

Phase Shifts of Electron-Atom Scattering Using J-Matrix Method for a Class of Short Range Potentials

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Abstract— This study deals with the non-relativistic J-matrix method in quantum scattering theory. The method is investigated for a class of short range scattering potentials (Yukawa, Hulthén, and Exponential-Cosine Screened Coulomb), and in two different L^2 basis (Laguerre and Gaussian) for elastic electron-atom scattering problem. The results of the scattering phase shifts non-relativistic case for this class of potentials are shown to be reasonable compared to analytical results.

Index Terms—Electron-Atom Scattering , Exponential-Cosine Screened Coulomb potential, Hulthén potential, J-Matrix Method , Phase Shift , Short Range Potentials, and Yukawa potential .

1 INTRODUCTION

Most of the computational efforts for describing electron scattering have concentrated on quantal methods. The numerical methods used in electron scattering generally falls into one of two categories, namely perturbation-series expansions based on variations of Born series or the non-perturbative close-coupling approach originating from the expansion of the trial wavefunction into a set of basis functions. [1]

Typically, Born- series expansions (Born approximation, distorted wave approximation...) [2] used successfully for high collision energies where the projectile-target interaction is a relatively small perturbation of the free-particle motion with large kinetic energy. On the other hand, close-coupling expansions were applied to simulate low-energy collision where the incident energy is such that only elastic scattering, or at most excitation of few low-lying target states is possible. However, this method may be extended to deal with higher collision energies.

Close-coupling expansions can be generalized to a relativistic framework, and the collision problem essentially consists of finding the solution to this system. This can be achieved by various iterative, noniterative, or algebraic methods such as R-matrix, and J-matrix. [1, 3].

The J-matrix theory of quantum scattering is an algebraic method which exploits the fact that the unperturbed reference

Hamiltonian can be tridiagonalized in a certain complete set of (L^2) basis functions. The resulting symmetric three-term recursion relation for the expansion coefficients of the unperturbed wave function is solved in terms of appropriate orthogonal polynomials. The method yields exact scattering information over a continuous range of energy for a model potential obtained by truncating the given short-range potential in a finite subset of this basis [4].

This method has been applied successfully to a large number of problems. It is shown to be free from the fictitious resonances that plague some algebraic variational scattering methods. The group-theoretical foundation of the theory has been exploited to account for the class of analytic potentials that are compatible with the formalism.

2 Potential Models

In our calculations we consider a class of short range potentials which are exponentially small in the asymptotic domain

$$V(r) \rightarrow O(e^{-\mu r}), \quad \mu > 0, \text{ for } r \rightarrow \infty \quad (1)$$

Through our consideration, it will be applicable to most of the potentials belonging to this class. We will illustrate our calculations by considering three specific potentials in detail [5].

Those potentials are the Yukawa potential,

$$V(r) = -Z \exp(-\lambda r) / r \quad (2)$$

The Exponential-Cosine Screened Coulomb potential,

$$V(r) = -Z \exp(-\lambda r) \cos(\lambda r) / r \quad (3)$$

And Hulthén potential,

$$V(r) = -Z \exp(-\lambda r) / (1 - \exp(-\lambda r)) \quad (4)$$

Those potentials have the behavior

$$V(r) \sim -1/r \text{ for } r \rightarrow 0 \quad (5)$$

And are exponentially small in the $r \rightarrow \infty$ limit, Where

Z : is the atomic number.

λ : is the screening parameter ($\lambda = \lambda_0 + Z^{1/3}$, $\lambda_0 = 0.97$) [6].

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first N basis functions.

To perform a calculation, we need merely augment this $N \times N$ matrix with the extra row and column shown and with the right-hand side driving term. Equation (10) can be immediately solved for t by standard techniques. An illuminating formula for $\tan \delta = t$ can be obtained by prediagonalizing the inner $N \times N$ matrix $(H_o + V^N - k^2 / 2)$, with the energy-independent transformation Γ , where

$$\tan \delta_N = - \frac{s_{N-1}^l + g_{N-1,N-1}(E) J_{N,N-1} s_N^l}{c_{N-1}^l + g_{N-1,N-1}(E) J_{N,N-1} c_N^l} \quad (11)$$

