

Fast and Efficient Solution of Scattering Integral Equations

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Abstract. In this work we propose a method for numerical treatment of integral equations describing scattering of low-energy electrons with atoms and molecules. The method is based on a combination of R-matrix approach with the Schwinger-Lanczos method proposed by the authors. It is shown on the example of scattering of electrons by hydrogen atoms in the static exchange approximation that the method is very fast, economic and very accurate. By using only 64 meshpoints the accuracy of 9 significant figures can be easily obtained.

Keywords: Numerical solution of integral equations, electron atom collisions

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INTRODUCTION

The scattering of electrons with atoms and molecules is in principle described by appropriate Schrödinger equation. This equation however contains "nonlocal", this means integral, terms. As a consequence the Schrödinger equation is no longer a differential equation but an integrodifferential equation. Because of the special boundary conditions describing scattering processes it is much more convenient to transform this integrodifferential equation into an Fredholm integral equation of the second type the so called Lipmann-Schwinger equation [1]. In the Dirac notation used in physics we can formulate it in the following way

$$|\phi\rangle = |u\rangle + G_0(E)(V+W)|\phi\rangle, \quad (1)$$

where $|u\rangle$ denotes the incident plane wave, $G_0(E)$ is the Green's function of the free particle's Hamiltonian defined as

$$G_0(E) = (E - H_0)^{-1},$$

V resp. W stands for the local resp. nonlocal part of the interaction under consideration and finally $|\phi\rangle$ represents the sought solution. Simple algebraic manipulations furnish another insight onto this equation. Explicitly written

$$|\phi\rangle = (1 - G_0(E)V)^{-1}|u\rangle + (1 - G_0(E)V)^{-1}G_0(E)W|\phi\rangle \equiv |\bar{u}\rangle + G(E)W|\phi\rangle, \quad (2)$$

where we have introduced the symbol $|\bar{u}\rangle$ for the "distorted" wave obeying an equation of the same structure as Eq. (1). Namely

$$|\bar{u}\rangle = |u\rangle + G_0(E)V|\bar{u}\rangle. \quad (3)$$

After solving Eq. (2), the quantity of principal interest is the matrix element $\langle u|V+W|\phi\rangle$, which is directly proportional to the tangent of the phase shift (proper normalisation condition on $|u\rangle$ is to be imposed). Simple algebra reveals, that this matrix element can be equivalently computed as $\langle u|V|\bar{u}\rangle + \langle \bar{u}|W|\phi\rangle$. The latter approach is more useful than the former because the second summand is naturally rendered as a byproduct of the Schwinger-Lanczos iterative algorithm described below.

RLS ALGORITHM

The proposed algorithm for solving Eq.(1) is based on a combination of two very distinct ideas: 1. R-matrix approach [3] used to construct the Green's function corresponding to the local part of the interaction, 2. the Schwinger-Lanczos approach proposed by the authors [4, 5] used for the treatment of nonlocal operators. Hereafter we will refer to this algorithm as the RLS algorithm.

The Green's function for the local part of the interaction V is taken in the form [3]

$$G(r, r', E) = \sum_n \frac{\Psi_n(r)\Psi_n(r')}{(E_n - E)} + \frac{A}{2(1 - A\mathcal{R})} \sum_{nm} \frac{\Psi_n(r_f)\Psi_m(r_f)\Psi_n(r)\Psi_m(r')}{(E_n - E)(E_m - E)}, \quad (4)$$

where

$$\mathcal{R} = \frac{1}{2} \sum_n \frac{\Psi_n(r_f)\Psi_n(r_f)}{(E_n - E)}, \quad (5)$$

$\Psi_n(r)$ are solutions of the R-matrix eigen-value problem

$$\tilde{K}\Psi_n(r) + \hat{V}\Psi_n(r) = E_n\Psi_n(r) \quad (6)$$

and A denotes the logarithmic derivative of the final solution at r_f . Here \tilde{K} is the symmetrized kinetic energy operator

$$\tilde{K}_{ij} = \frac{1}{2} \int_0^{r_f} \frac{d\Psi_i}{dx} \frac{d\Psi_j}{dx}, \quad (7)$$

where r_f (being presumably asymptotically large) represents the integration range.

