A NUMERICAL METHOD FOR SOLVING THE LIPPMANN-SCHWINGER INTEGRAL EQUATION WITH THE RADIAL INTERACTION POTENTIALS

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Abstract

In this article, a method is presented for transforming the singular Lippmann-Schwinger integral equation to a matrix algebraic equation. This method of computing the matrix elements of the reaction and transition operators is used on the real axis and on the complex plane, respectively. By specifying the elements value of the reaction and transition matrix on the energy-shell, both phase shifts and the differential scattering amplitudes and the differential cross sections are computable.

The presented method for the Gaussian quadratures is suitably based on

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Quantum scattering finds numerous applications in modern physics and technology including laser radiation modeling in semiconductor devices [1], optical fiber fabrication processes [2], superconductivity without phonons [3] (wherein strongly correlated electron materials are tuned close to a zero-temperature magnetic instability of itinerant charge carriers) and quantum-chemical analysis of factors controlling charge transport at the molecular scale in discotic liquid crystals [4] (for example, stacks composed of triphenylene, hexaazatriphenylene, hexaazatrinaphthylene, and hexabenzocoronene molecules and derivatives thereof). Numerous analytical studies of quantum scattering have been communicated. A seminal study was presented in the post-war period by Lippmann and Schwinger [5] wherein they developed a ground-breaking formulation of quantum scattering using variational principles. This study used a time-dependent theory and a pair of variational principles to generate an approximate calculation of the unitary (collision) operator which simulates the connection between the initial and final states of the system. The results of Fermi and Breit on the scattering of slow neutrons by bound protons were also analyzed using this variational formulation. Subsequently, tremendous interest has emerged in employing the so-called Lippmann-Schwinger integral equation which has become a fundamental equation for quantum scattering theory. The significance of this equation is due to the fact that in the quantum physics of collision processes, it replaces the Schrödinger differential equation and the corresponding boundary conditions. Additionally, the vast majority of presented formulations for solving scattering problems of three or multi-particle systems tend to result from the rearrangement of the Lippmann-Schwinger equation, as propounded by Dewangan and Eichler [6], Alvarez-Estrada and Villalon [7] (who considered applications in crystallography) and Afnan and Thomas [8]. Furthermore in numerous areas of atomic, nuclear and optical physics and fundamental particle physics, knowledge of phase shifts is necessary and this is greatly ameliorated with solutions of Lippmann-Schwinger integral equation.

In recent years, significant efforts have been exerted to provide a suitable numerical method for solving this equation which possesses an inherent singularity.
For instance, singular point and multipoint quadratures based on the characteristics of small-waves, for solving the integral equations have been described by Kessler et al. [9]. Kovacic et al. [10] discussed a similar method based on small-wave characteristics for solving integral equations. Methods based on the approximation theory and other numerical schemes are treated succintly by Chiang and Lee [11] and Lanzara et al. [12]. More recently Kadyrov et al. [13] have developed a numerical method for solving the Lippmann-Schwinger equation, directly, in three dimensions considering a coupled-channel approach and a robust static-exchange model of electron-hydrogen scattering.

In the present study, a method for transforming the Lippmann-Schwinger integral equation to a matrix equation is presented in the form of the product of one known matrix \((N + 1) \times (N + 1)\) in a one-column unknown matrix. To achieve this equation, we utilize \(N\) quadrative nodal points and an observable point which determines the value of reaction operator or transition operator on the energy-shell. Subsequent evaluation of Lippmann-Schwinger integral equation is highly amenable via the matrix inverse method and/or a Gaussian elimination method.

We furthermore derive the Lippmann-Schwinger integral equation for the transition and reaction operators in the momentum-space and for the radial interaction potentials, in one dimension form. An effective technique is presented for singular elimination of the resultant equation. Finally, a numerical method for solving the Lippmann-Schwinger integral equation is expounded with graphical solutions and accompanying discussion and evaluation. The present article constitutes, we feel, an important addition to theoretical modeling of quantum scattering problems and it is hoped will stimulate more attention among readers, using the present approach.