Where $g_{N-1,N-1}(E) = \sum_{m=0}^{N-1} (\Gamma_{N-1,m}^2 / E_m - E)$ with the matrix Γ diagonalizing the finite-dimensional problem

$$(\Gamma^\dagger P^\dagger (H_o + V - k^2 / 2) P \Gamma)_{mn} = (E_m - E) \delta_{mn} \quad [4, 8, 12, 16, 17]$$

4 RESULTS AND DISCUSSION

In order to visualize the effect of increasing the number of base N (i.e. $N \rightarrow \infty$) on the phase shift value δ , it is necessary to plot the phase shift δ versus the number of basis N to show that as the number of basis increase N (i.e. $N \rightarrow \infty$), the phase shift δ (i.e. δ_N) converges to correct value (i.e. $\tilde{\tau} = \tan \delta$ as $N \rightarrow \infty$).

The values of the parameters used in the numerical computations are the energy of the projectile electron $e=1$ Hartree, potential truncation (cut-off parameter) $r_o = 1$ a.u, atomic number of the target atom $Z = 1$, potential screening parameter $\lambda = 1$, base function scaling parameter $\lambda = 1$, numbers of base functions N extend from 1 to 550, and orbital angular quantum number $l = 0, 1$.

Since the phase shift has been calculated by using J-matrix method for Coulomb potential and they are identical to the analytical results [14, 12, 17], so taking $r \rightarrow 0$ the phase shift of this class of potentials using J-matrix method should converges to that of Coulomb calculated by the same method,

Table (I) shows the value of the phase shift for this class of potentials compared to the Coulomb potential for the same energy ($Z=1, \lambda=1, \kappa=1, e=1$ Hartree, gauss basis, $N=50, r_o = 0.0001$ a.u.)

Figures (2.a), and (2.b) illustrate the nonrelativistic phase shift convergence using Laguerre and Gauss basis function respectively to truncate the potential Hulthén for $l = 0$ and 1.

The figures show the effect of increasing the number of basis N on the phase shift value δ_N such that as the number of basis increase the accuracy of the phase shift increase and the convergence become faster.

For $l=1$ the convergence of phase shift value for Laguerre is faster than that for $l=0$ especially for $N > 50$, while for Gauss it convergence at $N < 100$.

One can notice that the convergence in Laguerre basis set has completely different nature if compared to convergence in Gaussian set. The convergence in Laguerre set appears to be more stable and regular, but is slower. In Gaussian basis, we have rather a quick convergence, but the numerical results "jump" around the analytical result.

TABLE 1

THE VALUE OF THE PHASE SHIFT FOR THIS CLASS OF POTENTIALS COMPARED TO THE COULOMB POTENTIAL FOR THE SAME ENERGY ($Z=1, \lambda=1, \kappa=1, E=1$ HARTREE, GAUSS BASIS, $N=50, r_o=0.0001$ A.U.)

Potential	Phase shift [rad]
Coulomb	1.64294×10^{-10}
Yukawa	1.64291×10^{-10}
Hulthén	1.64291×10^{-10}
Exponential cosine	1.64293×10^{-10}