The Schwinger-Lanczos method is based on the construction of Krylov basis set of vectors $|g_i\rangle$

$$\langle g_k | W | g_l \rangle = \delta_{kl} \quad (8)$$

chosen such that matrix WG_0W is tridiagonal

$$\langle g_{k-1} | WG_0W | g_k \rangle = \langle g_k | WG_0W | g_{k-1} \rangle = \beta_{k-1}, \quad (9)$$

$$\langle g_k | WG_0W | g_k \rangle = \alpha_k, \quad (10)$$

$$\langle g_k | WG_0W | g_l \rangle = 0 \quad \text{for } |k - l| \geq 2 \quad (11)$$

where W is the nonlocal part of the interaction [4]. This approach is very general and poses no restriction on the form of the nonlocality. This algorithm yields directly the nonlocal contribution to the final T -matrix in the form of a continued fraction [5]

$$T^N = \langle \bar{u} | W | g_1 \rangle (M^{-1})_{11} \langle g_1 | W | \bar{u} \rangle = \frac{\langle \bar{u} | W | \bar{u} \rangle}{1 - \alpha_1 - \frac{\beta_1^2}{1 - \alpha_2 - \frac{\beta_2^2}{1 - \alpha_3 - \dots - \frac{\beta_{N-1}^2}{1 - \alpha_N}}}}. \quad (12)$$

REFERENCE METHODS

In order to compare the numerical performance of the RLS approach with other methods we carried out calculations for four methods described in the literature:

- **S-IEM** is a spectral method for solving integral equation developed recently by G. H. Rawitscher et. al. Practical details can be found in [6, 7, 8].
- **M-IEM** is an iterative method originally introduced by B. T. Kim and T. Udagawa in [9]. Roughly speaking, the core of this method relies on utilising the Lanczos iterations for the complete LS equation.
- **N-IEM** stands for an older non iterative integral equation method based on the work by W. N. Sams and D. J. Kouri [10]. In principle, the final solution of the original one channel LS equation is expressed formally as a linear combination of two terms. The coefficients in this linear combination are profitably chosen (a linear set of two equations is to be solved to ensure this property) so that each of the two terms satisfies a Volterra integral equation of the second kind, which is then handled by standard means using e.g. trapezoidal quadrature rule.
- **MCFV** is an iterative method based on series of papers [11, 12, 13] by J. Horáček and T. Sasakawa. In this approach the local and nonlocal parts of the complete potential are also handled separately as in the RLS method. The Green's function is constructed in this case directly from the two independent solutions of the free Schrödinger equation. The implementation details can be found in [14].

NUMERICAL TESTS AND RESULTS

For the numerical test of the proposed algorithm we calculated the s-wave phase shift for scattering of electrons by ground-state hydrogen atoms in the static exchange approximation, both for the singlet $\delta^{(+)}$ and triplet $\delta^{(-)}$ state. We have chosen this model because similar calculations using different approaches (reference methods described above) can be found in the literature [7] offering the possibility to compare the results.

For the s-wave, the scattering problem reduces to solving an integral equation for the radial part of the corresponding partial wave. Namely

$$\left(\frac{d^2}{dr^2} + k^2\right)R_0(r) = V(r)R_0(r) \pm \int_0^\infty K(r,r')R_0(r')dr' \quad (13)$$

where

$$V(r) = -2re^{-2r} \left(1 + \frac{1}{r}\right) \quad (14)$$

$$K(r,r') = 2v(r)u(r') + \gamma u(r)u(r') \text{ for } r' < r \quad (15)$$

$$K(r,r') = 2u(r)v(r') + \gamma u(r)u(r') \text{ for } r' > r. \quad (16)$$

Here

$$u(r) = 2re^{-r}, \quad (17)$$

$$v(r) = \frac{u(r)}{r} = 2e^{-r} \quad (18)$$

and

$$\gamma = -k^2 - 1. \quad (19)$$

As we have already mentioned, our main goal is to compute the phase shift for the s-wave of the singlet as well as the triplet state. Since a relatively detailed study of the N-IEM method is found in [10], we tested the method presented in this paper for the same set of parameters. Results of the other mentioned methods for these parameters can be found in [7] and [14]. The case chosen is the singlet phase shift with exchange $\delta^{(+)}$. The wave number of the incident particle is $k = 0.2/a_0$, where a_0 is the Bohr radius ($a_0 = 1$ in atomic units), and the maximum radial distance (r_f , range of integration) is set to $20a_0$. As concerns the integration method used in the current implementation, we used the so called Clenshaw-Curtis quadrature, the details of which can be found e.g. in [2].

