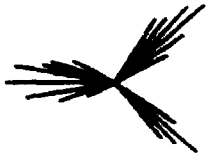

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May/95 IFT-P.025/95

Iterative numerical solution of scattering problems *

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*To appear in Chemical Physics Letters

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Iterative numerical solution of scattering problems

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An iterative Neumann series method, employing a real auxiliary scattering integral equation, is used to calculate scattering lengths and phase shifts for the atomic Yukawa and exponential potentials. For these potentials the original Neumann series diverges. The present iterative method yields results that are far better, in convergence, stability and precision, than other momentum space methods. Accurate result is obtained in both cases with an estimated error of about 1 in 10^{10} after some 8–10 iteration

PACS: 03.80.+r, 03.65.Nk, 34.40.+n

To appear in Chemical Physics Letters

Numerical solutions of the Lippmann-Schwinger-type scattering integral equation are usually performed by reducing this equation to a matrix equation of finite dimension [1]. Such a reduction is possible as the original integral equation has a compact kernel. However, this procedure needs a delicate treatment of a principal-value integral over a fixed point singularity in the kernel of this equation. Then remains the task of solving the finite dimensional matrix equation. In realistic situation the dimension of the matrix could be quite large. A direct solution of this discrete set of linear equation, for example, by matrix inversion, could involve large numerical effort for obtaining high precision result, due to the accumulation of numerical errors in this approach. Alternative variational methods deal with a small set of linear equations and have the advantage of yielding good results with relatively little numerical effort [2–16]. However, the appearance of spurious singularities [10, 17–20], and nonmonotonic and slow convergences of these methods have put a limitation on their use for obtaining high precision results.

Iterative solution of Fredholm integral equations are known for leading to rapidly convergent results for weak kernels [1]. The Lippmann-Schwinger equation permits iterative solution which converges for a sufficiently weak potential or at sufficiently high energies. Moreover, for most scattering energies the iterative solution of a realistic scattering equation is either divergent or very slowly convergent to be of any practical use.

The present Letter considers an iterative numerical method for scattering problems. The method relies on solving an auxiliary nonsingular equation whose kernel is free of the principal-value prescription needed in the K matrix equation, or the $\varepsilon \to 0$ outgoing wave limit needed in the t matrix equation. The kernel of this auxiliary equation, in contrast to that of the original t or the K matrix equations, is made of the difference between two terms which cancels the fixed point singularity of the momentum space Green's function. Consequently, by adjusting a free parameter, this kernel can be made sufficiently weak in order to yield a rapidly convergent iterative Neumann series for a wide class of scattering problems. The K or the t matrix elements are then obtained by performing an integral over the known solution of the auxiliary equation. This method was first suggested for nuclear scattering problems

[1, 21 25]. However, the accuracy of the method has really never been tested. In nuclear scattering problems, as the potential is not accurately known, usually, one is content with approximate solutions.

The situation is entirely different in atomic and molecular physics, where the basic interaction is known and this has led people to develop complicated models and perform high precision calculations. For this one needs intelligent and stable numerical methods. The iterative method involving nonsingular equation is here tested for two of the commonly used model potentials – the atomic exponential and the Yukawa potentials. After some 8 iterations we obtain results with estimated error of about 1 in 10^{10} for both these potentials. These results are more accurate than any currently available momentum space numerical results by several orders of magnitude. It is unlikely that the direct matrix inversion or the use of variational principles will lead to results with same precision.

The present iterative method can be applied both to single-channel and multi-channel scattering processes [22 24]. For real hermitian potentials, the method is formulated in terms of a real operator, called the Γ matrix, which satisfies a real nonsingular integral equation. No complex variables or principal-value prescriptions are needed for the numerical treatment of this equation. The t or the K matrix elements are then found out by evaluating an integral involving the Γ matrix. Details of this method have appeared in the literature [21- 23] and a description is given below.

In the single-channel case the partial wave t matrix (in units of $\hbar^2/2m$) satisfies

$$t(p,k;k^2) = V(p,k) + \frac{2}{\pi}\int_0^\infty q^2 dq \frac{V(p,q)t(q,k;k^2)}{k^2 - q^2 + i0}, \tag{1}$$

where V is the potential (in units of $\hbar^2/2m$), k the on-shell wave-number and m the reduced mass. The general scheme for the nonsingular reduction starts by introducing a real function $\gamma(k,q)$, such that $\gamma(k,k) = 1$. Then the Lippmann-Schwinger equation (1) can be rewritten as

$$\begin{aligned} t(p,k;k^2) = V(p,k) &+ \frac{2}{\pi}V(p,k)\int_0^\infty \frac{q^2 dq \gamma(k,q)}{k^2 - q^2 + i0} t(q,k;k^2) \\ &+ \frac{2}{\pi}\int_0^\infty q^2 dq A(p,q;k^2) t(q,k;k^2) \end{aligned} \tag{2}$$

where

$$A(p,q;k^2) = \frac{[V(p,q) - V(p,k)\gamma(k,q)]}{k^2 - q^2}, \tag{3}$$

is a nonsingular kernel.

The t matrix can be expressed in terms of the Γ matrix, which satisfies

$$\Gamma(p,k;k^2) = V(p,k) + \frac{2}{\pi}\int_0^\infty q^2 dq\, A(p,q;k)\Gamma(q,k;k^2). \tag{4}$$

The Γ matrix is not time-reversal symmetric: $\Gamma(q,q';k^2) \neq \Gamma(q',q;k^2)$. This is not a problem in numerical calculation.

