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Direct solution of the three-dimensional Lippmann–Schwinger equation

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Abstract

A standard technique for solving three-dimensional momentum-space integral equations in scattering theory is their transformation into one-dimensional equations in terms of partial waves. However, for some scattering systems where a large number of partial waves contribute this technique is not efficient. In this work we explore the alternative approach of solving these equations directly without partial-wave expansion. For illustrative purposes we adopt the coupled-channel approach and consider a well-studied static-exchange model of electron–hydrogen scattering.

The momentum-space integral-equation method in scattering theory is intrinsically powerful for a number of reasons. First of all the method deals directly with scattering amplitudes, the magnitude of which can be experimentally measured. In addition when formulated rigorously the method implicitly incorporates the correct asymptotic boundary conditions for the scattering problem of interest. Three-dimensional momentum-space integral equations emerge in such approaches to scattering problems like the coupled-channel (see, for example, [1]) and Faddeev formalisms [2, 3]. The standard technique for solving these equations is the use of a partial-wave expansion which transforms them into a sum of one-dimensional equations. With today's computer power, accurate solution of a large set of one-dimensional integral equations became a routine task [4]. However, for some collisional systems where an extremely large number of individual partial waves contribute this technique has disadvantages. At the same time progress in high-performance computing has reached the stage where it is opportune to assess direct solution approaches to the multidimensional integral equations. In this work we show that the three-dimensional momentum-space integral equations can be effectively and accurately solved without a recourse to partial-wave expansion. For illustrative purposes we adopt the coupled-channel formalism and consider the static exchange model of electron–hydrogen scattering [5]. Our ultimate goal is to develop an efficient method for solving scattering problems with heavy particles (ion–atom collisions) where several thousand partial waves can contribute. A similar method has been applied by Glöckle and collaborators

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[6] in nuclear physics. They solved the Faddeev equations for scattering of three identical bosons neglecting spin degrees of freedom. These authors have since presented a method of solving scattering integral equations for two nucleons with spins without partial-wave decomposition [7]. This is expected to be used in similar treatment of realistic three-nucleon Faddeev equations.

Consider the scattering of an electron with incident momentum $\boldsymbol{k}$ (atomic units are used unless otherwise specified) off a hydrogen atom in the ground state. We assume that the proton is infinitely heavy compared to the electrons and remains at rest. In the close-coupling approach to the problem the total scattering wavefunction is expanded in terms of channel functions with unknown coefficients. The spin of the proton is neglected. Singlet and triplet states of the total spin (of two electrons) are considered. After substituting the expansion into the Schrödinger equation for the scattering wavefunction and using the Bubnov–Galerkin principle [8] one obtains a system of integro-differential equations for the coefficients. Due to the conservation of the total spin the system of equations corresponding to singlet and triplet states decouples. This system can be transformed to a set of coupled effective two-body Lippmann–Schwinger equations [9].

We consider here a model that retains only the ground state of the atom, the so-called static exchange model. The momentum-space Lippmann–Schwinger equations for transition amplitudes $T^{\pm}$ corresponding to the singlet (+) and triplet (−) spin-states may be written as

$$T^{\pm}(\boldsymbol{k}', \boldsymbol{k}) = V^{\pm}(\boldsymbol{k}', \boldsymbol{k}) + \int \frac{\mathrm{d}\boldsymbol{k}''}{(2\pi)^3} \frac{V^{\pm}(\boldsymbol{k}', \boldsymbol{k}'')T^{\pm}(\boldsymbol{k}'', \boldsymbol{k})}{k^2/2 - k''^2/2 + \mathrm{i}0}, \tag{1}$$

where $\boldsymbol{k}'$ and $\boldsymbol{k}''$ are the off-the-energy-shell momenta of the free electron.