2. The Lippmann-Schwinger Equation in One-dimension

In two-body elastic scattering, the Lippmann-Schwinger equation, which is equivalent to the Schrödinger equation plus boundary conditions, is written, following Kopaleishvili [14] as

\[
\psi_k^{(\pm)} = \phi_k + G_0^{(\pm)} V \psi_k^{(\pm)}
\]  

(1)

in which \(V\) is the two-body interaction potential, \(|\psi_k^{(\pm)}\rangle\) is the two-body system wave function in the center of the mass, \(|\phi_k\rangle\) is the asymptotic wave function, and the Green operator \(G_0^{(\pm)} = \frac{1}{E - H_0 \pm i\varepsilon}\) shows the free dispersion equal to the free
Hamiltonian $H_0$, and, also, the very small value of $\varepsilon$. For clarity, we avoid using $(\pm)$ and use $+$ notation instead. By defining the two-body transition matrix as follows:

$$V|\psi_k\rangle = T|\phi_k\rangle$$  \hspace{1cm} (2)

and after implementing equation (2) in equation (1), we arrive at

$$|\psi_k\rangle = |\phi_k\rangle + G_0 T|\phi_k\rangle.$$  \hspace{1cm} (3)

By multiplying the two sides in $V$ and using the definition (2) again, we have

$$T|\phi_k\rangle = V|\phi_k\rangle + V G_0 T|\phi_k\rangle.$$  \hspace{1cm} (4)

Since equation (4) is true for each desired $|\phi_k\rangle$ which defines the asymptotic and free condition of the two-body system, therefore it follows that

$$T = V + V G_0 T$$ \hspace{1cm} (5)

which defines the Lippmann-Schwinger equation for the transition matrix. By writing equation (5) in the momentum-space, we have

$$\langle k | T | k' \rangle = \langle k | V | k' \rangle + (2\pi)^{-3} \int dk'^* \frac{\langle k | V | k'^* \rangle \langle k'^* | T | k' \rangle}{E - (k'^*^2 / 2 \mu) + i\varepsilon}$$ \hspace{1cm} (6)

in which we have used the atomic units and normalized the wave function of the free particle in the form of $\langle r | k \rangle = \exp(i k \cdot r) \cdot \mu$ denotes the reduced mass of the two-body system. By defining $E = \frac{p^2}{2\mu}$, extending the radial and angular parts, using the symmetrical characteristic of the spherical potential, characteristics and orthogonality condition of the Legendre polynomials and the spherical harmonics, and after mathematical computations, we eventually reach the following integral equation which is the Lippmann-Schwinger in one dimension

$$T_l(k, k') = V_l(k, k') + \frac{\mu}{4\pi^3} \int_0^\infty dk'^* \frac{k'^*^2}{p^2 - k'^*^2 + i\varepsilon} V_l(k, k'^*) T_l(k'^*, k').$$ \hspace{1cm} (7)

Except in rare cases, analytical solution of this equation is intractable and numerical methods must be employed. Here, it is necessary to refer to the relation which exists between the differential scattering amplitudes and the differential components of the
transition matrix. The scattering amplitude, based on the differential components, are written

$$f(k, \theta) = \frac{1}{k} \sum_{l} (2l + 1)f_{l}(k)P_{l}^{2} \cos \theta$$

(8)

in which $f_{l}(k)$ and $P_{l}(x)$ are differential amplitude and the $l$-order Legendre polynomial, respectively. $f_{l}(k)$ and $\delta_{l}$ of the $l$-order phase shift are related to the transition matrix elements by the following equations:

$$f_{l}(k) = -\frac{\mu k}{8\pi^{2}}T_{l}(k, k; E), t_{g} \delta_{l} = \frac{Im(T_{l})}{Re(T_{l})}.$$  

(9)

Also, the differential cross section of the scattering is arrived at using the following equation from the scattering amplitude:

$$\frac{d\sigma}{d\Omega} = |f(k, \theta)|^{2}.$$  

(10)

On occasion it is advisable to express the Lippmann-Schwinger equation on the basis of the reaction operator $R$. We can arrive at the following integral equation for the reaction matrix $R$:

$$R = V + VG_{0}^{(p)}R$$  

(11)

which is the familiar form of the Lippmann-Schwinger integral equation for the reaction matrix $R$. The Green operator $G_{0}^{(p)}$ is defined as $G_{0}^{(p)} = P \frac{1}{E - H_{0}}$ in which $P$ reads the Cauchy original value and also

$$G_{0}^{(p)} = G_{0}^{(p)} \mp i\pi\delta(E - H_{0}).$$  

(12)

