# THE J–MATRIX METHOD: NUMERICAL COMPUTATIONS

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**Abstract:** Numerical calculations of scattering phase shifts have been done using J–matrix method (both non–relativistic and relativistic versions). Results of computations for some simple potentials are described and discussed in this paper. In particular, it has been shown, that successive numerical approximations converge to results obtained using an analytical formula.

**Keywords:** atomic physics, scattering theory, J–matrix method, numerical computations

## 1. Introduction

The J–matrix method is an algebraic method in quantum scattering theory. It bases on the fact that the radial kinetic energy operator is tridiagonal in some suitable bases. Non–relativistic version of the method was introduced in1974 by Heller and Yamani [1], [2] and developed by Yamani and Fishman [3] a year later. The relativistic version was introduced in 1998 by P. Horodecki [4]. Theoretical basis of the method is described in Section 1. The aim of this paper is to check if the method properly describes the scattering problem on square–well potentials. Preliminary computations which have been introduced in [5], are extended and completed. The results are presented and described in Section 2 of the present paper. Computations have been performed using Fortran 90 programming language and compiler.

## 2. J–matrix method — theory

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

$$V^N = P_N^\dagger V P_N$$

with the generalized projection operator

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

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

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

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

$$\left(H_0 - \frac{k^2}{2}\right)\sum_{n=0}^{\infty} u_n^l \phi_n^l(\lambda r) = \Omega_u \bar{\phi}_n^l(\lambda r); \quad u = s, c; \quad \Omega_u = 0; \quad \Omega_c = -\frac{k}{2s_0^l}.$$

Here, $k \equiv \sqrt{\frac{2m\mathcal{E}}{\hbar^2}}$ the wave number related to the energy $\mathcal{E}$ and mass $m$ of the projectile. The basis set $\{\bar{\phi}_n^l\}$ is biorthonormal to set $\{\phi_n^l\}$ with respect to unitary scalar product, i.e. $\langle \bar{\phi}_m^l | \phi_n^l \rangle = \delta_{mn}$.

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

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

In some suitable bases, such as the Gaussian or Laguerre set, the above matrix is tridiagonal (and is called Jacobi or J–matrix). This enables one to find the 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 forms of these coefficients and elements of basis sets are collected in Table I.

$N$ is the number of the 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 $P_N^{\dagger}\left(H_0 + V^N - k^2/2\right)P_N$ restricted to the $N$–dimensional space, where it doesn't vanish. For $N \to \infty$, what is connected with reduction of the approximation error of the potential, $\delta_N$ should converge to the exact value.

In the relativistic case we have a very similar formula for tangent of the approximated phase shift:

$$\tan\tilde{\delta}_N = -\frac{s_{N-1}^l(\tilde{k}) + 2\varepsilon/\tilde{k} G_{N-1,N-1}^{++}(E) J_{N,N-1}(\tilde{k}) s_N^l(\tilde{k})}{c_{N-1}^l(\tilde{k}) + 2\varepsilon/\tilde{k} G_{N-1,N-1}^{++}(E) J_{N,N-1}(\tilde{k}) c_N^l(\tilde{k})}$$

Here, we have the same coefficients of the expansion and the elements of the J–matrix as in the non–relativistic case, but taken with the relativistic number $\tilde{k} \equiv \sqrt{(E - mc^2)(E + mc^2)}/c\hbar$, related to the total energy $E = \mathcal{E} + mc^2$. For the de-

tailed explanation of the symbol $G^{++}_{N-1,N-1}$ see [4]. As in the non–relativistic case, it can be viewed as a matrix element of the inverse of some truncated operator, but here restricted to the $2N$–dimensional space. To complete the definitions, $\varepsilon \equiv \sqrt{\frac{E-mc^2}{E+mc^2}}$.

## 3. Numerical computations

One can expect, that, approximate phase shift converges to the exact value for $N \to \infty$. The main task of the present work is to study this convergence by calculations of the phase shifts for some simple potentials and comparison with analytical results. To execute this task, the author wrote a computer program in Fortran 90, which computes all the needed quantities (such as the Gegenbauer and Laguerre polynomials, hypergeometric functions, Bessel, spherical Bessel, Neumann and spherical Neumann functions and their derivatives, Gamma function and more) to evaluate the basis functions $\phi_n^l$ and the coefficients $s_n^l$ and $c_n^l$. Moreover, the program truncates the scattering potential in the selected basis by numerical inte-gration, inverses the matrix by diagonalisation (using some orthogonal matrix) and finally, computes approximate phase shift for the given number N. To check if the results are correct, an additional procedure has been written to calculate the phase shifts using an analytical formula for potentials with shape of a potential well.