Fully off-shell effective potentials corresponding to the singlet and triplet spin-states are given by

$$V^{\pm}(\boldsymbol{q}, \boldsymbol{p}) = F(\boldsymbol{q}, \boldsymbol{p}) \pm G(\boldsymbol{q}, \boldsymbol{p}), \tag{2}$$

with

$$F(\boldsymbol{q}, \boldsymbol{p}) = \int \mathrm{d}\boldsymbol{r}_1 \, \mathrm{d}\boldsymbol{r}_2 \, \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}_1} \psi^*(\boldsymbol{r}_2)(H - E) \, \mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}_1} \psi(\boldsymbol{r}_2), \tag{3}$$

$$G(\boldsymbol{q}, \boldsymbol{p}) = \int \mathrm{d}\boldsymbol{r}_1 \, \mathrm{d}\boldsymbol{r}_2 \, \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}_2} \psi^*(\boldsymbol{r}_1)(H - E) \, \mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}_1} \psi(\boldsymbol{r}_2), \tag{4}$$

where $H = H_0 + v_1 + v_2 + v_3$ is the total three-body Hamiltonian, H_0 is the free three-body Hamiltonian, v_1 and v_2 are the interactions of the electrons with the proton, v_3 is the interaction between the electrons, E is the total energy of the system, ψ is the ground-state wavefunction of the atom, $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ are the coordinates of the electrons relative to the proton.

At this stage conventional approaches use expansion of $V^{\pm}(\boldsymbol{q}, \boldsymbol{p})$ and $T^{\pm}(\boldsymbol{q}, \boldsymbol{p})$ into partial waves. This transforms equation (1) into a sum of one-dimensional integral equations for each partial-wave amplitude. This method is very effective for collisions of light particles such as electrons and positrons scattering from atoms. In these cases a small number of partial waves (as a rule less than 20 in a wide energy range) give the main contribution to the sum. This result can be reliably extrapolated to incorporate the contribution from all remaining partial waves. Therefore all important atomic states (eigen and pseudo) can easily be included into the scheme. Let us assume now a situation where the contribution from a thousand partial waves is significant. This is the case, for example, in ion–atom collisions. Though the partial-wave approach is still valid, however it is impractical. Firstly, too many partial-wave amplitudes need to be calculated. Secondly, and most importantly, there is no practical angular-momentum algebra for such large angular momenta and, therefore, inclusion

of necessary atomic states is problematic. This essentially limits the utility of the partial-wave approach to ion–atomic processes to one-state calculations. One alternative is to transform the integral equations using an impact-parameter approach [10, 11]. The impact-parameter approach works well at sufficiently high energies but is not reliable at low energies. Therefore, at low energies the only alternative to the partial-wave approach is solving equation (1) in three-dimensional momentum space. In order to do this we first calculate the potentials in a closed form.

The off-shell direct amplitude (3) is calculated easily and the result is similar to the on-shell one

$$F(\boldsymbol{q},\boldsymbol{p}) = -4\pi\frac{\Delta^2+8}{(\Delta^2+4)^2}, \tag{5}$$

where $\Delta = |\boldsymbol{p}-\boldsymbol{q}|$ is the momentum transfer.

The exchange amplitude (4) for the on-shell case has been calculated by Corinaldesi and Trainor [12]. The fully off-shell amplitude which we need in our integral equations is quite different. After applying H_0 on the incoming state, $G(\boldsymbol{q},\boldsymbol{p})$ can be written as

$$G(\boldsymbol{q},\boldsymbol{p}) = -\frac{32\pi(k^2+1)}{(q^2+1)^2(p^2+1)^2} + I(\boldsymbol{q},\boldsymbol{p}), \tag{6}$$

where

$$I(\boldsymbol{q},\boldsymbol{p}) = \frac{32}{\pi}\int\frac{\mathrm{d}\boldsymbol{x}}{x^2}\frac{1}{(|\boldsymbol{x}-\boldsymbol{q}|^2+1)^2(|\boldsymbol{x}+\boldsymbol{q}|^2+1)^2}. \tag{7}$$

In the on-shell case the last integral has been calculated [13] using the Feynman parametrization technique. Similar way we calculate it for the general off-shell case to get

$$I(\boldsymbol{q},\boldsymbol{p}) = \frac{16\pi}{s^5}(I_0+I_1+I_2), \tag{8}$$

with

$$I_0 = \frac{(P+Q)}{PQ}[2(P-Q)^2+PQ\Delta^2]s - \left[4(P-Q)^2+2((P-Q)^2+PQ)\Delta^2-\frac{1}{2}PQ\Delta^4\right]t, \tag{9}$$

$$I_1 = -\frac{2}{4+\Delta^2}[8(P-Q)^2+(3(P-Q)^2+4PQ)\Delta^2]s+(P+Q)[2(P-Q)^2+PQ\Delta^2]t, \tag{10}$$

