2)\ G_o\ (k, r, r') = \delta\ (r - r') \tag{9b}$$

Choice of Green Function

The Green function plays a vital role in trying to solve (9b), since the inhomogeneous equation is an influence function of infinite space (Fayyazuddin and Riazuddin, 1990; Ni ad Chew, 2002).

Hence, we expand the delta function as:

$$\delta(r-r') = \left(\frac{1}{2\pi}\right)^3 \int \exp\{iK.(r-r')\}\,dK' \tag{10}$$

But the Fourier expansion for G_o (k, r, r') is

$$G_o(k,r,r') = \left(\frac{1}{2\pi}\right)^3 \int g_o(k',r')\exp iK.(r-r')\,dK' \tag{11}$$

where $g_o(k',r') = \frac{\exp(-ik'.r')}{k^2-k'^2}$. Hence, we obtain

$$G_o(k,r,r') = \left(\frac{1}{2\pi}\right)^3 \int \frac{\exp\left[ik'(r-r')\right]}{k^2-k'^2}dK' \tag{12}$$

PROTOTYPE SCATTERING PROCESS

A simple scattering process which forms the basis of more complex processes of Hamiltonian H has the solution of its equation of motion (in interaction picture) in terms of the eigenstates of H_o given by:

$$|\psi(t)\rangle = \sum_{k,s} |k\rangle\langle k|\tilde{T}(t,t_O)|s\rangle\langle s||\psi(t_o)\rangle \tag{13}$$

But basically, in scattering problems, the transition amplitude is the sought parameter of interest with equation of motion:

$$\langle k|\tilde{T}(t,t_o)|s\rangle = \delta_{ks} - \frac{i}{\hbar}\sum_n \langle k|V|n\rangle \int_0^t e^{i\omega_{kn}t'}\langle n|\tilde{T}(t',t_o)|s\rangle dt' \tag{14}$$

From (12), assuming an initial state $|\Psi(t_o)\rangle$ to represent a freely moving wave packet towards the interaction region, we can assume the transition matrix element $\langle k|\tilde{T}(t,t_o)|s\rangle$ between incident state, s at $t \to -\infty$ and a scattered state, k at $\to +\infty$ with recourse to the first order perturbation:

$$\langle k|\tilde{T}(t,t_o)|s\rangle = \delta_{ks} - \frac{i}{\hbar}\langle k|V|s\rangle \int_{t_o}^t e^{i\omega_{ks}t'}dt' \tag{15}$$

to obtain the transition matrix as:

$$\langle k|\tilde{T}(t,t_o)|s\rangle = \delta_{ks} - \frac{i}{\hbar}T_{ks}\int_{t_o}^t e^{i\omega_{ks}t'+\zeta t'}dt' \tag{16}$$

provided $|t| \ll (1/\zeta)$, where $1/\zeta$ measures approximately the time interval of an impact between the wave packet and the scatterer, T_{ks} is the transition matrix element. Assuming (14) is the solution of (12), then, if the solution exists, integrating (14) (as $\zeta \to 0$; $t_o \to -\infty$: $e^{\zeta t_o} = 0$) gives:

$$\langle k|\tilde{T}(t,-\infty)|s\rangle = \delta_{ks} + \frac{T_{ks} e^{i\omega_{ks}t+\alpha t}}{\hbar(-\omega_{ks}+i\zeta)} \tag{17}$$

However, as $t \to +\infty$ and $\zeta \to 0$, provided that $|t| \ll (1/\zeta)$, we establish that the S-matrix and the transition matrix is related by:

$$S_{ks} = \langle k|\tilde{T}(+\infty,-\infty)|s\rangle = \delta_{ks} - 2\pi i\delta(E_k - E_s)T_{ks} \tag{18}$$

Using (17) in (14), we obtain (provided that $|t| \ll (1/\zeta)$ at $\zeta\, t = 0$) that

$$T_{ks} = \langle k|V|s\rangle + \frac{1}{\hbar}\sum_n \frac{\langle k|V|n\rangle T_{ns}}{-\omega_{ns}+i\zeta} \tag{19}$$

Equation (19) is valid only if the stationary state has a quasi-continuum energy states of very close value, close enough to the energy of the initial state E_s. This is however not a problem as such cases are predominant in scattering processes where $E_s \approx E_k$. Putting (19) in the needed frame for the discussion of formal scattering theory, we define in Hilbert space set of vectors $\psi_s^{(+)}$ by the homogeneous equation:

$$T_{ks} = \sum_j (\psi_k, V\psi_j)\left(\psi_j, \psi_s^{(+)}\right) = \left(\psi_k, V\psi_s^{(+)}\right) \tag{20}$$

