The relativistic J-matrix method: theory and numerical computations

P. Syty[1], P. Horodecki and J. E. Sienkiewicz
Katedra Fizyki Teoretycznej i Metod Matematycznych
Politechnika Gdańska, ul. Narutowicza 11/12, 80-952 Gdańsk, Poland
[1] *e-mail: sylas@task.gda.pl*

Abstract

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. Non-relativistic version of the method was introduced in 1974 by Heller and Yamani and developed by Yamani and Fishman a year after. Relativistic version was introduced in 1998 by P. Horodecki. For a first time numerical calculations of scattering phase shifts have been done using relativistic version of the J-matrix method. Here, we introduce results of computations performed for square-type potential. Adequate computations have been performed using Fortran 90 programming language and compiler.

What is the J-matrix method?

The main 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:

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

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 that tangent of approximated phase shift is given by the formula:

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

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

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

Here, $k \equiv \sqrt{\frac{2m\mathcal{E}}{\hbar^2}}$ 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. $\left\langle\bar{\phi}_m^l|\phi_n^l\right\rangle = \delta_{mn}$.

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

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

In some suitable bases, such as Gaussian or Laguerre 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.

N is the quantity of base functions ϕ_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. When $N \to \infty$, what is connected with reduction of the approximation error of the potential, δ_N should converge to the exact value.

The relativistic case

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

$$\tan\tilde{\delta}_N = -\frac{s_{N-1}^l(\tilde{k}) + \frac{2\epsilon}{k}\mathcal{G}_{N-1,N-1}^{++}(E) J_{N,N-1}(\tilde{k}) s_N^l(\tilde{k})}{c_{N-1}^l(\tilde{k}) + \frac{2\epsilon}{k}\mathcal{G}_{N-1,N-1}^{++}(E) J_{N,N-1}(\tilde{k}) c_N^l(\tilde{k})}.$$

Here, we have the same coefficients of the expansion and J-matrix element as in the non-relativistic case, only taken with the relativistic number $\tilde{k} \equiv \frac{\sqrt{(E-mc^2)(E+mc^2)}}{c\hbar}$, related to the total energy $E = \mathcal{E} + mc^2$. See [4] for detailed explanation of the symbol $\mathcal{G}_{N-1,N-1}^{++}$. As in the non-relativistic case, it can be viewed as a matrix element of the inverse of some trucated operator, but here restricted to the $2N$-dimensional space. To complete definitions, $\epsilon \equiv \sqrt{\frac{E-mc^2}{E+mc^2}}$. When $c \to \infty$, the relativistic formula for $\tan\tilde{\delta}_N$ converges to the non-relativistic one.

The model

Let's consider spherically symmetric potential $V(r)$ defined by the square-well with respect to the radial coordinate:

$$V(r) = \begin{cases} 0 & \text{for } r \in (0, a) \\ V_0 & \text{for } r \in [a, b) \\ 0 & \text{for } r \in [b, \infty) \end{cases} .$$

The analytical formula for tangent of the phase shift can be simply found to be

$$\tan \delta = \frac{B}{A}.$$

The numbers A, B (depending on the energy of the projectile, the relativistic number κ, and parameters of the potential) can be defined as coordinates of the following vector