As with the transition matrix $T$, the Lippmann-Schwinger equation for the reaction matrix $R$ can be written in this integral form:

$$R_{l}(k, k') = V_{l}(k, k') + \frac{\mu}{4\pi^{2}} P \int_{0}^{\infty} dk' \frac{k'^{2}}{p^{2} - k'^{2}} V_{l}(k, k')R_{l}(k', k')$$

(13)

which is arrived at by using the definition of $G_{0}^{(p)}$. The advantage of using this equation is that, unlike equation (7), only real quantities are dealt with. Also, by applying equation (12) in equation (5) and doing the same computations or by direct
application on equation (7), we reach the following integral equation which is, of course, equal to equation (7):

\[
T_i(k, k') = V_i(k, k') + \frac{i\mu}{4\pi^3} \int_0^\infty dk'' \frac{k''^2}{p^2 - k''^2} V_i(k, k'')T_i(k'', k')
\]

\[
- \frac{i\pi\mu}{(2\pi)^3} pV_i(k, p)T_i(p, k').
\] (14)

Here, it is necessary to refer to the relation between the transition matrix \( T \) and the reaction matrix \( R \):

\[
T_i(k, k') = R_i(k, k') - \frac{i\pi\mu p R_i(k, p) R_i(p, k')}{(2\pi)^3 + i\pi\mu p R_i(p, p)}.
\] (15)

The experimental observables and the theoretical results which are arrived at by solving equation (7) or (13) or (14), will be related together by phase shifts. The phase shifts are given by equation (9) and based on the components of the transition matrix on the energy-shell \((p = k = k')\). Equation (15) can be written on the energy-shell as such

\[
T_l = \frac{(2\pi)^3 R_l}{(2\pi)^6 + \pi^2 \mu^2 p^2 R_l^2} \times \left[(2\pi)^3 - i\pi\mu p R_l\right].
\] (16)

Therefore, considering the second equality in equation (9), phase shifts are given based on the differential components of the interaction matrix \( R \) as follows:

\[
t_g \delta_l = \frac{\pi\mu p R_i(p, p; E)}{(2\pi)^3}.
\] (17)

Implicit in this analysis is the assumption that interaction potential has a spherical symmetry. By extending the plane-wave functions, based on the first type of spherical Bessel functions \( j_l(x) \), and the spherical harmonies, integrating on the angular part, and adding on the Kronecker deltas, we have

\[
\langle k | V | k' \rangle = \sum_{l=0}^{+l} \sum_{m=-l}^{l} Y_{lm}(\hat{k})V_i(k, k')Y_{l'm'}(\hat{k}')
\] (18)

in which
\[ V_l(k, k') = (4\pi)^2 \int_0^\infty dr r^2 j_l(kr) j_l(k'r) V(r). \] (19)

However, due to oscillatory nature of the spherical Bessel functions, the above-mentioned integral computation is extremely difficult if not impossible. Therefore, for the radial potentials, one can use the Legendre functions. In equation (18), by adding on \( m \), we have

\[ \langle k \mid V \mid k' \rangle = \sum_{l=0}^\infty \frac{2l + 1}{4\pi} j_l(k, k') P_l(\cos \gamma); \quad \cos \gamma = \hat{k} \cdot \hat{k}'. \] (20)

Multiplying the two sides by \( P_l(\cos \gamma) \) and integrating on \( \cos \gamma \), by using the orthogonality of the Legendre functions, gives

\[ V_l(k, k') = 2\pi \int_{-1}^{+1} \langle k \mid V \mid k' \rangle P_l(x) dx; \quad x = \cos \gamma. \] (21)

By inserting the closure relation in the position-space, leads to

\[ V_l(k, k') = 2\pi \int_{-1}^{+1} dx P_l(x) \int dr V(r) e^{-i(k-k')r} \]

\[ = (2\pi)^{5/2} \int_{-1}^{+1} dx P_l(x) \tilde{V}(k-k') \] (22)

in which \( \tilde{V}(k-k') \) is the potential Fourier transformation to \( \Delta = k - k' \). Assuming a radial potential, the following is generated:

\[ V_l(k, k') = -4\pi \int_{-1}^{+1} dx P_l(x) \frac{1}{\Delta} \int_0^\infty dr V(r) (e^{i\Delta r} - e^{-i\Delta r}). \] (23)