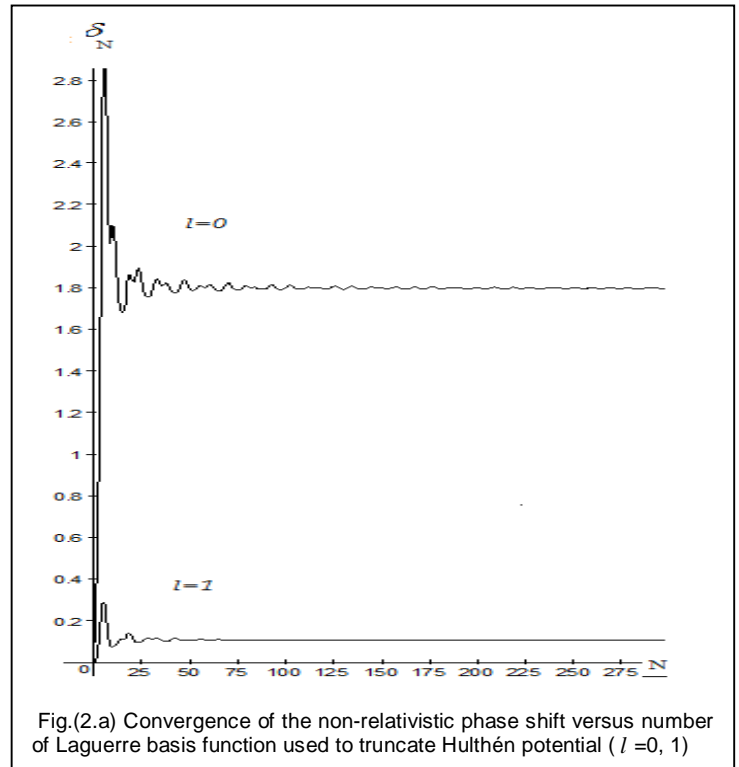


Fig.(2.a) Convergence of the non-relativistic phase shift versus number of Laguerre basis function used to truncate Hulthén potential ($l = 0, 1$)

Figures (3.a), and (3.b) illustrate the nonrelativistic phase shift convergence using Laguerre and Gauss basis function respectively to truncate Exponential- cosine screened coulomb potential for $l = 0$ and 1.

The figures show the effect of increasing the number of basis N on the phase shift value δ_N such that as the number of basis increase the accuracy of the phase shift increase and the convergence become faster.

For $l=1$ the convergence of phase shift using Laguerre basis function is faster than that for $l=0$ especially for $N < 75$ which is the same number of Gauss basis function needed to achieve the convergence.

One can notice that the convergence in Laguerre basis set has completely different nature if compared to convergence in Gaussian set.

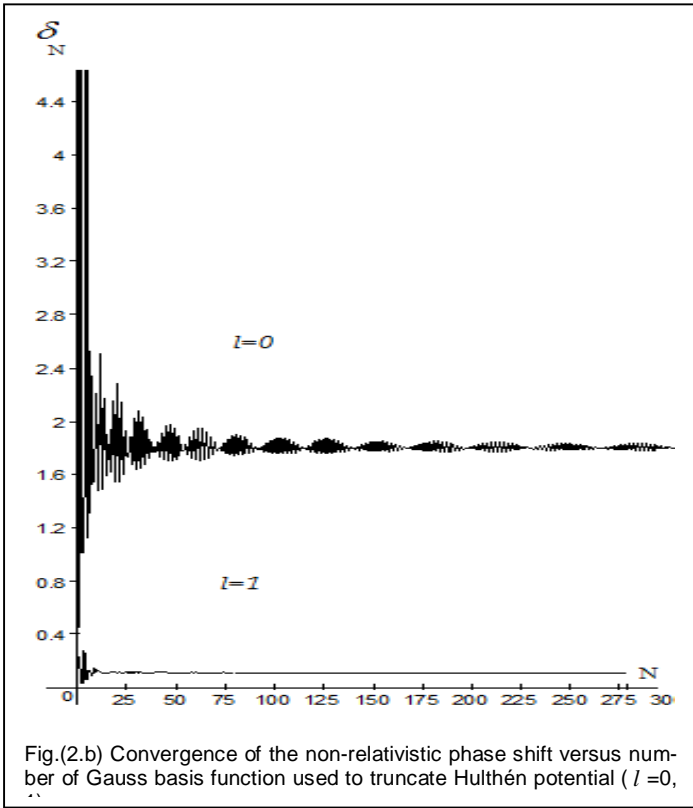


Fig.(2.b) Convergence of the non-relativistic phase shift versus number of Gauss basis function used to truncate Hulthén potential ($l=0, 1$).