The results are summarised in Tab. 1 (typical number of sectors to obtain this accuracy was 4-5, while cca. 20 R-matrix basis functions per sector and 5-6 Lanczos iterations were needed), where the number of significant figures in the second column is determined from the stability of the phase shift value after rounding, when compared to the result corresponding to higher number of mesh points. It is seen that as few as 64 meshpoints yield the accuracy of at least 9 significant digits whereas the most recent approach of Rawitscher et al. [7] requires at least 80 digits to reach similar accuracy. Other methods require significantly larger number of meshpoints. Moreover, the RLS method is very advantageous in case when the calculation for more than one value of energy is required. The core of the calculation, the construction of the R-matrix basis, has to be done only once and then used for an arbitrary energy.

A more transparent overview of the convergence properties of these methods is depicted in Fig. (1), in which we are dealing with the "inverse" task, i.e. with determining the number of mesh points necessary to obtain a prescribed number of significant digits.

As can be seen from this picture, the proposed RLS method is very accurate even for very low number of mesh points. We believe, that it is primarily due to the accurate construction of the Green's function via the R-matrix approach. The problem of electron scattering with hydrogen atom in the static exchange approximation discussed here is in fact a very simple problem. The integral kernel is a real smooth non-oscillatory function with only one cusp. The problem of scattering of electrons with molecules is much more difficult. This will be discussed in a forthcoming paper.

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TABLE 1. Calculated phase shift $\delta^{(+)}$ for several reference methods. In the last column the number of mesh points used in the calculation is shown. Details are described below.

method	$\delta^{(+)}$	number of m.p.
RLS	1.87015788	64
S-IEM	1.8701579	80
MCFV	1.8701579	128
M-IEM	1.870156	4000
N-IEM	1.87015	4000

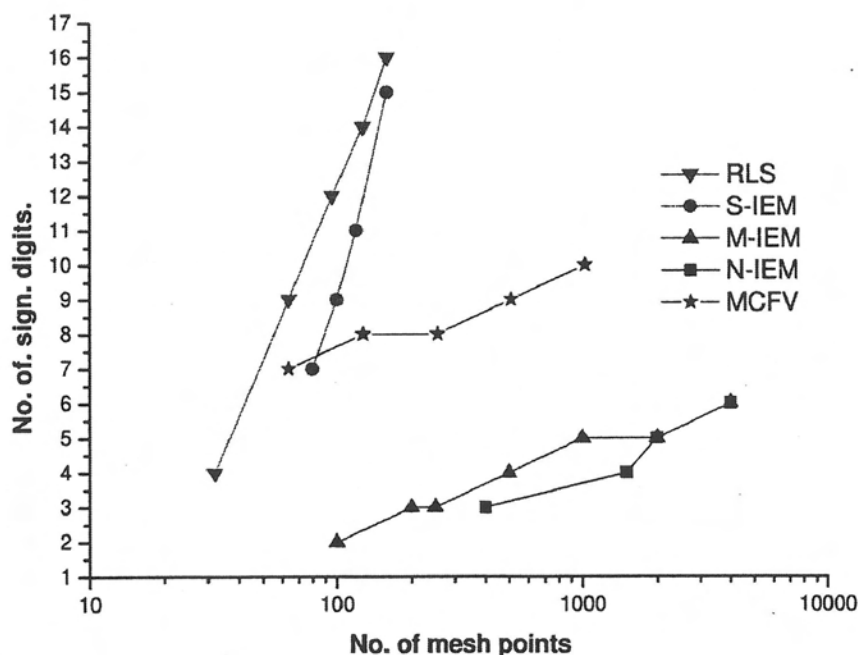


FIGURE 1. This figure shows the number of significant digits in the calculation of the triplet $\delta^{(+)}(k)$ phase shift as obtained by different methods.

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