As a simple example for the Yukawa potential \( V(r) = V_0 \frac{e^{-\lambda r}}{r} \), we get

\[ V_l(k, k') = -4\pi V_0 \int_{-1}^{+1} dx P_l(x) \frac{1}{\Delta} \int_0^\infty dr e^{-\lambda r} (e^{i\Delta r} - e^{-i\Delta r}) \] (24)
or

\[ V_I(k, k') = 8\pi V_0 \int_{-1}^{+1} dx \frac{P_I(x)}{k^2 + \Delta^2}; \quad \Delta^2 = k^2 + k'^2 - 2kk'x. \] \tag{25}

For such a potential, the zero-order component of the potential is

\[ V_0(k, k') = -\frac{4\pi V_0}{kk'} \ln \left( \frac{\lambda^2 + (k - k')^2}{\lambda^2 + (k + k')^2} \right). \] \tag{26}

3. A Numerical Method for Solving the Lippmann-Schwinger Equation

Let us now consider the numerical solution of the Lippmann-Schwinger integral equation. The purpose of solving the Lippmann-Schwinger equation is to evaluate the transition matrix elements \( T_I(p, p) \), or, equally, the relation matrix elements \( R_I(p, p) \), on the energy-shell, which are true in the above-mentioned equation. By arriving at these matrix elements on the energy-shell, we can compute all the information related to the scattering problem, e.g., the differential and whole amplitudes of the scattering, phase shifts, the differential and whole cross sections, etc. In general, in integral equations, depending on the integrand’s approach, the method of computing, too, varies. In particular, the singular integrals and, also, oscillatory integrals have their own particular methods. The degree of error, also, depends on the method of computing. For the present case we start from the solution (13). We implement the equation

\[ P \int_{0}^{\infty} \frac{f(x)dx}{x^2 - x_0^2} = \int_{0}^{\infty} \frac{(f(x) - f(x_0))dx}{x^2 - x_0^2} \] \tag{27}

and eliminate the major value sign

\[ R_I(k, k') = V_I(k, k') + \frac{\mu}{4\pi^3} \int_{0}^{\infty} dk'' \frac{1}{p^2 - k''^2} \]

\[ \times \{ k''^2 V_I(k, k'') R_I(k'', k') - p^2 V_I(p, k) R_I(p, k') \}. \] \tag{28}

In this equation, the \( k \) and \( k' \) parameters can possess their favorite values. However, owing to the fact that the values on the energy-shell have physical importance, we
elect a $k'$ value equal to $p$, i.e., $k' = p$. In addition, by using a proper
quadratic relation, we approximate the present integral to the following set:

\[
R_l(k, p) \approx V_l(k, p) + \frac{\mu}{4\pi^3} \sum_{j=1}^{N} w_j
\]

\[
\times \left\{ k_j^2 V_l(k, k_j) R_l(k_j, p) - p^2 V_l(k, p) R_l(p, p) \right\}
\]

(29)

in which the whole points of \( \{k_j; j = 1, 2, \ldots, N\} \) are integration points and the whole constant values of \( \{w_j; j = 1, 2, \ldots, N\} \) are weight coefficients in the integration method, the values of which depend on the kind of quadrature chosen. Usually, in this case, Gaussian quadratures are chosen. Assuming $k_{N+1} = p$ and considering the discrete values of \( \{k_i; i = 1, 2, \ldots, N + 1\} \) for the parameter $k$ in the above-mentioned equation in this form, gives

\[
k_i = \begin{cases} 
k_j; i = j = 1, 2, \ldots, N, \
p; i = N + 1.
\end{cases}
\]

(30)

We therefore reach $N + 1$ algebraic equations with the same number of unknowns. These unknowns are $N$ quadratic values $R_l(k_j, p)$ and observable values $R_l(p, p)$ which equal the value of the reaction matrix on the energy-shell. These unknowns are coupled with all the resulting linear equations. These equations are

\[
R_l(k_i, p) \approx V_l(k_i, p) + \frac{\mu}{4\pi^3} \sum_{j=1}^{N} w_j
\]

\[
\times \left\{ k_j^2 V_l(k_i, k_j) R_l(k_j, p) - p^2 V_l(k_i, p) R_l(p, p) \right\}
\]

\[
i = 1, 2, \ldots, N + 1.
\]