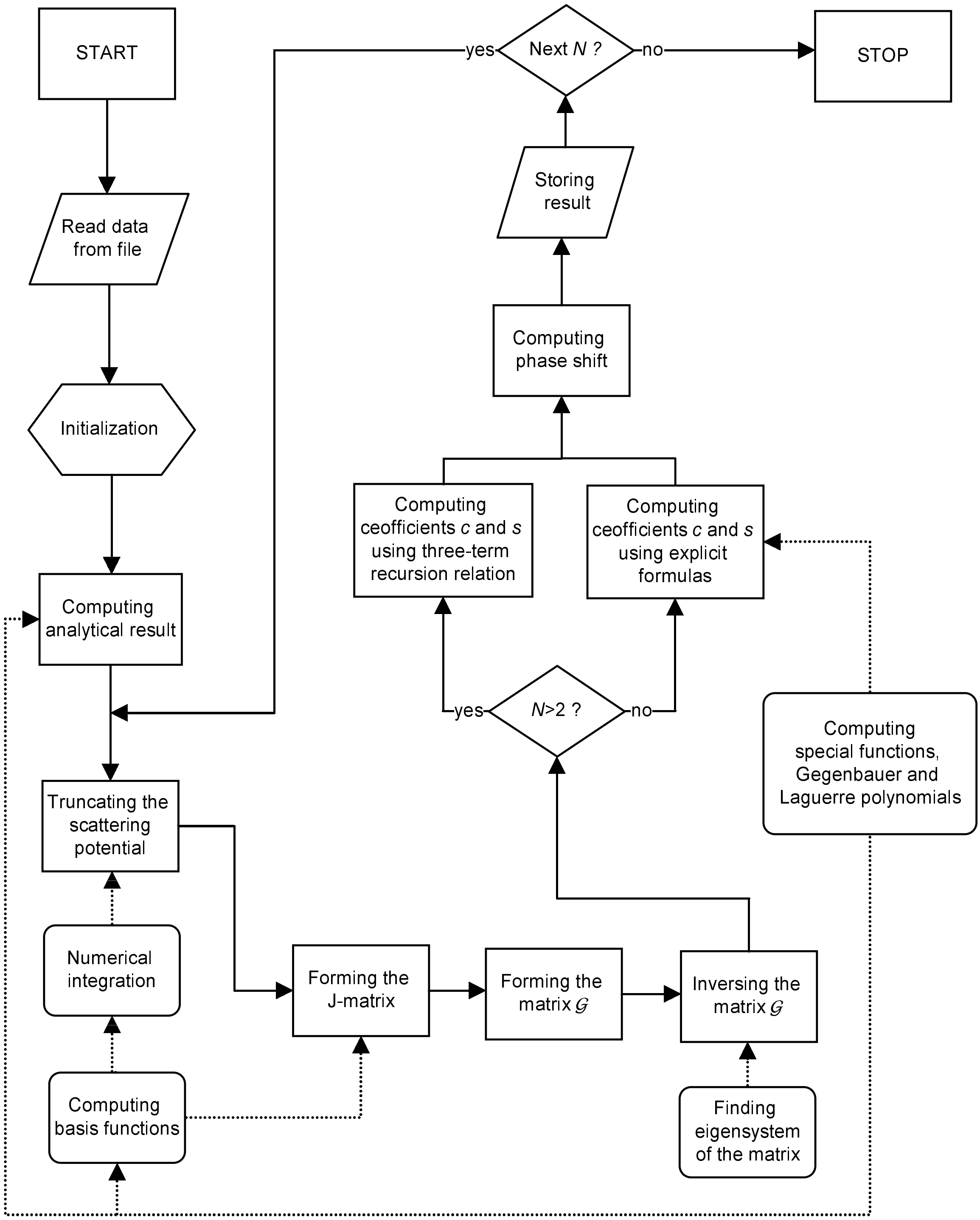
$$\begin{bmatrix} A \\ B \end{bmatrix} = N(b)^{\tilde{k},\kappa} M(b)^{\tilde{k}',\kappa} N(a)^{\tilde{k}',\kappa} M(a)^{\tilde{k},\kappa} \begin{bmatrix} 1 \\ 0 \end{bmatrix},$$

where the 2×2 matrices M, N depending on the position are defined with aid of Ricatti-Bessel and Ricatti-Neumann functions $j_l(r)$, $n_l(r)$ as follows