Using (20) in (19), we obtain

$$\begin{aligned}\psi_s^{(+)} &= \psi_s + \sum_n \psi_n \frac{\left(\psi_n, V\psi_s^{(+)}\right)}{E_s - E_n + i\hbar\zeta} \\ &= \psi_n + \sum_n \frac{1}{E_s - H_0 + i\hbar\zeta}\psi_n\left[\left(\psi_n, V\psi_s^{(+)}\right)\right]\end{aligned} \tag{21}$$

Equation 21 is known as the Lippmann-Schwinger equation with operator form:

$$\psi_s^{(+)}(E_s) = \psi_s + G^{(+)}(E_s)V\psi_s \tag{22}$$

A vital point to note in handling (21) is in the limit $\zeta \to 0$, it is clearly noted that an inhomogeneous equation:

$$(E_s - H_o)\psi_s^{(+)} = V(r)\psi_s^{(+)} \tag{23a}$$

is established depicting that $\psi_s^{(+)}$ is an eigenspace of $H = H_o + V$ with corresponding eigenvalue, E_s which is also the eigenvalue of H_o (Fayyazuddin and Riazuddin, 1990; Omnes, 1994). Hence, rewrite in its formal form taking cognizance of H as:

$$\left(E_s - H_o - V(r)\right)\psi_s^{(+)} = \delta(r - r') \tag{23b}$$

RIGOROUS T-MATRIX ELEMENT

Taking into account the correct boundary condition of the outgoing wave vector, the Lippmann-Schwinger (L-S) Eq. 21 can be written in terms of the free Green function as:

$$\psi_s^{(+)} = (2\pi)^{\frac{3}{2}} e^{ikr} + \int G_o^{(+)} \langle r|r'\rangle V(r')\psi_s^{(+)}(r')dr' \tag{24a}$$

with an operator form:

$$\psi_s^{(+)} = \psi_s + \frac{1}{E_s - \hat{H}_o + i\hbar\zeta} \tag{24b}$$

which is the fundamental problem we dare to solve in scattering theory as its solution is used to determine the transition matrix which is directly related to the cross section.

Since generally, the solution of the nonhomogeneous Eq. 23 has a solution of the form:

$$\psi_s^{(+)} = \psi_s + G^+(E_s)V\psi_s^{(+)} \tag{25a}$$

where $G^+(E_s)$ is the given solution of the operator equation:

$$\left(E_s - \hat{H}_o\right)G^+(E_s) = 1 - P_s \tag{25b}$$

Now, defining the total Green function $G^{(+)}\langle r|r'\rangle$, a consequence of the potential interaction as a solution of (23) with a particular operator form:

$$G^{(+)}(E_s) = \frac{1}{E_s - \hat{H}_o + i\hbar\zeta}\left(\frac{\hbar^2}{2\mu}\right) \tag{26}$$

which permits the solution of (25a) to be:

$$\psi_s^{(+)} = \int G^{(+)}\langle r|r'\rangle V(r')\psi_s(r')dr' \tag{27}$$

Hence, the difficulty in establishing the rigorous solution of the L-S equation is reduced to finding the total Green function, $G^{(+)}\langle r|r'\rangle$ of the scattering system. Rewriting (23b) and making use of the free Green function $G_o^{(+)}$, the formal solution:

$$G^{(+)}\langle r|r'\rangle = G_o^{(+)}\langle r|r'\rangle + \int G_o^{(+)}\langle r|r''\rangle V(r'')G^{(+)}\langle r''|r'\rangle dr'' \tag{28}$$

is obtained which in its present form is known as the Dyson's equation with operator form:

$$G^{(+)} = G_o^{(+)} + G_o^{(+)} V G^{(+)} \tag{29}$$

The advantage of the Dyson's equation in dealing with scattering problems over the L-S equation is its obvious independent of the initial boundary condition of the scattering process (Ni and Chen, 2002). Hence, more adequate for discussing most rigorous theoretical scattering phenomena e.g., the Levinson theorem.

