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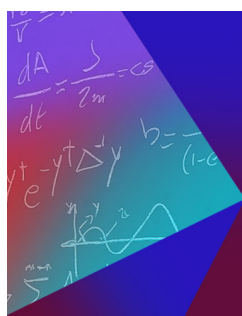
# Solution of coupled integral equations for quantum scattering in the presence of complex potentials ⊘

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# Solution of coupled integral equations for quantum scattering in the presence of complex potentials

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In this paper, we present a method to compute solutions of coupled integral equations for quantum scattering problems in the presence of a complex potential. We show how the elastic and absorption cross sections can be obtained from the numerical solution of these equations in the asymptotic region at large radial distances. © *2015 AIP Publishing LLC.* [http://dx.doi.org/10.1063/1.4905734]

## I. INTRODUCTION

The formalism of non-Hermitian quantum mechanics offers some simplifications in the formulation and computation of scattering processes, which might be difficult to solve within the Hermitian quantum scattering theory (see, e.g., Moiseyev[2] and Chapter 8 in the book by Moiseyev[1]). The use of complex absorption potentials offers an efficient way to obtain cross section for reactive and short-lived channels (see, e.g., Chapter 18 in the book by Calogero[3]). The use of complex absorption potentials has been discussed for various solution methods for the time independent Schrödinger equation for scattering problems. For example, Calogero[3] shows how to extend the variable phase approach and Huarte-Larranage *et al.*[4] have generalized the *R*-matrix method, just to name a few.

In this paper, we present a method to solve the time independent Schrödinger equation for scattering equations in the presence of a complex absorbing potential via the numerical integration of coupled Volterra integral equations. Sams and Kouri[5–7] have shown that for real potentials, the scattering cross section can be obtained by solving a system of coupled Volterra integral equations. In matrix form, the integral equations can be written as (see, e.g., Chapter 5 in the book by Gianturco[13])

$$\mathbf{U}(R) = \int_{R_0}^{R} \{ \mathbf{J}(R) \cdot \mathbf{N}(x) + \mathbf{N}(R) \cdot \mathbf{J}(x) \} \cdot \mathbf{V}(x) \cdot \mathbf{U}(x)\, dx \ . \tag{1}$$

Here, $\mathbf{J}$ and $\mathbf{N}$ are diagonal matrices containing the spherical Riccati-Bessel and Riccati-Neumann functions, respectively, $\mathbf{V}$ is the potential matrix, and $\mathbf{U}(R)$ is a matrix containing the radial wavefunction. The formulation of Sams and Kouri via Volterra integral equations has a number of advantages. The boundary conditions are automatically included. The equations can be solved by non-iterative procedures.[7] The method can be used for local and non-local potentials.[7] The formulation can be extended to obtain other scattering quantities directly, like the $\mathbf{T}$ and $\mathbf{K}$ matrix[8,9] and to reactive scattering.[10–12]

Curik *et al.* have shown that the method can result in very efficient computer implementations to obtain cross sections for electron molecule collisions[14] and positron molecule collisions.[15] Recently, we have applied this method to positron scattering from biomolecules[16–19] employing the recent computer implementation of Sanna *et al.*[20]

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The good features of the integral equation method of Sams and Kouri motivate us to extend it for complex potentials. The paper is organized as follows: in Sec. II, we show how to solve Eq. (1) for real potentials and how to extract scattering cross sections, as discussed in the literature. In Sec. III, we will show how Eq. (1) can be solved for complex potentials and how elastic and absorption cross sections can be obtained from the asymptotic solutions of the wavefunction.

## II. SOLUTION FOR REAL POTENTIALS

### A. Integral equations

Equation (1) can be rewritten in the following equivalent form (see Chapter 5 in Gianturco[13]):

$$\mathbf{G}(R) = \mathbf{V} \cdot (\mathbf{J} \cdot \mathbf{Q} + \mathbf{N} \cdot \mathbf{P}) \,, \tag{2}$$

with the auxiliary matrices

$$\mathbf{P}(R) = \int_{R_0}^{R} \mathbf{J}(x) \cdot \mathbf{G}(x) \, dx \tag{3}$$

and

$$\mathbf{Q}(R) = \int_{R_0}^{R} \mathbf{N}(x) \cdot \mathbf{G}(x) \, dx \,. \tag{4}$$