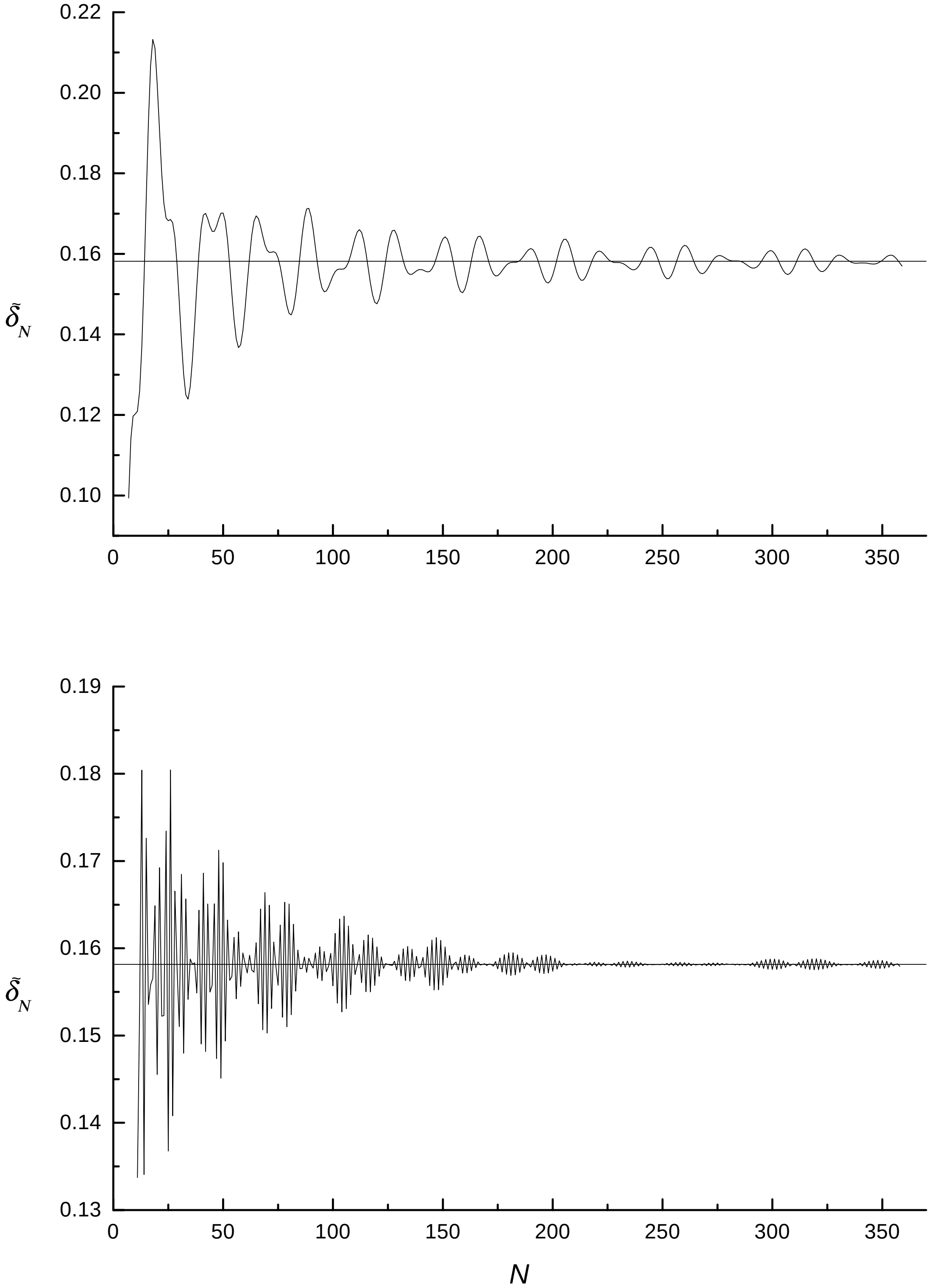
$$M(r)^{\tilde{k},\kappa} = \begin{bmatrix} j_l(kr) & -n_l(kr) \\ \mp\epsilon(\tilde{k}) j_{l\pm1}(\tilde{k}r) & \pm\epsilon(\tilde{k}) n_{l\pm1}(\tilde{k}r) \end{bmatrix}, \; N(r)^{\tilde{k},\kappa} = \begin{bmatrix} \pm\epsilon(\tilde{k}) n_{l\pm1}(\tilde{k}r) & n_l(\tilde{k}r) \\ \mp\epsilon(\tilde{k}) j_{l\pm1}(\tilde{k}r) & j_l(\tilde{k}r) \end{bmatrix}$$

with the relativistic quantum number $\kappa = l$ ($\kappa = -l - 1$) for upper (lower) sign of indices in the above formula. $\tilde{k}'$ is defined in the same way as $\tilde{k} \equiv \frac{\sqrt{(E-mc^2)(E+mc^2)}}{c\hbar}$, but with shifted energy $E' = \mathcal{E} + V_0 + mc^2$ instead of E. The number ϵ is defined as previously.