Recalling (24b), we note in particular that it has a formal solution of the form:

$$\psi_s^{(+)} = \psi_s + \frac{1}{E_s - \hat{H}_0 + i\hbar\zeta} V\psi_s \tag{30}$$

a consequence of $\psi_s^{(+)}$ given in terms of the known state Ψ_s. Let the transition matrix be defined as T with matrix element:

$$T_{ks} = \left(\psi_k, V\psi_s\right) + \left(\psi_k, V\frac{1}{E_s - \hat{H}_0 + i\hbar\zeta} V\psi_s\right) \tag{31}$$

which enables the scattering cross section $|T_{ks}|^2$ in principle for any scattering process to be obtained directly from (31). But in practice, since we know nothing about the eigenvalues of H (unless in cases where it has already been specified), the effect of $\frac{1}{E_s - \hat{H}_0 + i\hbar\zeta}$ is not always known. To resolve this discrepancy, we resort to approximation method which is conveniently achieved by introducing the Green's (resolvent) operator:

$$\varsigma_o^{(+)}\left(E_s\right) = \frac{1}{E_s - H_0 + i\hbar\zeta} \tag{32a}$$

$$\varsigma^{(+)}\left(E_s\right) = \frac{1}{E_s - H + i\hbar\zeta} \tag{32b}$$

to obtain from (30) that:

$$\psi_s^{(+)} = \psi_s + \varsigma_o^{(+)}\left(E_s\right) V\psi_s \tag{33a}$$

with a formal solution:

$$\psi_s^{(+)} = \psi_s + \varsigma^{(+)}\left(E_s\right) V\psi_s \tag{33b}$$

Using the identity: 1/A-1/B = 1/B (B-A) 1/A; where $A = E_s - H + i\hbar\zeta$; $B = E_s - H_0 + i\hbar\zeta$, we obtain:

$$\varsigma^{(+)}\left(E_s\right) = G_o^{(+)}\left(E_s\right) + G_o^{(+)}\left(E_s\right) V\varsigma^{(+)}\left(E_s\right) \tag{34}$$

which is solved using perturbative expansion to obtain:

$$\varsigma^{(+)}(E_s) = G_0^{(+)}(E_s) + G_0^{(+)}(E_s)VG_0^{(+)}(E_s) + G_0^{(+)}(E_s)VG_0^{(+)}(E_s)VG_0^{(+)}(E_s) + \cdots \quad (35)$$

such that:

$$\psi_s^{(+)}(E_s) = \psi_s + G_0^{(+)}(E_s)V\psi_s + G_0^{(+)}(E_s)VG_0^{(+)}(E_s)V\psi_s + \cdots \quad (36)$$

The formal solution (30) depicts the orthogonality of the scattering states, hence, we obtain from the implicit Eq. 23b that:

$$\left(\psi_k^{(-)}, \psi_s^{(-)}\right) = \delta_{ks} \quad (37a)$$

analogous to:

$$\left(\psi_k^{(+)}, \psi_s^{(+)}\right) = \delta_{ks} \quad (37b)$$

which is valid only when the eigenvalues of H and H_o is quasi-continuous (Eugen, 2003). Consequently, due to the presence of the interaction potential V, discrete eigenvalues of bound states may be produced that has no counterpart in the solutions of (32a) in the Hamiltonian of the unperturbed spectrum H_o which are part of the spectrum of the perturbed Hamiltonian, H_o. Again, these bound states have energies lower than that in the scattering process and as such, said to be orthogonal to the scattering state, hence must be added to $\psi_s^{(+)}$ or $\psi_s^{(-)}$ to complete the set of the eigenvectors as:

$$\sum_{\xi} \left|\xi^{(+)}\right\rangle\left\langle\xi^{(+)}\right| + \sum_{B} |B\rangle\langle B| = 1 \quad (38)$$

where $|B^{(+)}\rangle$ is the bound states (Fayyazuddin and Riazuddin, 1999).

CONCLUSIONS

We have in this study presented the rigorous solution of the quantum scattering theory. It was noted that in scattering problems, the transition amplitude (and the transition matrix) are the most sought parameter in resolving scattering problems because of their direct relation with the cross section. It was established for a quasi-continuum scattering processes that the complexity of finding the solution of the Lippmann-Schwinger equation can be reduced to finding the total Green function for such process normally for convenience, recast in the more appropriate Dyson's equation that has the advantage of being independent of the initial boundary conditions of the scattering process and obtained the transition matrix as:

$$T_{ks} = \left(\psi_k, V\psi_s\right) + \left(\psi_k, V\frac{1}{E_s - \hat{H}_0 + i\hbar\zeta}V\psi_s\right)$$

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