(31)

Now, we transfer all of the unknowns to the left side. With some mathematical manipulation, we have

\[
\sum_{j=1}^{N} \left[ \delta_{ij} - \frac{\mu}{4\pi^3} \frac{w_j}{p^2 - k_j^2} k_j^2 V_l(k_i, k_j) \right] R_l(k_j, p)
\]

\[
\sum_{j=1}^{N} \left[ \delta_{ij} - \frac{\mu}{4\pi^3} \frac{w_j}{p^2 - k_j^2} k_j^2 V_l(k_i, k_j) \right] R_l(k_j, p)
\]
\[
\begin{align*}
+ \left[ \delta_i, N+1 + \frac{\mu}{4\pi^3} p^2 V_i(k_i, p) \sum_{m=1}^{N} \frac{w_m}{p^2 - k_m^2} \right] R_i(p, p) &= V_i(k_i, p), \\
i &= 1, 2, \ldots, N + 1
\end{align*}
\]

or, in a more compact form

\[
\sum_{j=1}^{N+1} D(k_i, k_j) R_j(k_j, p) = V_i(k_i, p), \quad i = 1, 2, \ldots, N + 1
\]  \hspace{1cm} (32)

in which

\[
D(k_i, k_j) = \begin{cases} 
\delta_{ij} - \frac{\mu}{4\pi^3} \frac{w_j}{p^2 - k_j^2} \sum_{m=1}^{N} \frac{w_m}{p^2 - k_m^2}, & 1 \leq j \leq N, \\
\delta_{i, N+1} + \frac{\mu}{4\pi^3} p^2 V_i(k_i, p) \sum_{m=1}^{N} \frac{w_m}{p^2 - k_m^2}, & j = N + 1.
\end{cases}
\]  \hspace{1cm} (33)

All the coupled equations in equation (33) can be expressed using matrix multiplication

\[
DR = V
\]  \hspace{1cm} (34)

in which \( D \) is the square matrix of the order \((N + 1) \times (N + 1)\). Also, \( R \) and \( V \) are column matrices, each possessing \((N + 1)\) rows. The elements of these matrices, considering the equation (33) and (34) are defined thus

\[
D_{ij} = D(k_i, k_j),
\]

\[
R_{ii} = R_i(k_i, p), \quad i, j = 1, 2, \ldots, N + 1,
\]

\[
V_{ii} = V_i(k_i, p).
\]  \hspace{1cm} (35)

There are two ways to identify the unknown elements of the column matrix \( R \). The first method is solving the matrix equation (35) using the matrix inverse method. By multiplying the two sides of this equation in the inverse form of the matrix \( D \), from the left side, we have

\[
R = D^{-1}V.
\]  \hspace{1cm} (36)

Owing to the fact that in linear algebraic, the inverse forms of the complex matrices, too, follow the standard and current method, equation (37) offers a direct and simple
solution for the matrix. The second method encapsulates finding an \( R \) matrix that arrives at equation (37) without the need to compute the inverse matrix. This method is termed the Gaussian elimination method.

When the matrix elements \( R \) are known, one can compute the differential components of the transition matrix \( T \) by using equation (15), and \( l \)-order equal phase shift by equation (17). By determining the equal phase shifts with different orders of \( l \), all pertinent characteristics will be evaluated for two-body scattering.