$$I_2 = \left[2PQ(P+Q)+\frac{8(P+Q)^3}{(4+\Delta^2)^2}+\frac{(P+Q)((P-Q)^2-16PQ)}{4+\Delta^2}\right]s-\frac{3}{2}PQ(P-Q)^2t, \tag{11}$$

where

$$s = \sqrt{(P-Q)^2-PQ\Delta^2}, \tag{12}$$

$$t = \log\left[\frac{P}{Q}\right]+\log\left[\frac{2(P-Q)+2s-Q\Delta^2}{2(P-Q)+2s+P\Delta^2}\right], \tag{13}$$

$$P = 1+p^2, \tag{14}$$

$$Q = 1+q^2. \tag{15}$$

It is not difficult to verify that on the energy shell the off-shell amplitude reproduces the Corinaldesi–Trainor amplitude [12].

We solve equation (1) both in partial waves and directly in three-dimensional space. For the three-dimensional calculations we use the spherical coordinate system $\boldsymbol{k} = \{k, \theta, \varphi\}$. For simplicity we put the z-axis along the incident momentum and set $T^{\pm}(k', \theta', \varphi') \equiv T^{\pm}(k', \theta', \varphi'; k, 0, 0)$. Then in spherical coordinates equation (1) reads as

$$T^{\pm}(k', \theta', \varphi') = V^{\pm}(k', \theta', \varphi'; k, 0, 0) + \int_0^{\infty} \mathrm{d}k'' \int_{-\pi}^{\pi} \mathrm{d}\theta'' \int_0^{2\pi} \mathrm{d}\phi'' \times \frac{2k''^2 \sin\theta''}{(2\pi)^3} \frac{V^{\pm}(k', \theta', \varphi'; k'', \theta'', \varphi'') T^{\pm}(k'', \theta'', \varphi'')}{k^2 - k''^2 + \mathrm{i}0}. \tag{16}$$

Using the Cauchy principal-value (PV) formulae for the singular integral in equation (16) we have

$$\begin{aligned} T^{\pm}(k', \theta', \varphi') = {} & V^{\pm}(k', \theta', \varphi'; k, 0, 0) + \mathrm{PV} \int_0^{\infty} \frac{\mathrm{d}k''}{k - k''} \int_{-\pi}^{\pi} \mathrm{d}\theta'' \int_0^{2\pi} \mathrm{d}\phi'' \\ & \times K^{\pm}(k', \theta', \varphi'; k'', \theta'', \varphi'') T^{\pm}(k'', \theta'', \varphi'') \\ & - \mathrm{i}\pi \int_{-\pi}^{\pi} \mathrm{d}\theta'' \int_0^{2\pi} \mathrm{d}\phi'' K^{\pm}(k, \theta', \varphi'; k, \theta'', \varphi'') T^{\pm}(k, \theta'', \varphi''), \end{aligned} \tag{17}$$

where

$$K^{\pm}(k', \theta', \varphi'; k'', \theta'', \varphi'') = \frac{2k''^2 \sin\theta''}{(2\pi)^3} \frac{V^{\pm}(k', \theta', \varphi'; k'', \theta'', \varphi'')}{k + k''} \tag{18}$$

is the kernel of the equation. Integrals over variables φ and θ have been discretized using the standard Gauss–Legendre quadrature. For the principal-value integral over k-variable a composite mesh has been used. The mesh included a subquadrature consisting of an even number of Gauss–Legendre points, symmetrically distributed around the singular point. This subquadrature was designed to ensure high accuracy for the principal-value integral.

Applying the quadrature rules to equation (17) and evaluating the result at the mesh points we get

$$\begin{aligned} T^{\pm}\big(k_{i_k}, \theta_{i_\theta}, \varphi_{i_\varphi}\big) = {} & V^{\pm}\big(k_{i_k}, \theta_{i_\theta}, \varphi_{i_\varphi}; k_0, 0, 0\big) \\ & + \sum_{j_k=0}^{N_k} \sum_{j_\theta=1}^{N_\theta} \sum_{j_\varphi=1}^{N_\varphi} \tilde{K}^{\pm}\big(k_{i_k}, \theta_{i_\theta}, \varphi_{i_\varphi}; k_{j_k}, \theta_{j_\theta}, \varphi_{j_\varphi}\big) T^{\pm}\big(k_{j_k}, \theta_{j_\theta}, \varphi_{j_\varphi}\big), \end{aligned} \tag{19}$$