### B. Numerical solution

The Eqs. (2)–(4) can easily be solved numerically. As an example, we show explicitly the one-step advancing procedure for the trapezoidal integration rule, given in Chapter 5 of Gianturco.[13] The formulation using alternative integration rules can be done in a straightforward manner. If we assume a constant step size $h$, we can define

$$\mathbf{G_t} = \mathbf{G}(R_0 + th) \,, \tag{5}$$

with $t \in \{0, 1, 2, \ldots, N\}$. Quantities $\mathbf{V}_t, \mathbf{J}_t, \mathbf{N}_t, \mathbf{P}_t$, and $\mathbf{Q}_t$ can be formulated in an equivalent way. Here, the point $R_0$ is chosen either at the origin or deep enough in the classically forbidden region. The last radial grid point $R_N = R_0 + N \cdot h$ is in the asymptotic region, where the influence of the potential can be neglected. This procedure can easily be generalized to non-uniform radial grids. The stepping procedure is given by (see Chapter 5 in Gianturco[13])

$$\mathbf{G_t} = \mathbf{V_t} \cdot (\mathbf{J_t} \cdot \mathbf{Q_{t-1}} + \mathbf{N_t} \cdot \mathbf{P_{t-1}}) \,. \tag{6}$$

The computation of $\mathbf{G_t}$ at the radial grid point $t$ only requires the knowledge of the matrices $\mathbf{P_{t-1}}$ and $\mathbf{Q_{t-1}}$ at the grid points $t-1$. The two auxiliary matrices can be computed as

$$\mathbf{P_t} = \mathbf{P_{t-1}} + h \cdot \mathbf{J_t} \cdot \mathbf{G_t} \tag{7}$$

and

$$\mathbf{Q_t} = \mathbf{Q_{t-1}} + h \cdot \mathbf{N_t} \cdot \mathbf{G_t}. \tag{8}$$

The initial conditions are given by

$$\mathbf{P_0} = \mathbf{0} \text{ and } \mathbf{Q_0} = \mathbf{1} \,, \tag{9}$$

where $\mathbf{0}$ and $\mathbf{1}$ are the zero matrix and the unit matrix, respectively.

### C. Computation of the cross sections

At the final radial grid point $R = N \cdot h$, which is in the asymptotical region, the **K**-matrix can be obtained by

$$\mathbf{K} = \mathbf{P_N} \cdot \mathbf{Q_N}^{-1} \,. \tag{10}$$

One should note that the matrices $\mathbf{P_t}$ and $\mathbf{Q_t}$ can be parametrized in the following way:

$$\mathbf{P_t} = \sin\mathbf{d_t} \tag{11}$$

and

$$\mathbf{Q_t} = \cos\mathbf{d_t} . \tag{12}$$

This parametrization is never explicitly used in the procedure, however, it is instructive to see that the $\mathbf{K}$ matrix can be expressed as

$$\mathbf{K} = \tan\mathbf{d_N} , \tag{13}$$

where the matrix $\mathbf{d}$ is a matrix containing the partial-wave phase shifts. This parametrization directly motivates the initial conditions for $\mathbf{P_0}$ and $\mathbf{Q_0}$ given in Eq. (9).

From the $\mathbf{K}$-matrix, we can obtain the $\mathbf{S}$-matrix as

$$\mathbf{S} = (1 - i\mathbf{K}) \cdot (1 + i\mathbf{K})^{-1} . \tag{14}$$

The elastic integral cross section is computed in terms of the $\mathbf{S}$-matrix as

$$\sigma_{\text{el}} = \frac{\pi}{k^2} \sum_{mn} |\delta_{mn} - \mathbf{S}_{mn}|^2 , \tag{15}$$

where $k = \sqrt{2E}$ and $E$ is the collision energy. The above sum runs over all $\mathbf{S}$-matrix channels $m$ and $n$.