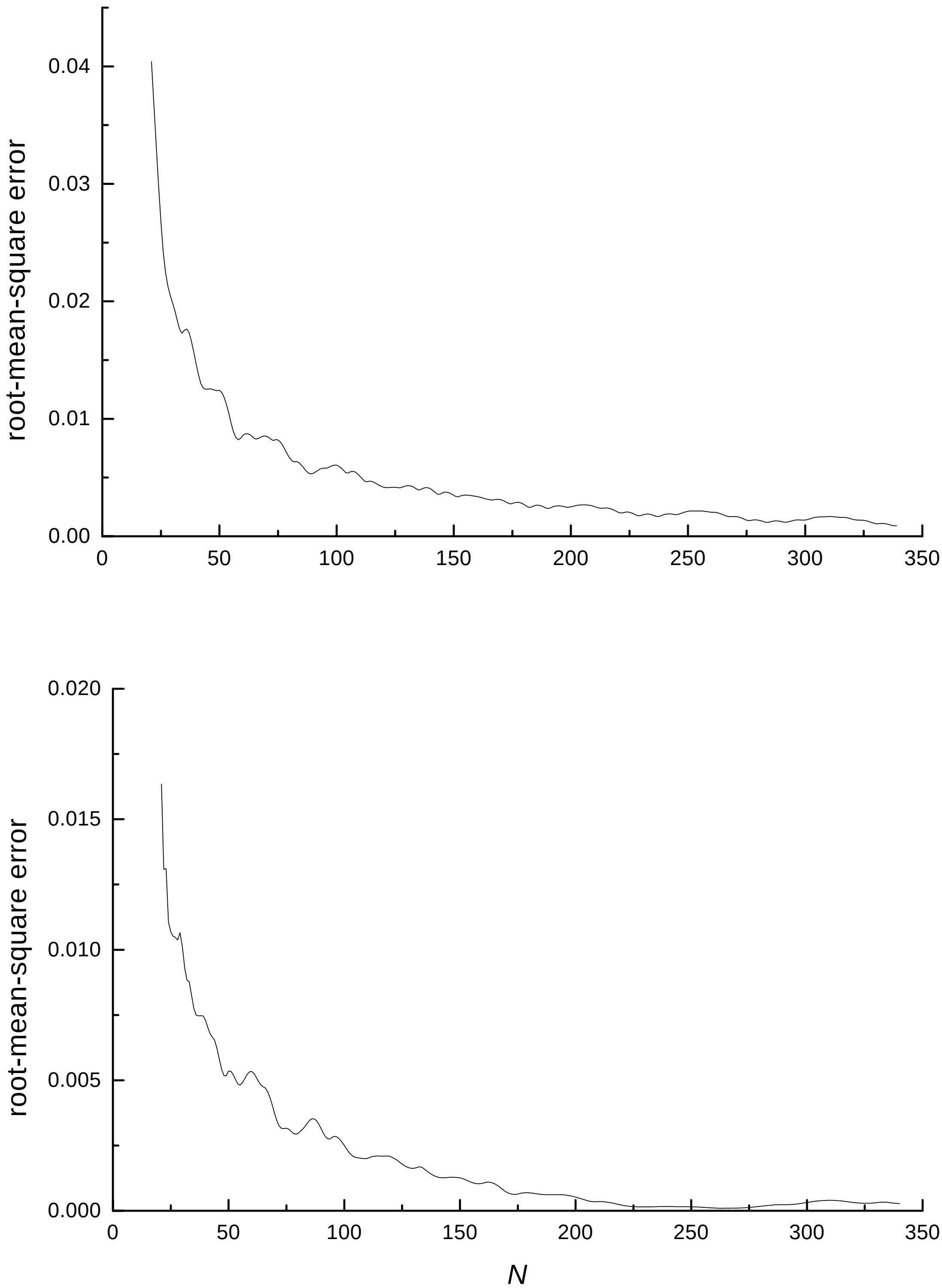
Numerical computations - scheme



Results



Convergence of the phase shift versus number of Laguerre and Gaussian (respectively) basis functions N used to truncate the scattering potential. Straight line – analytical result.



Root-mean-square error, averaging 20 points backwards and 20 forwards. Laguerre and Gaussian basis set, respectively.

References

[1] E. Heller, H. Yamani, *New L2 approach to quantum scattering: Theory*, Phys. Rev. A **9** (1974) 1201

[2] E. Heller, H. Yamani, *J-matrix method: Application to s-wave electron-hydrogen scattering*, Phys. Rev. A **9** (1974) 1209

[3] H. Yamani, L. Fishman, *J-matrix method: Extensions to arbitrary angular momentum and to Coulomb scattering*, J. Math. Phys. **16** (1975) 410

[4] P. Horodecki, *The relativistic J-matrix method*, submitted to J. Phys. B: At. Mol. Opt. Phys.

[5] P. Syty, *Programowanie metody J-macierzy*, praca dyplomowa, Politechnika Gdańska, 1999

[6] P. Syty, *The relativistic J-matrix method: Numerical computations*, TASK Quarterly, vol 3, nr 3

[7] P. Syty, P. Horodecki and J. E. Sienkiewicz, *The relativistic J-matrix method: Numerical computations*, submitted to Phys. Lett. A