with

$$\begin{aligned} \tilde{K}^{\pm}\big(k_{i_k}, \theta_{i_\theta}, \varphi_{i_\varphi}; k_{j_k}, \theta_{j_\theta}, \varphi_{j_\varphi}\big) = {} & \big(\big(1 - \delta_{j_k 0}\big) - \mathrm{i}\pi\delta_{j_k 0}\big) w_{j_k} u_{j_\theta} v_{j_\varphi} \\ & \times K^{\pm}\big(k_{i_k}, \theta_{i_\theta}, \varphi_{i_\varphi}; k_{j_k}, \theta_{j_\theta}, \varphi_{j_\varphi}\big), \end{aligned} \tag{20}$$

where $k_{j_k}, \theta_{j_\theta}, \varphi_{j_\varphi}$ and $w_{j_k}, u_{j_\theta}, v_{j_\varphi}$ are the quadrature points and relevant weights, N_k, N_θ and N_φ are the number of points in the k, θ and φ quadratures, respectively. We assigned index 0 to the on-shell momentum and set $w_0 = 1$. Equation (19) is easily transformed to a standard matrix equation

$$(\mathbf{1} - \tilde{\boldsymbol{K}}^{\pm}) \cdot \boldsymbol{T}^{\pm} = \boldsymbol{V}^{\pm}, \tag{21}$$

where $\boldsymbol{V}^{\pm}$ and $\boldsymbol{T}^{\pm}$ are N-dimensional vectors and $\tilde{\boldsymbol{K}}^{\pm}$ is a $N \times N$ matrix with $N = (N_k + 1)N_\theta N_\varphi$. At all incident energies we used 24 points for φ and 18 for θ variable. Meanwhile k-grid for the principal-value integral required 32 points.

The partial-wave calculations were made using the K-matrix method. In solving the one-dimensional integral equations for K-matrix a composite k-grid similar to the one described

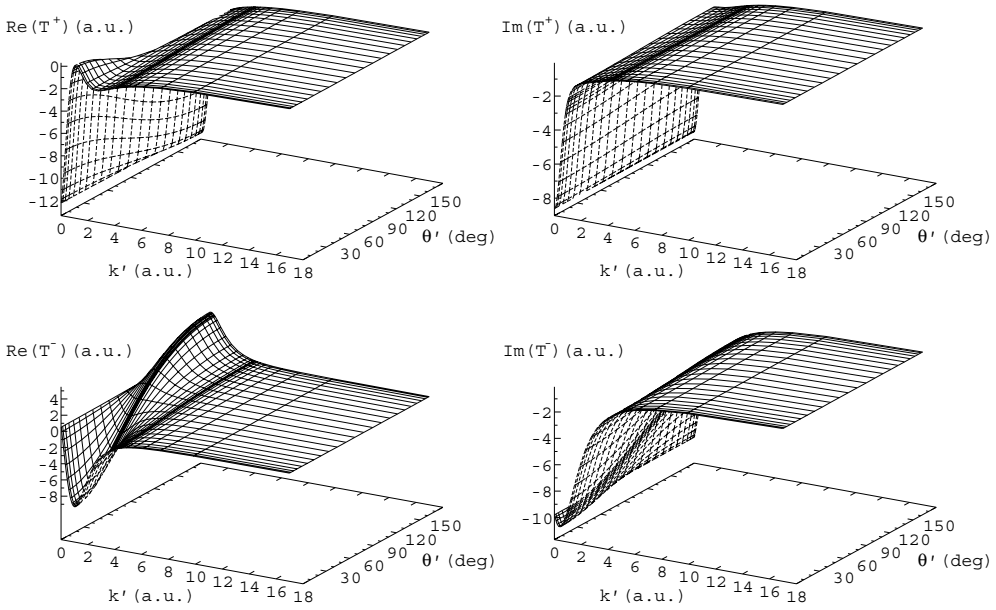

Figure 1. Singlet and triplet half-off-shell scattering amplitudes at 10 eV incident energy.

Table 1. Total cross section for elastic electron–hydrogen scattering within the static exchange approximation (au).