Most of the procedures and functions in the program have been written by the author using [6] and [7], but some (Bessel, Neumann and Gamma functions, numerical integration and searching for eigenvalues and eigenvectors of real, symmetric matrix) have been taken from the free Fortran 77 libraries and rewritten in Fortran 90.

The author has been faced with the following difficulties during his work:

1. Numerical instability for $N > 50$. This problem is connected with the properties of hypergeometric functions. It is difficult to count these functions, especially for big arguments. To avoid this problem, coefficients $s_n^l$ and $c_n^l$ for small $N$ have been calculated using explicit formulas contained in Table I, but for $N > 50$ using three–term recursion relation (see [2]).
2. Factorial and Gamma function for big arguments (see Table I). These functions have been replaced by their logarithms.
3. Long time of the computations. There are many integrals to be calculated, especially in the relativistic case. They are used to truncate the potential. To minimize their quantities, the author utilized symmetry of the J–matrix, integrals calculated in the previous step and specific shape of the potential (square–well).

Program has been compiled using AIX Fortran Compiler and run on the IBM SP/2 machine at the TASK Computer Center in Gdansk. Calculations have been performed for various sets of parameters. The results for two sets of parameters are

***Table I.*** *Elements of the Laguerre and Gaussian basis sets and elements of expansion of sine–like and cosine–like solutions in these bases. $L_n^{(\omega)}$ and $C_n^{(\omega)}$ are Laguerre and Gegenbauer polynomials, respectively. ${}_2F_1$ and ${}_1F_1$ are hypergeometric functions, $\lambda > 0$ is a scaling parameter ($\lambda \neq 0.5$)*

| | ***Laguerre set*** | ***Gaussian set*** |
|---|---|---|
| $\phi_n^l$ | $(\lambda r)^{l+1}\exp\left(-\frac{\lambda r}{2}\right)L_n^{(2l+1)}(\lambda r)$ | $(\lambda r)^{l+1}\exp\left(-\frac{\lambda^2 r^2}{2}\right)L_n^{(l+\frac{1}{2})}(\lambda^2 r^2)$ |
| $\bar{\phi}_n^l$ | $\frac{n!}{\lambda^2\Gamma(n+2l+2)}\frac{1}{r}\phi_n^l(\lambda r)$ | $\frac{n!}{\lambda^2\Gamma(n+l+\frac{3}{2})}\phi_n^l(\lambda r)$ |
| $s_n^l$ | $\frac{2^l\Gamma(l+1)n!(\sin\theta)^{l+1}}{\Gamma(n+2l+2)}C_n^{(l+1)}(\cos\theta)$ | $\frac{\sqrt{2\pi}\,n!(-1)^n}{\Gamma(n+l+\frac{3}{2})}\exp\left(-\frac{\eta^2}{2}\right)\eta^{l+1}L_n^{(l+\frac{1}{2})}(\eta^2)$ |
| $c_n^l$ | $\frac{-2^l\Gamma(l+\frac{1}{2})n!}{\sqrt{\pi}\,\Gamma(n+2l+2)(\sin\theta)^l}$ $x_2F_1\left(-n-2l-1,n+1,\frac{1}{2}-l;\sin^2\left(\frac{\theta}{2}\right)\right)$ | $\frac{\sqrt{\frac{2}{\pi}}\,\Gamma(l+\frac{1}{2})(-1)^n n!}{\Gamma(n+l+\frac{3}{2})}\exp\left(-\frac{\eta^2}{2}\right)\eta^{-l}$ $x_1F_1\left(-n-l-\frac{1}{2},\frac{1}{2}-l;\eta^2\right)$ |
| | $\sin\theta\equiv\frac{k\lambda^{-1}}{k^2\lambda^{-2}+\frac{1}{4}};\cos\theta\equiv\frac{k^2\lambda^{-2}-\frac{1}{4}}{k^2\lambda^{-2}+\frac{1}{4}}$ | $\eta\equiv\frac{k}{\lambda}$ |

presented in this paper. The results for these two sets have been obtained using relativistic scheme with parameters of the scattering potential, quantum numbers, energy of projectile and basis given in Table II.

In Figures 1 and 2 we have results for the first set of parameters, whereas in Figures 3 and 4 — for the second set. Analysing Figures 1–4 it is easy to notice that the convergence in the Laguerre basis set has completely different nature if compared to convergence in the Gaussian set. The convergence in set is faster, but there are some intervals with unexpected behaviour–systematic (though little) increase of the distance between the expected and the obtained results. The

***Table II.*** *Parameters of the scattering potential, quantum numbers, energy of projectile and basis used in the calculations*

| ***parameter*** | ***set 1*** | ***set 2*** |
|---|---|---|
| depth of potential well | –1.0 [au] | –1.5 [au] |
| left bound of potential well | 1.0 [au] | 1.0 [au] |
| right bound of potential well | 1.2 [au] | 1.5 [au] |
| energy of projectile | 5.0 [Hartree] | 2.5 [Hartree] |
| quantum numbers of projectile | $l = 2$, $\kappa = -3$ | $l = 1$, $\kappa = -2$ |
| scaling parameter ($\lambda$) | 1.0 | 1.0 |
| initial value of $N$ | 1 | 250 |
| final value of $N$ | 1 | 230 |

convergence in the Laguerre set is more stable and regular. However, in general, in both the investigated cases it is not difficult to see that phase shifts computed numerically converge to the phase shift obtained using an analytical formula, marked in Figures by the straight line.