## III. SOLUTION FOR COMPLEX POTENTIALS

### A. Integral equations

In this section, we will explore the possibility of using a complex potential matrix

$$\mathbf{V^c} = \mathbf{V^r} + i\,\mathbf{V^i}, \tag{16}$$

which can contain a real part $\mathbf{V^r}$ and an imaginary part $\mathbf{V^i}$. For the above matrices $\mathbf{G}$, $\mathbf{P}$, and $\mathbf{Q}$, we are making the Ansatz

$$\mathbf{G^c} = \mathbf{G^r} + i\,\mathbf{G^i}, \tag{17}$$

$$\mathbf{P^c} = \mathbf{P^r} + i\,\mathbf{P^i}, \tag{18}$$

$$\mathbf{Q^c} = \mathbf{Q^r} + i\,\mathbf{Q^i}. \tag{19}$$

Inserting these equations into Eq. (2) and separating real and imaginary quantities, we obtain for the $\mathbf{G}$ matrices

$$\begin{aligned}\mathbf{G^r} = \mathbf{V^r} \cdot (\mathbf{J} \cdot \mathbf{Q^r} + \mathbf{N} \cdot \mathbf{P^r}) \\ - \mathbf{V^i} \cdot (\mathbf{J} \cdot \mathbf{Q^i} + \mathbf{N} \cdot \mathbf{P^i})\end{aligned} \tag{20}$$

and

$$\begin{aligned}\mathbf{G^i} = \mathbf{V^r} \cdot (\mathbf{J} \cdot \mathbf{Q^i} + \mathbf{N} \cdot \mathbf{P^i}) \\ + \mathbf{V^i} \cdot (\mathbf{J} \cdot \mathbf{Q^r} + \mathbf{N} \cdot \mathbf{P^r}).\end{aligned} \tag{21}$$

For the real and imaginary parts of the $\mathbf{P}$ and $\mathbf{Q}$ matrices, we obtain

$$\mathbf{P^r}(R) = \int_{R_0}^{R} \mathbf{J}(x) \cdot \mathbf{G^r}(x)\, dx, \tag{22}$$

$$\mathbf{P^i}(R) = \int_{R_0}^{R} \mathbf{J}(x) \cdot \mathbf{G^i}(x)\, dx \tag{23}$$

and

$$\mathbf{Q}^{\mathbf{r}}(R) = \int_{R_0}^{R} \mathbf{N}(x) \cdot \mathbf{G}^{\mathbf{r}}(x)\, dx, \tag{24}$$

$$\mathbf{Q}^{\mathbf{i}}(R) = \int_{R_0}^{R} \mathbf{N}(x) \cdot \mathbf{G}^{\mathbf{i}}(x)\, dx\ . \tag{25}$$

## B. Numerical solution

The Eqs. (20)–(25) can be solved in a similar way as shown in the previous section for the case of real potentials. As an example, we show the one-step advancing procedure for the trapezoidal integration rule. The formulation using other integration rules is again straightforward. Let

$$\mathbf{G}^{\mathbf{r}}_{\mathbf{t}} = \mathbf{G}^{\mathbf{r}}(R_0 + th)\,, \tag{26}$$

with $t \in \{0, 1, 2, \ldots, N\}$. All other quantities with a subscript are defined equivalently. The stepping procedure can now be formulated as

$$\begin{aligned}
\mathbf{G}^{\mathbf{r}}_{\mathbf{t}} &= \mathbf{V}^{\mathbf{r}}_{\mathbf{t}} \cdot \left(\mathbf{J_t} \cdot \mathbf{Q}^{\mathbf{r}}_{\mathbf{t-1}} + \mathbf{N_t} \cdot \mathbf{P}^{\mathbf{r}}_{\mathbf{t-1}}\right) \\
&\quad - \mathbf{V}^{\mathbf{i}}_{\mathbf{t}} \cdot \left(\mathbf{J_t} \cdot \mathbf{Q}^{\mathbf{i}}_{\mathbf{t-1}} + \mathbf{N_t} \cdot \mathbf{P}^{\mathbf{i}}_{\mathbf{t-1}}\right)
\end{aligned} \tag{27}$$

and

$$\begin{aligned}
\mathbf{G}^{\mathbf{i}}_{\mathbf{t}} &= \mathbf{V}^{\mathbf{r}}_{\mathbf{t}} \cdot \left(\mathbf{J_t} \cdot \mathbf{Q}^{\mathbf{i}}_{\mathbf{t-1}} + \mathbf{N_t} \cdot \mathbf{P}^{\mathbf{i}}_{\mathbf{t-1}}\right) \\
&\quad + \mathbf{V}^{\mathbf{i}}_{\mathbf{t}} \cdot \left(\mathbf{J_t} \cdot \mathbf{Q}^{\mathbf{r}}_{\mathbf{t-1}} + \mathbf{N_t} \cdot \mathbf{P}^{\mathbf{r}}_{\mathbf{t-1}}\right),
\end{aligned} \tag{28}$$