We emphasize here that via a direct solution of the integral equation (14), we may accumulate all the necessary information for the intended two-body scattering. In this case, too, by a method similar to that discussed above, we reach the following equation:

\[
\sum_{j=1}^{N+1} D(k_i, k_j) T_j(k_j, p) - \frac{i \pi \mu}{(2\pi)^3} p V_i(k_i, p) T_j(p, p) = V_i(k_i, p), \quad i = 1, 2, \ldots, N + 1. \tag{38}
\]

By inserting the second term in the sigma (\( \Sigma \)), we have

\[
\sum_{j=1}^{N+1} F(k_i, k_j) T_j(k_j, p) = V_i(k_i, p), \quad i = 1, 2, \ldots, N + 1 \tag{39}
\]

in which

\[
F(k_i, k_j) = \begin{cases} 
D(k_i, k_j), & 1 \leq j \leq N, \\
D(k_i, p) - \frac{i \pi \mu}{(2\pi)^3} p V_i(k_i, p), & j = N + 1.
\end{cases} \tag{40}
\]

Equation (39), also has the \( (N+1) \) unknowns, i.e., \( N \) is the quadrative unknowns \( T_j(k_j, p) \) and one is the observable unknown \( T_j(p, p) \) which equals the differential component value of the transition matrix on the energy-shell.

This equation may also be written in the form of the following matrix multiplication based on the square matrix \( F \) of the order \((N+1) \times (N+1)\), and the column matrices \( T \) and \( V \), each possessing \((N+1) \) rows:

\[
FT = V \tag{41}
\]
in which the matrix elements of different components are designated as follows:

\[ F_{ij} = F(k_i, k_j), \]
\[ T_{ij} = T(k_i, p), \quad i, j = 1, 2, \ldots, N + 1, \]
\[ V_{ii} = V(k_i, p). \]  

Equation (41) can also be solved by the two processes explained above, the only difference being that here we deal with the complex matrix \( F \) defined in equation (40). Therefore, the values which we arrive at for unknown elements \( T \), too, will be complex.

By solving equation (41), different values of the \( l \)-order component of the transition matrix are arrived at for different energies external to and on the energy-shell. By knowing the component value on the energy-shell, we can find the \( l \)-order phase shift by using equation (9) and, also, by knowing the phase shifts, the scattering problem is solved completely.

### 4. Results and Discussion

The Schrödinger equation for two-particle scatterings in which the interaction potential reduces quicker than \( \frac{1}{r} \), has a singular, limited, and determined answer. Consequently, the Lippmann-Schwinger equation has such characteristics. However, as we saw, this equation has an inherent singularity which can be eliminated as described by Joachain [15]. A method has been suggested above for the elimination of the above-mentioned singularity and the result is equation (28) which can be solved, in most cases, using a numerical method. The numerical method offered in this article relies on the Gaussian quadrature for solving the above-mentioned equation and leads to equation (29). The weight coefficients \( w_i \) are based on the chosen quadrature. The infinity of the upper limit of an integral does not mean the whole integral’s infinity, especially when it is known that the Laguerre polynomials-based quadrature can be, directly, used for integrals in the interval \([0, \infty]\). Although the method mentioned in this article can be used for all the Gaussian quadratures, we use the Gauss-Jacobi quadrature for our computations hereafter. In this method, by a simple changing of variable, the interval \([0, \infty]\) is mapped on the interval \([-1, +1]\) (further elucidation of weight coefficients and Gaussian quadratures is provided in Press et al. [16]).
The method offered in the previous section can be used for the well-behaved radial scattering potentials. What results from the algebraic equations (35) and (41), and possesses physical importance, is the numerical value of the transition matrix $T_l(p, p)$, or the reaction matrix $R_l(p, p)$, on the energy-shell. In this section, as an example of the uses of the above-mentioned method, we compute the phase shifts, the real and imaginary parts of the transition matrix on the energy-shell, the amplitudes and differential cross sections of the scattering for a particle scattering to the individual mass in the Yukawa scattering potential to the equation

$$2 \exp\left[-\frac{2r}{r}\right]$$

for $l = 0$ to $l = 10$. The reason for this choice is that researchers working in atomic scattering theory, often approximate the complex potential of the interaction with the sum of a Coulomb potential and a short-range potential. In simple atoms and especially for K-shell electrons, the Yukawa potential is a good approximate for the short-range part. We assumed the scattering energy changes spectrum from 10 eV to 500 eV which is equivalent to momentum changes of 0.86 a.u. to 6 a.u.. Gauss-Jacobi quadrature with nine nodal points is used in computations. Therefore, the $F$ and $D$ matrices are $10 \times 10$ matrices and by the Gaussian elimination method, we may compute their inverse form so that we solve 10 coupled algebraic equations simultaneously.