Some numerical results are presented in Table III. They have been selected as we have *the biggest* deviations from the analytical results for them.

Some computations using the non–relativistic method have also been done. There is no need to present them here in detail, because both the results and the

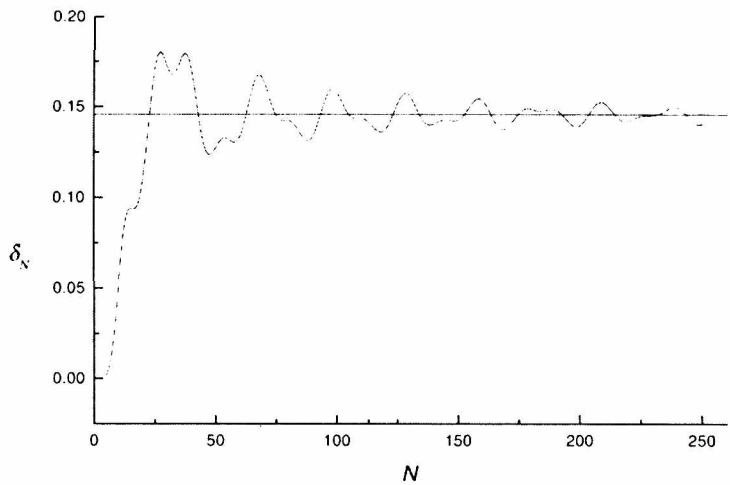


***Figure 1.*** *Convergence of the phase shift versus the number of Laguerre basis function N used to truncate the scattering potential for the first set of parameters*

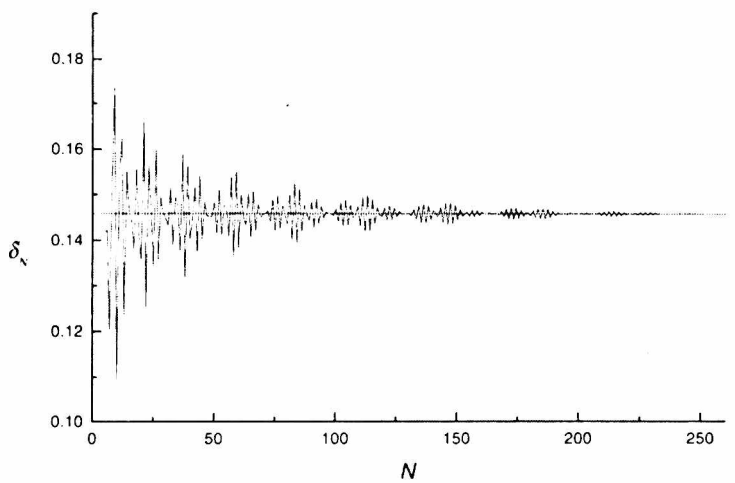


***Figure 2.*** *Convergence of the phase shift versus the number of Gaussian basis function N used to truncate the scattering potential for the first set of parameters*