with

$$\mathbf{P}^{\mathbf{r}}_{\mathbf{t}} = \mathbf{P}^{\mathbf{r}}_{\mathbf{t-1}} + h \cdot \mathbf{J_t} \cdot \mathbf{G}^{\mathbf{r}}_{\mathbf{t}}, \tag{29}$$

$$\mathbf{P}^{\mathbf{i}}_{\mathbf{t}} = \mathbf{P}^{\mathbf{i}}_{\mathbf{t-1}} + h \cdot \mathbf{J_t} \cdot \mathbf{G}^{\mathbf{i}}_{\mathbf{t}}, \tag{30}$$

$$\mathbf{Q}^{\mathbf{r}}_{\mathbf{t}} = \mathbf{Q}^{\mathbf{r}}_{\mathbf{t-1}} + h \cdot \mathbf{N_t} \cdot \mathbf{G}^{\mathbf{r}}_{\mathbf{t}}, \tag{31}$$

$$\mathbf{Q}^{\mathbf{i}}_{\mathbf{t}} = \mathbf{Q}^{\mathbf{i}}_{\mathbf{t-1}} + h \cdot \mathbf{N_t} \cdot \mathbf{G}^{\mathbf{i}}_{\mathbf{t}}\ . \tag{32}$$

The initial conditions are

$$\mathbf{P}^{\mathbf{r}}_{\mathbf{0}} = \mathbf{0} \text{ and } \mathbf{P}^{\mathbf{i}}_{\mathbf{0}} = \mathbf{0} \tag{33}$$

and

$$\mathbf{Q}^{\mathbf{r}}_{\mathbf{0}} = \mathbf{1} \text{ and } \mathbf{Q}^{\mathbf{i}}_{\mathbf{0}} = \mathbf{0}\ . \tag{34}$$

## C. Computation of the cross sections

In order to formulate an expression for the **K**-matrix in the asymptotic region, it is instructive to introduce some parametrization of the matrices $\mathbf{P^i}$ and $\mathbf{Q^i}$. We choose the following parametrization of the **S**-matrix (see, e.g., Chapter 18 in Calogero[3]):

$$\mathbf{S}(R) = \mathbf{A}(R) \cdot e^{2i\mathbf{d}(R)}. \tag{35}$$

Here, $\mathbf{d}(R)$ is the matrix containing the phase shifts, and the matrix $\mathbf{A}(R)$ can be parametrized as

$$\mathbf{A}(R) = e^{-2\mathbf{b}(R)}, \tag{36}$$

where $\mathbf{b}(R)$ is a matrix of complex phase shifts. With this parametrization, the matrices $\mathbf{P^c}$ and $\mathbf{Q^c}$ in Eqs. (18) and (19) can be expressed in term of the matrices **P** and **Q**, given in Eqs. (11) and (12).

$$\begin{aligned}
\mathbf{P^c} &= \mathbf{P} \cdot \cos i\mathbf{b} + \mathbf{Q} \cdot \sin i\mathbf{b} \\
&= \sin\mathbf{d} \cdot \cos i\mathbf{b} + \cos\mathbf{d} \cdot \sin i\mathbf{b} \\
&= \sin\mathbf{d} \cdot \cosh\mathbf{b} + i\cos\mathbf{d} \cdot \sinh\mathbf{b}
\end{aligned} \tag{37}$$

and

$$
\begin{aligned}
\mathbf{Q^c} &= -\mathbf{P}\cdot\sin i\mathbf{b} + \mathbf{Q}\cdot\cos i\mathbf{b} \\
&= -\sin\mathbf{d}\cdot\sin i\mathbf{b} + \cos\mathbf{d}\cdot\cos i\mathbf{b} \\
&= \cos\mathbf{d}\cdot\cosh\mathbf{b} - i\sin\mathbf{d}\cdot\sinh\mathbf{b}.
\end{aligned}
\tag{38}
$$