	0.1 eV	1 eV	10 eV	100 eV
Partial-wave	208.42	86.477	18.670	1.2044
Three-dimensional	208.40	86.475	18.671	1.2045

above has been used. At the highest energy the first 20 partial waves were taken into account explicitly. Further details on partial-wave calculations can be found in [4].

Figure 1 shows typical solutions of equation (16) obtained in three-dimensional calculations for singlet and triplet cases. The off-shell amplitudes $T^{\pm}(k', \theta', \varphi')$ shown in this figure correspond to the 10 eV incident energy. It is noteworthy that the method does not assume the rotational symmetry about the beam direction which is known but does reproduce that symmetry. Therefore, the final results do not depend on variable φ'. This is an important test of the method. The physical (on-shell) amplitudes and differential cross sections ($\mathrm{d}\sigma^{\pm}/\mathrm{d}\Omega = 1/(2\pi)^2|T^{\pm}|^2$) at the same energy are shown in figure 2 (curves) and compared with the corresponding partial-wave calculations (points). The spin-averaged differential cross section is also shown.

Table 1 shows the results for elastic electron–hydrogen scattering total (spin-averaged) cross section obtained in the partial-wave and three-dimensional calculations. Generally, we achieved 4 digit agreement between the partial-wave and three-dimensional results in a wide energy range. The agreement can be refined simply by increasing the quadrature points.

The presented results show that the Lippmann–Schwinger equations can be reliably solved in a three-dimensional quadrature without partial-wave expansion. Similar integral equations emerge also in the quasi-particle Alt–Grassberger–Sandhas (AGS) approach [3, 14] to the Faddeev equations. However, in this formalism the effective potentials (driving terms) are different and slightly more complicated. In the so-called unitarized Born approximation

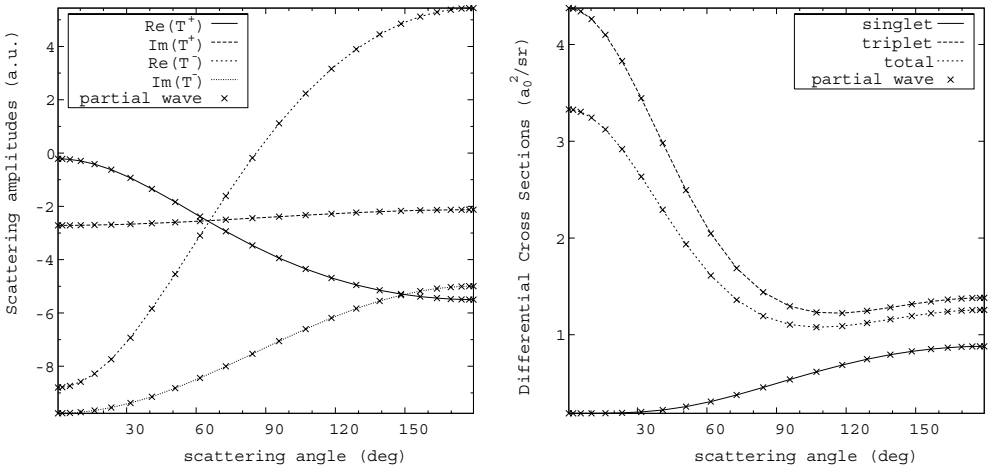

Figure 2. Scattering amplitudes and differential cross sections at 10 eV incident energy.

(the first-order K-matrix approach) the AGS and coupled-channel approaches coincide if in the former multiple-scattering terms are also neglected [9]. The calculations described in this work can be performed for the AGS equations as well by using the corresponding effective potentials. The conclusions drawn here are equally applicable to the AGS equations.

A similar direct approach has been suggested by Shertzer and Temkin [15]. However, they solve a two-dimensional integro-differential equation for the scattering wavefunction in configuration space using a finite element method. These authors were also able to reproduce the scattering amplitude for the static-exchange model, obtained from the partial-wave expansion approach to the corresponding coordinate space equation.

Summarizing, we solved three-dimensional momentum-space Lippmann–Schwinger equations directly without the partial-wave expansion. The results reproduce ones obtained with the partial-wave method indicating that with the power of today's computers direct solution of the three-dimensional integral equations for scattering can be a reliable alternative to the partial-wave expansion method. This conclusion is important for the theory of ion–atom and atom–atom collisions where the partial-wave expansion becomes inefficient. We are now in the process of extending this approach to such collisions.

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