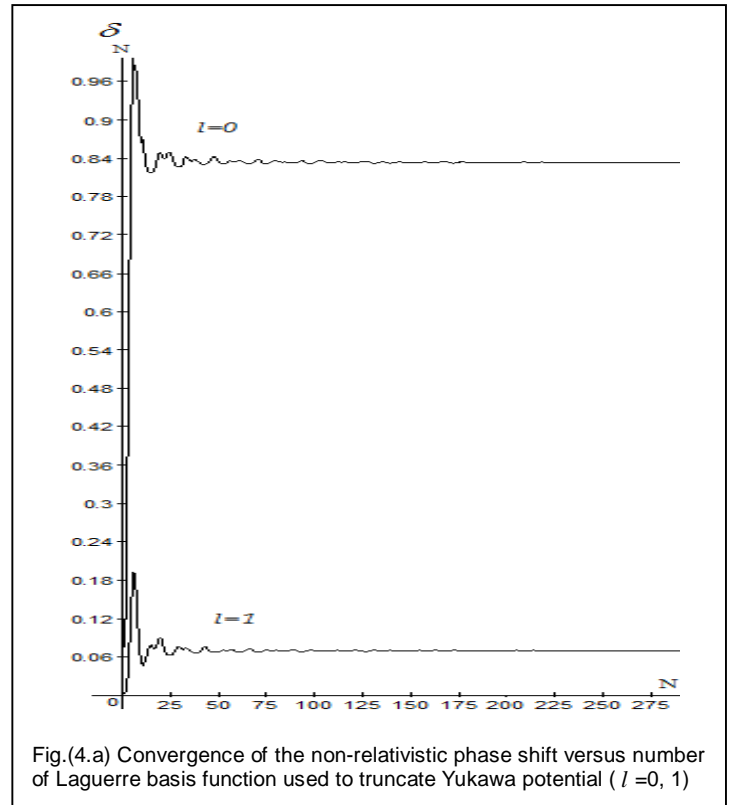


Fig.(4.a) Convergence of the non-relativistic phase shift versus number of Laguerre basis function used to truncate Yukawa potential ($l=0, 1$).

For phase shift convergence in Yukawa potential, figures (4.a), and (4.b) show the nonrelativistic case using Laguerre and Gauss basis function to truncate the potential for $l=0$ and 1 respectively.

For $l=1$ the convergence of phase shift value is faster than that for $l=0$ especially for $N < 50$ using Laguerre while for Gauss basis function the convergence is $N < 50$.

In general, in both investigated cases ($l=0$ and 1) it is not difficult to see that phase shifts computed numerically converge to phase shift obtained using an analytical formula, the convergence in this basis is rather slow but systematic.

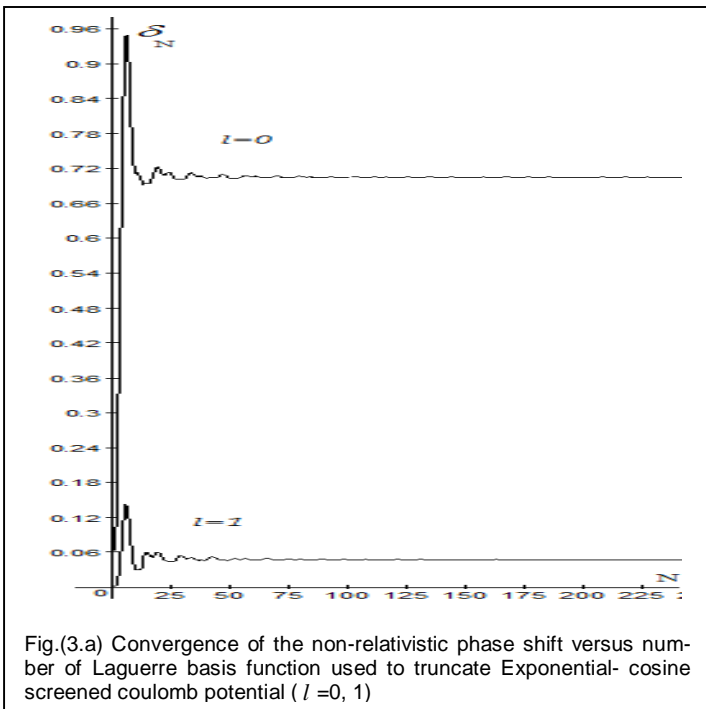


Fig.(3.a) Convergence of the non-relativistic phase shift versus number of Laguerre basis function used to truncate Exponential-cosine screened coulomb potential ($l=0, 1$).