For the real and imaginary parts of the matrices $\mathbf{P^c}$ and $\mathbf{Q^c}$, we get the following set of expressions:

$$
\mathbf{P^r} = \sin\mathbf{d}\cdot\cosh\mathbf{b}, \tag{39}
$$
$$
\mathbf{P^i} = \cos\mathbf{d}\cdot\sinh\mathbf{b}, \tag{40}
$$
$$
\mathbf{Q^r} = \cos\mathbf{d}\cdot\cosh\mathbf{b}, \tag{41}
$$
$$
\mathbf{Q^i} = -\sin\mathbf{d}\cdot\sinh\mathbf{b} . \tag{42}
$$

With the definition of the $\mathbf{K}$-matrix,

$$
\mathbf{K} = \tan\mathbf{d_N}, \tag{43}
$$

we can express the $\mathbf{K}$-matrix as either

$$
\mathbf{K} = \mathbf{P^r_N}\cdot\left(\mathbf{Q^r_N}\right)^{-1} \tag{44}
$$

or as

$$
\mathbf{K} = -\mathbf{Q^i_N}\cdot\left(\mathbf{P^i_N}\right)^{-1} . \tag{45}
$$

For the computation of the absorption cross section, we need the asymptotic value of the matrix $\mathbf{A}$. Using the relations between hyperbolic functions, we can derive the following identity:

$$
\mathbf{A} = e^{-2\mathbf{b}} \tag{46}
$$
$$
= (\cosh\mathbf{b} + \sinh\mathbf{b})\cdot(\cosh\mathbf{b} - \sinh\mathbf{b})^{-1}. \tag{47}
$$

With the quantities given in Eqs. (39) – (42), the matrix $\mathbf{A}$ can be expressed as

$$
\mathbf{A} = \left(\mathbf{Q^r} + \mathbf{P^i}\right)\cdot\left(\mathbf{Q^r} - \mathbf{P^i}\right)^{-1} \tag{48}
$$

or alternatively as

$$
\mathbf{A} = \left(\mathbf{P^r} - \mathbf{Q^i}\right)\cdot\left(\mathbf{P^r} + \mathbf{Q^i}\right)^{-1}. \tag{49}
$$

From the $\mathbf{K}$-matrix and the $\mathbf{A}$-matrix, computed in the asymptotic region, we can obtain the $\mathbf{S}$-matrix as

$$
\mathbf{S} = \mathbf{A}\cdot(1 - i\mathbf{K})\cdot(1 + i\mathbf{K})^{-1}. \tag{50}
$$

The elastic integral cross section is computed in terms of the $\mathbf{S}$-matrix as

$$
\sigma_{\mathrm{el}} = \frac{\pi}{k^2}\sum_{mn}|\delta_{mn} - \mathbf{S}_{mn}|^2 , \tag{51}
$$

with $k = \sqrt{2E}$ and $E$ being the collision energy. The absorption cross section is given by

$$
\sigma_{\mathrm{abs}} = \frac{\pi}{k^2}\sum_{mn}\left\{\delta_{mn} - |\mathbf{S}_{mn}|^2\right\} . \tag{52}
$$

The total cross section is given by

$$
\sigma_{\mathrm{total}} = \frac{2\pi}{k^2}\sum_{mn}\{\delta_{mn} - \mathrm{Re}(\mathbf{S}_{mn})\} , \tag{53}
$$

where $\mathrm{Re}(\mathbf{S}_{mn})$ denotes the real part of $\mathbf{S}_{mn}$. The sums in Eqs. (51) – (53) run over all channels $m$ and $n$.

## IV. CONCLUSIONS

In this paper, we are presenting a method to solve the system of coupled Volterra integral equations in the presence of a complex potential. Explicit equations are derived for the numerical implementation. We have derived expressions for computing the elastic and absorption cross sections from the solutions in the asymptotic region. The equations can be easily implemented into existing computer program packages, like VOLSCAT.[20]

In the future, we plan to use this method to describe processes like the ionization of atoms and molecules by electron or positron impact and the formation of Positronium, the bound system of an electron and a positron, by positron collisions with atoms and molecules. Complex absorption potentials have been utilized to describe these processes (see, e.g., for electron potentials Staszewska[21] and Blanco and Garcia[22,23] and for positron potentials Reid and Wadehra[24,25]).

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