Figure 1 shows the phase shifts based on energy and quantum number. Phase shift changes on the basis of the scattering energy for different orbital quantum numbers and orbital quantum number for different incidental energies are, also, shown in Figure 2. Inspection of these figures indicates that differential phase shifts for large $l$ are for all possible energy values tend toward zero and for the energy 100 eV, the phase shift absolute value $\delta_0$ is greater than other energies. Figure 3 shows the real and imaginary parts of the transition matrix for the same energies and for the scattering angles of 0 to 180 degrees. The real part of the scattering amplitude for big angles and in low energies possesses the lowest value possible. In higher energies, this value grows dramatically. In contrast to the low energies in which the real value of the transition matrix is greater in the small scattering angles, for high scattering energies, in big scattering angles, this value is more than the equivalent values in small scattering angles. The imaginary part of the scattering amplitude, also, has the highest value in high energies and high scattering angles but possesses the lowest value in low energies and big scattering angles.

Figure 4 shows the angular distribution of the scattering cross section for the
same incidental energies for all possible scattering angles, considering eleven
differential components \((l = 0, 10)\), and by computing the equal scattering
amplitudes using the present numerical method. For all incidental energies, the
differential cross section of the scattering possesses the highest value in small angles,
and in large angles, the cross section tends toward zero.

In Figure 5, the angular distribution of the differential cross sections of the
scattering for different incidental energies are compared with each other. As can be
seen from the figure, the peak of the differential cross section of the scattering in the
scattering angles arises in the vicinity of zero, and, also, by increasing the incidental
energy, this peak increases. Also, by increasing the scattering angle, the cross section
decreases dramatically and by increasing the energy, the cross section reduction rate
increases due to angular change of the scattering.

Figure 6 and Figure 7 depict the real and imaginary parts of the transition matrix
and the differential cross section of the scattering, respectively, for the incidental
energy 100 eV. The values arrived at from this method are compared to the
equivalent values via direct solution of the Schrödinger equation. As anticipated, the
differential cross section in small angles reaches its peak, but reduces dramatically by
increasing the angle. Also we note that there is very good correlation between the
values arrived at using the present numerical approach and the values arrived at from
solving the Schrödinger equation.

5. Conclusions

In the above-mentioned method, we transformed the singular Lippmann-
Schwinger integral equation, for the radial interaction potentials, to a one-dimension
integral equation. By using the Cauchy major value, we eliminated the singularity in
this equation. Thereafter we described a suitable method to transform the integral
equation to a simple algebraic equation, such that the solution of the relatively simple
algebraic equation is equivalent to the singular and complex Lippmann-Schwinger
equation. Knowledge of the interaction potential, thererby, allows solution of the
algebraic equation for evaluating the differential components of the transition and
interaction matrices with each desired \(l\) on the energy-shell. The component values of
the reaction matrix are real and of the transition matrix are imaginary. By knowing
the value of the reaction and transition matrixes elements on the energy-shell, phase
shifts, the differential scattering amplitudes and the differential cross sections are
computable. The scattering cross section is a physical observable which is theoretically computable and can be measured by an experimental method.

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References


Figure 1. Phase shifts changes on the basis of the scattering energy for different values of quantum number $l$. 
Figure 2. Phase shifts changes: (a) on the basis of the scattering energy for the orbital quantum numbers 0-5, and (b) on the basis of the orbital quantum number for the incidental energies 100 eV, 300 eV, and 500 eV.
Figure 3. (a) The real and (b) the imaginary values of the transition matrix on the energy-shell for the energy spectrum of 10-500 eV and the scattering angles of 0-180 degrees.
Figure 4. The angular distribution of the differential cross section of the scattering in the energy spectrum 10-500 eV and the scattering angles of 0-180 degrees.

Figure 5. The angular distribution of the differential cross sections of the scattering for the incidental energies of 50 eV, 100 eV, 150 eV, and 200 eV.
Figure 6. Comparing the present results, using the present method, with the results of the Schrödinger equation for the real and imaginary values of the transition matrix on the energy-shell for 100 eV energy and the scattering angles of 0-180 degrees.

Figure 7. Comparing the present results, using the present method, with the results of the Schrödinger equation for the angular distribution of the differential cross section of the scattering for the incidental energy 100 eV and the scattering angles of 0-180 degrees.