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# Application of the J-matrix method to multichannel scattering

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**Abstract**

In this contribution we describe the multichannel extension to the nonrelativistic J-matrix method, and present differential cross sections for scattering of slow electrons from Argon atoms. Nonrelativistic phase shifts, then the S-matrix and the cross sections have been calculated using newly developed Fortran code, JMATRIX-MULTI. We applied the model Hartree-Fock potential as the scattering potential, which was truncated in the oscillatory basis functions.

## 1 Introduction

The J-matrix method is an algebraic method in quantum scattering theory. It is based on fact that the radial kinetic energy operator is tridiagonal in some suitable bases, so the physical scattering problem is replaced by well-defined model which is solved exactly. Non-relativistic version of the method was introduced in 1974 by Heller and Yamani [1], [2] and developed by Yamani and Fishman [3] in 1975. Relativistic version was introduced by Horodecki [4] and extended by Alhaidari *et al* [5]. Theoretical basis of the method is described in section 2.

The main task of the present work was to use the multichannel extension of the method to atomic calculations. The non-relativistic phase shifts obtained by the J-matrix method method are used to calculate inelastic differential cross sections of electron scattering by argon in its ground state at a few selected energies.

# 2 Theoretical method

## 2.1 The J-matrix method of scattering

In this section we give only a short review of the J-matrix theory of scattering, but it should be sufficient for understanding the main idea of the method. Detailed description of the method can be found in publications [1] – [6].

Our task is to find an approximate solution of the scattering problem on the radial potential $V = V(r)$ vanishing faster than the Coulomb one. Let us replace this scattering potential by a truncated potential operator:

$$V^N = P_N^\dagger V P_N \tag{1}$$

with the generalized projection operator

$$P_N = \sum_{n=0}^{N-1} \left|\phi_n^l\right\rangle \left\langle\phi_n^l\right|. \tag{2}$$

Then, using expansion of the solution of the new problem in the basis $\{\phi_n^l\}$, one can find that tangent of approximated phase shift is given by the formula

$$\tan\delta_N = -\frac{s_{N-1}^l(k) + g_{N-1,N-1}(\mathcal{E}) J_{N,N-1}(k) s_N^l(k)}{c_{N-1}^l(k) + g_{N-1,N-1}(\mathcal{E}) J_{N,N-1}(k) c_N^l(k)}, \tag{3}$$

where $s_n^l$ and $c_n^l$ are coefficients of sine-like and cosine-like solutions of the following equation

$$\left(H_0 - \frac{k^2}{2}\right) \sum_{n=0}^{\infty} u_n^l \phi_n^l(\lambda r) = \Omega_u \bar{\phi}_n^l(\lambda r), \tag{4}$$

where $H_0 - \frac{k^2}{2} \equiv -\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} - \frac{k^2}{2}$ is the radial kinetic energy operator; $u = s, c;\ \ \Omega_s = 0;\ \ \Omega_c = -\frac{k}{2s_0^l}$. $k \equiv \sqrt{\frac{2M\mathcal{E}}{\hbar^2}}$ is the wave number related to the energy $\mathcal{E}$ and mass $M$ of the projectile.

Basis set $\{\bar{\phi}_n^l\}$ is biorthonormal to set $\{\phi_n^l\}$ with respect to unitary scalar product, i.e. $\langle\bar{\phi}_m^l|\phi_n^l\rangle = \delta_{mn}$, where $\delta_{mn}$ is, as usual, Kronecker delta.

$J_{N,N-1}$ is an element of the following matrix

$$\begin{aligned} J_{mn} &\equiv \left\langle\phi_m^l\right| H_0 - \frac{k^2}{2} \left|\phi_n^l\right\rangle \equiv \\ &\equiv \left\langle\phi_m^l\right| -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{l(l+1)}{2r^2} - \frac{k^2}{2} \left|\phi_n^l\right\rangle. \end{aligned} \tag{5}$$

In some suitable bases, such as Gaussian, Laguerre (biorthonormal) or the complete oscillator set, the above matrix is tridiagonal (and is called Jacobi or J-matrix). This enables us to find coefficients $s_n^l$ and $c_n^l$, using three-term recursion relation between them and the J-matrix (see [2] for details). The explicit