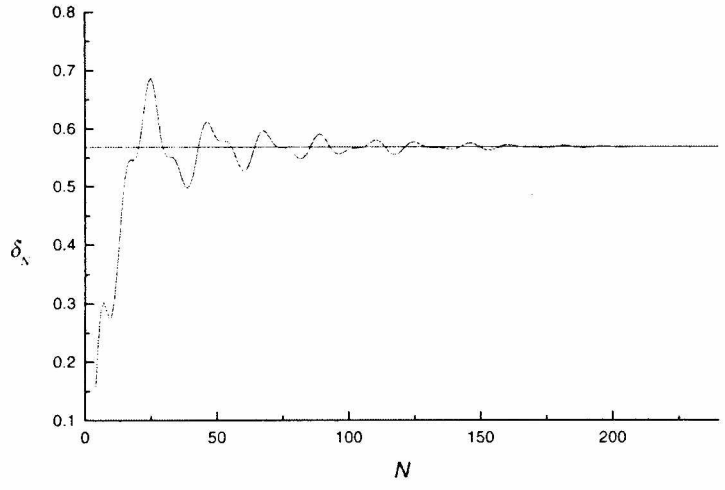


***Figure 3.*** *Same as Figure 1, the second set of parameters*

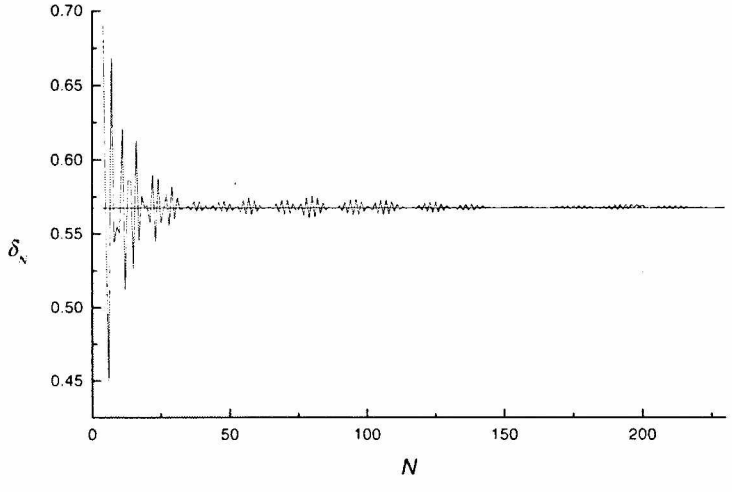


***Figure 4.*** *Same as Figure 2, the second set of parameters*

nature of convergence obtained using relativistic and non–relativistic schemes are very similar. Moreover, it has been verified that the relativistic results converge to the non–relativistic limit as the speed of light approaches infinity. This fact was expected as the basis sets used in relativistic calculations satisfy so called kinetic balance condition (see [4] and references therein).

## 4.Conclusions

For the first time, the numerical computations of scattering phase shifts using a relativistic version of the J–matrix method have been performed. The results presented and discussed in this paper indicate that the method properly describes the scattering problem on the square–well potentials.

***Table IIIa.*** *Selected values of N and* $\widetilde{\delta}_N$ *with* ***the biggest*** *deviations from the analytical result* ($\widetilde{\delta}_N$ = 0.145873580427407 *[rad]*, $\Delta = |\widetilde{\delta}_N - \widetilde{\delta}|$). *The first set of parameters*

| ***Laguerre set*** | | | ***Gaussian set*** | | |
|---|---|---|---|---|---|
| $N$ | $\widetilde{\delta}_N$ [rad] | $\Delta$ [rad] | $N$ | $\widetilde{\delta}_N$ [rad] | $\Delta$ [rad] |
| 27 | 0.180116968924908 | $3.42E-2$ | 22 | 0.125326918382050 | $2.05E-2$ |
| 68 | 0.167500450016762 | $2.16E-2$ | 58 | 0.136310080222280 | $9.56E-3$ |
| 98 | 0.159852856829423 | $1.39E-2$ | 84 | 0.139518247283100 | $6.35E-3$ |
| 128 | 0.157467517312117 | $1.15E-2$ | 114 | 0.141995122583362 | $3.87E-3$ |
| 158 | 0.154452733003588 | $8.57E-3$ | 148 | 0.143636098164198 | $2.23E-3$ |
| 208 | 0.152525948826599 | $6.65E-3$ | 173 | 0.144593474760792 | $1.28E-3$ |
| 238 | 0.149877031960159 | $4.00E-3$ | 215 | 0.145327120893617 | $5.46E-4$ |

***Table IIIb.*** *Selected values of N and* $\widetilde{\delta}_N$ *with* ***the biggest*** *deviations from the analytical result* ($\widetilde{\delta}_N$ = 0.567566818088086 *[rad]*, $\Delta = |\widetilde{\delta}_N - \widetilde{\delta}|$). *The second set of parameters*

| ***Laguerre set*** | | | ***Gaussian set*** | | |
|---|---|---|---|---|---|
| $N$ | $\widetilde{\delta}_N$ [rad] | $\Delta$ [rad] | $N$ | $\widetilde{\delta}_N$ [rad] | $\Delta$ [rad] |
| 25 | 0.687042152693040 | $1.19E-1$ | 24 | 0.587827932939388 | $2.02E-2$ |
| 46 | 0.611692202423948 | $4.41E-2$ | 57 | 0.574352289141600 | $6.78E-3$ |
| 68 | 0.595916896485416 | $2.83E-2$ | 80 | 0.575660438081612 | $8.09E-3$ |
| 89 | 0.590288836859340 | $2.27E-2$ | 107 | 0.572959922365968 | $5.39E-3$ |
| 110 | 0.579004291590615 | $1.14E-2$ | 138 | 0.569993342445206 | $2.23E-3$ |
| 146 | 0.574252933464510 | $6.68E-3$ | 194 | 0.569957348652832 | $1.28E-3$ |
| 196 | 0.569042211762838 | $1.47E-3$ | 212 | 0.568910508862311 | $5.46E-3$ |

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