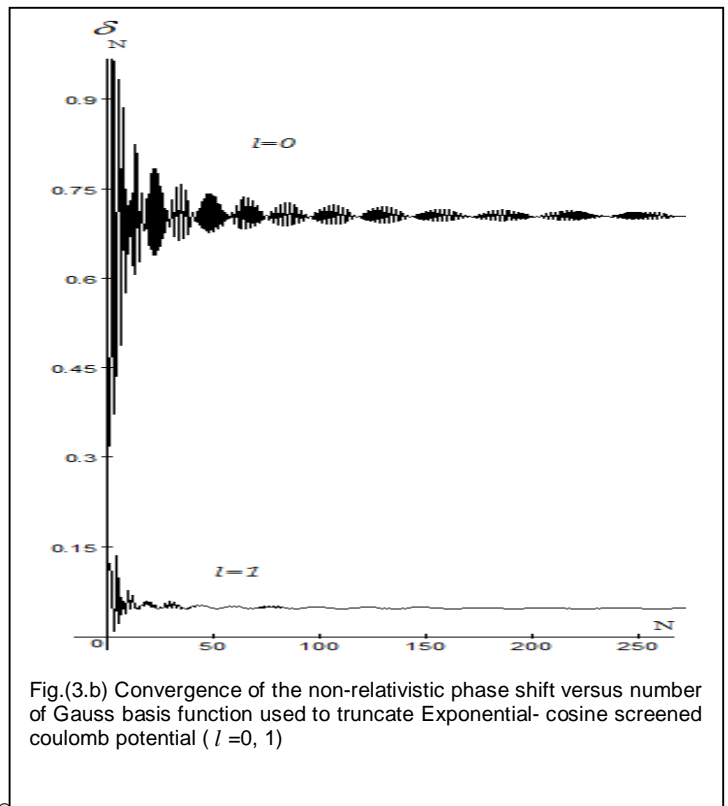
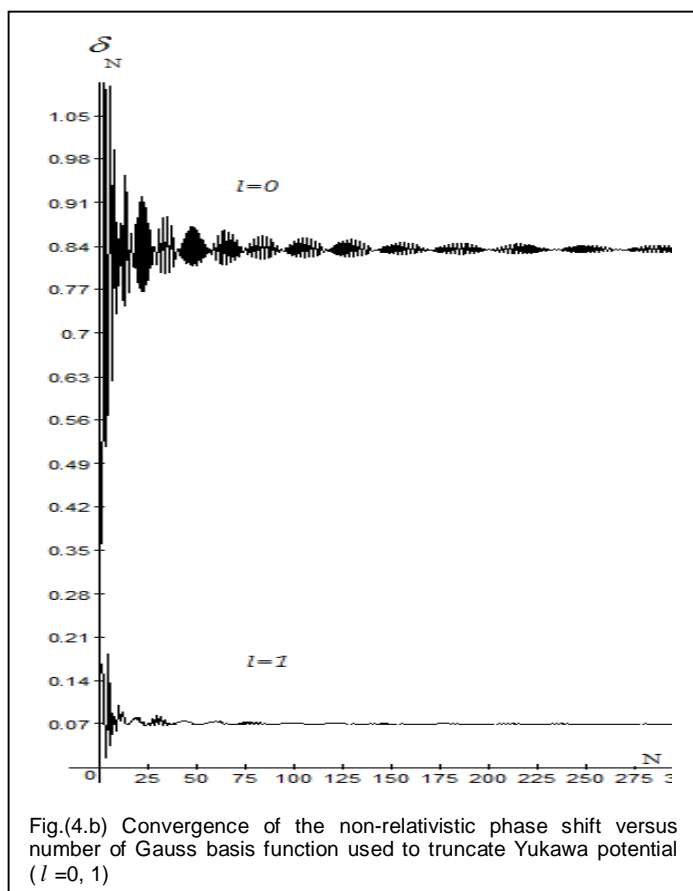


Fig.(3.b) Convergence of the non-relativistic phase shift versus number of Gauss basis function used to truncate Exponential-cosine screened coulomb potential ($l=0, 1$).