| | Laguerre basis |
|---|---|
| $\phi_n^l$ | $(\lambda r)^{l+1}\exp\left(-\frac{\lambda r}{2}\right)L_n^{(2l+1)}(\lambda r)$ |
| $\bar{\phi}_n^l$ | $\frac{n!}{\lambda^2\Gamma(n+2l+2)}\frac{1}{r}\phi_n^l(\lambda r)$ |
| $s_n^l$ | $\frac{2^l\Gamma(l+1)n!(\sin\theta)^{l+1}}{\Gamma(n+2l+2)}C_n^{(l+1)}(\cos\theta)$ |
| $c_n^l$ | $\frac{-2^l\Gamma(l+\frac{1}{2})n!}{\sqrt{\pi}\Gamma(n+2l+2)(\sin\theta)^l}\ {}_2F_1\left(-n-2l-1,n+1,\frac{1}{2}-l;\sin^2\left(\frac{\theta}{2}\right)\right)$, $\sin\theta\equiv\frac{k\lambda^{-1}}{k^2\lambda^{-2}+\frac{1}{4}}$ |
| | Gaussian basis |
| $\phi_n^l$ | $(\lambda r)^{l+1}\exp\left(-\frac{\lambda^2r^2}{2}\right)L_n^{(l+\frac{1}{2})}(\lambda^2r^2)$ |
| $\bar{\phi}_n^l$ | $\frac{2n!}{\lambda^2\Gamma(n+l+\frac{3}{2})}\phi_n^l(\lambda r)$ |
| $s_n^l$ | $\frac{\sqrt{2\pi}n!(-1)^n}{\Gamma(n+l+\frac{3}{2})}\exp\left(-\frac{\eta^2}{2}\right)\eta^{l+1}L_n^{(l+\frac{1}{2})}(\eta^2)$ |
| $c_n^l$ | $\frac{\sqrt{\frac{2}{\pi}}\Gamma\left(l+\frac{1}{2}\right)(-1)^n n!}{\Gamma(n+l+\frac{3}{2})}\exp\left(-\frac{\eta^2}{2}\right)\eta^{-l}\ {}_1F_1\left(-n-l-\frac{1}{2},\frac{1}{2}-l;\eta^2\right),\ \ \eta\equiv\frac{k}{\lambda}$ |
| | Oscillator basis |
| $\phi_n^l$ | $r(-1)^n\sqrt{\frac{2n!\lambda^3}{\Gamma(n+l+3/2)}}(\lambda r)^l\exp\left(-\frac{\lambda^2r^2}{2}\right)L_n^{(l+1/2)}\left(\lambda^2r^2\right)$ |
| $s_n^l$ | $\sqrt{\frac{\pi n!}{\lambda k\Gamma(n+l+\frac{3}{2})}}\left(\frac{k}{\lambda}\right)^{l+1}\exp\left(-\frac{k^2}{2\lambda^2}\right)\right)L_n^{(l+\frac{1}{2})}\left(\frac{k^2}{\lambda^2}\right)$ |
| $c_n^l$ | $\frac{-1^l}{\Gamma(-l+\frac{1}{2})}\sqrt{\frac{\pi n!}{\lambda k\Gamma(n+l+\frac{3}{2})}}\left(\frac{k}{\lambda}\right)^{-l}\exp\left(-\frac{k^2}{2\lambda^2}\right)\right)\ {}_1F_1\left(-n-l-\frac{1}{2},\frac{1}{2}-l,\frac{k^2}{\lambda^2}\right)$ |

Table 1: Elements of Laguerre, Gaussian (biorthonormal) and oscillator (complete) basis set and elements of expansion of sine-like and cosine-like solutions. $L_n^{(\alpha)}$ and $C_n^{(\alpha)}$ are Laguerre and Gegenbauer polynomials, respectively; ${}_2F_1$ and ${}_1F_1$ are hypergeometric functions, $\lambda>0$ is a scaling parameter ($\lambda\neq 0.5$).

forms of these coefficients as well as elements of basis sets are collected in Table 1.

In above formulas, $N$ is the number of base functions $\phi_n^l$ used to truncate scattering potential, $g_{N-1,N-1}(\mathcal{E})$ is a matrix element of the inverse of the truncated operator $P_N^\dagger\left(H_0+V^N-\frac{k^2}{2}\right)P_N$, restricted to the $N$-dimensional space, where it doesn't vanish. In short, this matrix can be viewed as the matrix approximating the Green function.

For $N\to\infty$, what is connected with reduction of inaccuracy in approximating of the scattering potential, $\tan\delta_N$ should converge to the exact value $\tan\delta$, and, simultaneously, approximate $\delta_N$ should approach the exact scattering phase, $\delta$.

Once we have calculated the phase shifts for different angular momenta $l$, we are ready to employ partial-wave analysis, and calculate non-relativistic cross sections. Formulas for the cross sections can be found elsewhere, i.e. in [8].

# 3 Multichannel extension

## 3.1 Elements of the S-matrix

The elements of the S-matrix (which allows for calculations of cross sections for different channel configurations) are given as follows [7]:

$$S_{\alpha\beta}(E) = T_{N_\alpha}\delta_{\alpha\beta} - \sqrt{\frac{J^{(\alpha)}_{N_\alpha-1,N_\alpha}}{J^{(\beta)}_{N_\beta-1,N_\beta}}\frac{R_\alpha}{R_\beta}}\times \tag{6}$$

$$\sqrt{T_{N_\alpha-1} - T_{N_\alpha}}\sqrt{\frac{D^{(+)}_{\alpha\beta}(E)}{\Delta^{(+)}(E)}}\sqrt{T_{N_\beta-1} - T_{N_\beta}}, \tag{7}$$

where $\alpha$ and $\beta$ denotes initial and final channels, respectively. If we put $\alpha = \beta$, we can obtain [7]:

$$S_{\alpha\beta}(E) = T_{N_\alpha} - (T_{N_\alpha-1} - T_{N_\alpha})\sqrt{\frac{D^{(+)}_{\alpha\beta}(E)}{\Delta^{(+)}(E)}}. \tag{8}$$

In the above equations

$$\Delta^{(+)}(E) = \begin{vmatrix} (1-Y_{1,1}) & -Y_{1,2} & \dots & -Y_{1,M} \\ -Y_{2,1} & (1-Y_{2,2}) & \dots & -Y_{2,M} \\ \dots & \dots & \dots & \dots \\ -Y_{M,1} & -Y_{M,2} & \dots & (1-Y_{M,M}) \end{vmatrix},$$

and

$$D^{(+)}_{\alpha\beta}(E) = \begin{vmatrix} 0 & \delta_{\alpha,1} & \delta_{\alpha,2} & \dots & \delta_{\alpha,M} \\ \delta_{1,\beta} & & & & \\ \delta_{2,\beta} & & \Delta^{(+)}(E) & & \\ \dots & & & & \\ \delta_{M,\beta} & & & & \end{vmatrix},$$

where, in turn,

$$Y_{\alpha\beta} = -g^{(\alpha,\beta)}_{N_\alpha-1,N_\beta-1}J^{(\beta)}_{N_\beta-1,N_\beta}R^{+}_{N_\beta}. \tag{9}$$

The function $g$ is dependent on the selected basis, so we need to find the eigensystem of the full Hamiltonian to calculate this function. For oscillatory basis set we obtain:

$$g^{(\alpha,\beta)}_{N_\alpha-1,N_\beta-1}(E) = \sum_{\mu=1}^{N_c}\frac{\Lambda^{(\alpha)}_{N_\alpha-1,\mu}\Lambda^{(\beta)}_{N_\beta-1,\mu}}{E_\mu - E}, \tag{10}$$

where $E_\mu$ are the eigenvalues of the full Hamiltonian, and

$$\left(\Lambda^{(1)}_{0,\mu}, \Lambda^{(1)}_{1,\mu}, \dots, \Lambda^{(1)}_{N_1-1,\mu}, \Lambda^{(2)}_{0,\mu}, \dots, \Lambda^{(2)}_{N_2-1,\mu}, \dots, \Lambda^{(M)}_{0,\mu}, \dots, \Lambda^{(M)}_{N_M-1,\mu}\right)$$

is the eigenvector.

J-matrix elements are written in the form (in oscillatory basis):

$$J_{n,n} = (2n + l + 3/2)(\lambda^2/2) - (E - E_\alpha),$$
$$J_{n,n-1} = \sqrt{n(n + l + 1/2)}(\lambda^2/2).$$

Let's now define:

$$u_n = -J_{n,n}/J_{n,n-1}, \quad v_n = -J_{n,n-1}/J_{n,n+1}, \tag{11}$$

so the coefficients $R_N^{\pm}(E)$ and $T_{N-1}(E)$ are given as

$$R_{n+1}^{\pm} = u_n + \frac{v_n}{R_n^{\pm}} \quad (n \geq 1),$$
$$T_n = T_0 \left( \prod_{j+1}^{n} \frac{R_j^-}{R_j^+} \right).$$

They are given in recurrence form, with initial terms:

$$R_1^{\pm} = (c_1 \pm is_1)/(c_0 \pm is_0), \; T_0 = (c_0 - is_1)/(c_0 + is_0). \tag{12}$$

### 3.2 Hartree-Fock potential for Argon

The general formula for scattering potential is as follows [9]:

$$V(r) = -Ze^2 r^{-1} Z_p/Z. \tag{13}$$

For Argon, the index $m = 2$, with screening factor:

$$Z_p/Z = \sum_i^2 {}^a\gamma_i \exp^{-{}^a\lambda_i r} + r \sum_j^m {}^b\gamma_j \exp^{-{}^b\lambda_j r}, \tag{14}$$

where:

- $r$ is a distance from atom,
- $Z_p$ is a effective atomic number for HF potential,
- $Z$ is atomic number
- ${}^a\gamma_i$, ${}^a\lambda_i$, ${}^b\gamma_j$ i ${}^b\lambda_j$ are given in Table 2.