5. CONCLUSIONS

Applying the J-matrix method to a class of short range potentials for describing the scattering phenomena was the fundamental purpose of the work. For this purpose the JMATRIX program is modified and used to carry out numerical calculations for scattering phase shifts for potentials in the shape of the Yukawa potential, Hulthén potential and exponential-cosine screened potential. Performed calculations of scattering phase shifts show, that:

The J-matrix method is an effective method for describing the scattering phenomena for any scattering potential vanishing faster than the Coulomb one given in analytical form (short range potential) and especially for this class of short range potentials (Yukawa potential, Hulthén potential and exponential-cosine screened potential),

The convergence in Laguerre basis set has completely different nature if compared to convergence in Gaussian set. The convergence in Laguerre set appears to be more stable and regular, but is slower. In Gaussian basis, we have rather a quick convergence, but the numerical results "jump" around the analytical result. The difference between the Laguerre and Gaussian basis is in the "r". The Gaussian basis squares the "r" [see table I] so the (r) dependence in the exponent in the Gaussian basis is a poorer representation than that of the Laguerre basis. Gaussian basis also falls off more rapidly with distance than Laguerre basis. These factors suggest that more Gaussian basis are needed to form a suitable basis set than Laguerre basis,

roughly three times as many are needed to achieve the same accuracy,

As the angular momentum quantum number l increases, the convergence of the scattering phase shift values become faster in both Laguerre and Gaussian basis because this increasing makes the basis decay faster due to the (r) dependence in the exponent in the both basis,

As the angular momentum quantum number l increases, the effect of the repulsive centrifugal potential increases and become more dominants, so phase shift values decrease.

The convergence of phase shift values for Hulthén potential are slower than those of Yukawa and Exponential Cosine-Screened Coulomb potential because the fall off of Hulthén potential is slower than that of the other potentials.

REFERENCES

- [1] N. Anderson, K. Bartschat, Polarization, Alignment, and Orientation in Atomic Collision, Springer Verlag, New York (2001)
- [2] I. Ladawa, Aspect of Atomic Structure in Atomic Collisions, Ph.D. Thesis, University of Bergen (2000).
- [3] A. D. Alhaidari, H. Bahlouli, M. S. Abdelmonem, F. S. Al-Ameen and T. H. Al-Abdulaal, Scattering theory with a natural regularization: Rediscovering the J-matrix method, Physics Letters A, 364.5, 372, (2007)
- [4] A.D. Alhaidari, H.A. Yamani, and M.S. Abdelmonem, J-matrix method of scattering in any L^2 basis, Phys. Rev. A, 64, 042703, (2001)
- [5] S.H. Patil, U.I. patil, Asymptotically correct basis for a class of short range potentials, Physica Scripta, 48, 641, (1993)
- [6] B. H. Alias, E. M. Ahmad, Energy Calculation of S-State for some Atoms using Hulthén and exponential Cosine Screened Coulomb Potentials, J.Edu.Sci. 34, 45 (1998)
- [7] H. A. Yamani, The J-matrix reproducing kernel: Numerical weights at the Harris energy eigenvalues, J. Math. Phys., 25, 317, (1984)
- [8] E. J. Heller and H. A. Yamani, New L^2 approach to quantum scattering: Theory, Phys. Rev. A, 9, 1201, (1974)
- [9] E. J. Heller and H. A. Yamani, J-matrix method: Application to s-wave electron-hydrogen scattering, Phys. Rev. A, 9, 1209, (1974)
- [10] H.A. Yamani, L. Fishman, J. Math. Phys., J-matrix method: Extensions to arbitrary angular momentum and to Coulomb scattering, 16, 410 (1975)
- [11] J.T. Broad and W. P. Reinhardt, J-matrix method: multichannel scattering and photoionization, J. Phys., B, 9, 1491 (1976)
- [12] P. Syty, The J-matrix method: numerical computations, TASK Quarterly 3 No. 3 (1999)
- [13] S. K. Adhikari, Variational Principles and the Numerical Solution of Scattering Problems, John Wiley & Sons, Inc., New York (1998)
- [14] P. Horodecki, Relativistic J-matrix method, Phys. Rev. A, 62, 052716 (2000)
- [15] A. D. Alhaidari, H. A. Yamani, and M. S. Abdelmonem, Relativistic J-matrix theory of scattering, Phys. Rev. A, 63, 062708, (2001)
- [16] H. A. Yamani, The J-matrix reproducing kernel: Numerical weights at the Harris energy eigenvalues, J. Math. Phys., 25, 317, (1984)
- [17] P. Syty, Programming the J-matrix method, MSc thesis, Gdansk University of Technology (1999)