## 4 Results and discussion

To test the multichannel extension of the J-matrix method, we have applied the derived multichannel formulas to the case of one-channel scattering, for two selected energies of incident electron. Results are presented on Fig. 1 and Fig. 2. All the calculations have been performed by using the newly

| constant | value |
|---|---|
| ${}^a\lambda_1$ | 2.0636 |
| ${}^a\lambda_2$ | 32.485 |
| ${}^b\lambda_1$ | 4.853 |
| ${}^b\lambda_2$ | 19.772 |
| ${}^a\gamma_1$ | $1 - {}^a\gamma_2 = 1.3740$ |
| ${}^a\gamma_2$ | $-0.3740$ |
| ${}^b\gamma_1$ | $-4.2960$ |
| ${}^b\gamma_2$ | $-8.916$ |

Table 2: Constants for HF potential for Argon [9].

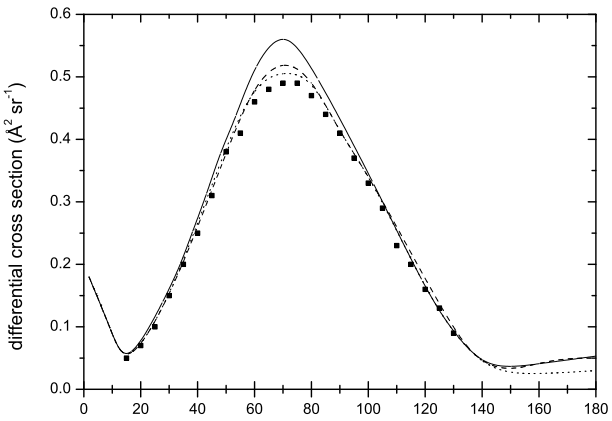


Figure 1: Differential cross sections versus scattering angle. Solid line: current results, full squares: experimental results of Gibson *et al* [11], dashed line: McEachran and Stauffer [12] (relativistic polarized-orbital method), dotted line: Syty and Sienkiewicz [13] (CI-MCDF).

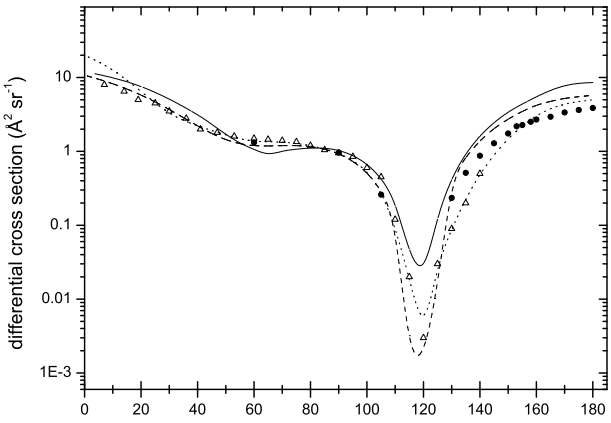


Figure 2: Differential cross sections versus scattering angle. Solid line: current results, full circles: experimental results of Mielewska [14], empty triangles: experimental results of Furst *et al* [15], dashed line: Plenkiewicz *et al* [16] (pseudopotential approach), dotted line: Syty and Sienkiewicz [13] (CI-MCDF).

developed JMATRIX-MULTI program [10]. It allows for multichannel calculations of numerical phase shifts for a wide range of energies, then uses standard partial-waves analysis to calculate cross sections. Program implements both non-relativistic and relativistic J-matrix method and is suitable to study the non-relativistic limit in relativistic calculations.

Our test results show both the limitations and advantages of the multichannel J-matrix method. The main computational problem is to achieve the proper convergence of the phase shifts – it is connected with increasing of the numerical errors while increasing the basis sets used to truncate the scattering potential. Bearing in mind these convergence problems, the results are in a surprisingly well agreement with other theoretical and experimental data. It was because we have used relatively large basis set ($N = 2000$) to minimize the computational errors.

The main advantage of the method is that we are able to calculate phase shifts and cross sections for wide energy range, with relatively small computational effort. This is because we need to truncate the scattering potental only once, and this is the most time-consuming part of the J-matrix calculations. This is a very important progress comparing e.g. to the multiconfiguration Hartree(Dirac)-Fock method, where calculations for each different energy of incident electrons require large-scale, thus time-consuming calculations (detailed study is given i.e. in [17]).

# 5 Acknowledgements

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