The formal manipulation needed to relate the t matrix with the Γ matrix becomes transparent in the operator form. In operator form Eqs. (2) and (4) are written as

$$t = V + At + V\mathcal{G}_0 t, \tag{5}$$

$$\Gamma = V + A\Gamma, \tag{6}$$

with $V(p,q) = V(p,k)$, and $\mathcal{G}_0(p,q) = \delta(q-p)(k^2 - q^2 + i0)^{-1}\gamma(k,q)$. Then t is expressed in terms of Γ by

$$t = \Gamma + \hat{\Gamma}\mathcal{G}_0 t, \tag{7}$$

with $\hat{\Gamma}(p,q;k^2) = \Gamma(p,k;k^2)$. Equation (7) leads to the following on-shell t matrix element [1, 21]

$$t(k,k;k^2) = \frac{\Gamma(k,k;k^2)}{1 - (2/\pi)\int_0^\infty q^2 dq (k^2 - q^2 + i0)^{-1}\gamma(k,q)\Gamma(q,k;k^2)}. \tag{8}$$

Once the real nonsingular equation (4) is solved, the t matrix can be calculated by performing the complex integral of (8). The zeros of the denominator of Eq. (8) correspond to bound states and this t-matrix does not have spurious poles. This fact has been used to develop a related method for the binding energy and bound state wave function [26]. The only principal-value prescription or the $i\epsilon \to 0$ limit appears in Eq. (8), which can be handled easily. For numerical purpose Eq. (8) can be rewritten as

$$\frac{1}{t(k,k;k^2)} = \frac{1}{\Gamma(k,k;k^2)} - \frac{2}{\pi}\int_0^\infty dq \frac{[q^2\gamma(k,q)\Gamma(q,k;k^2)/\Gamma(k,k;k^2) - k^2]}{(k^2 - q^2 + i0)} + ik. \tag{9}$$

While arriving at Eq. (9) the integral in the denominator of Eq. (8) has been broken up into its principal-value and imaginary delta function parts and the principal-value integral eliminated by the following identity:

$$\mathcal{P}\int_0^\infty \frac{dp}{k^2-p^2}=0, \tag{10}$$

where k is any real positive number and $\mathcal{P}$ denotes the principal-value prescription.

The inverse of the on-shell K matrix is also essentially given by Eq. (9) but with the imaginary part deleted. Explicitly,

$$\frac{1}{K(k,k;k^2)}=\frac{1}{\Gamma(k,k;k^2)}-\frac{2}{\pi}\int_0^\infty dq\,\frac{[q^2\gamma(k,q)\Gamma(q,k;k^2)/\Gamma(k,k;k^2)-k^2]}{(k^2-q^2+i0)}. \tag{11}$$

With the present partial wave projection one has, for S wave at zero energy, the scattering length a given by

$$a=K(0,0;0)=t(0,0;0). \tag{12}$$

At other energies the phase shifts δ are defined by

$$\frac{1}{K(k,k;k^2)}=\Re\left(\frac{1}{t(k,k;k^2)}\right)=-k\cot\delta. \tag{13}$$

The present method relies on the solution of the auxiliary nonsingular Γ matrix equation (4). The real nonsingular kernel of this equation, given by Eq. (3), involves a difference of two terms. At the on-shell point, $q=k$, and the expression in the square bracket of this equation vanishes, which makes the kernel A both nonsingular at the on-shell point and weak compared to that of the original nonsingular equation. This property of the kernel A will be used for the iterative solution of the scattering Γ matrix equation (4), defined by

$$\Gamma_n=V+A\Gamma_{n-1},\quad n=1,2,\ldots. \tag{14}$$

where $\Gamma_0=V$.

The range of momentum integration in Eq. (4) covers the whole phase space, e.g., 0 to ∞. So one encounters an infinite integral. The Fredholm nature of the problem guarantees that the kernel decays rapidly to zero as the momentum variables tend to

infinity. It is often useful, from a practical point of view, to transform the infinite integral to a finite integral. Given the Gauss-Legendre points between $-1 < x < 1$, this is achieved by the transformation

$$q = c\left(\frac{1+x}{1-x}\right), \tag{15}$$

which maps $0 < q < \infty$ into $-1 < x < 1$ where the images of points $x = -1, 0, 1$ are $q = 0, c, \infty$, respectively. The differential dq in Eq. (4) is directly obtained from the transformation. Obviously, one can have an infinite class of transformations, each one distributing the integration points in a different fashion. In fact all of these mappings correspond to a maximum value of q in momentum space which is efficiently controlled by the parameter c. This corresponds to a cut-off in the infinite integral. Otherwise, the choice of the parameter c is entirely arbitrary. Generally, the parameter c is dictated by special features of the kernel and should be chosen in order to get the most accurate numerical result with a given number of mesh points.

In order to illustrate the method we consider the S wave scattering of an electron by the following exponential and Yukawa attractive potentials

$$V(r) = -\frac{\hbar^2}{ma_0^2}\exp(-r/a_0), \tag{16}$$

and

$$V(r) = -\frac{\hbar^2}{ma_0^2}\frac{\exp(-r/a_0)}{(r/a_0)}, \tag{17}$$

where a_0 is the Bohr radius of the hydrogen atom. Both these potentials have been used in numerous tests of various computational methods in atomic physics [8, 10–12, 16, 27, 28]. After factorization of $\hbar^2/2m$, the S wave momentum space matrix elements of the above potentials are, respectively, given in atomic units (a.u.) by

$$V(p,q) = -4[1+(p+q)^2]^{-1}[1+(p-q)^2]^{-1}, \tag{18}$$

and

$$V(p,q) = -\frac{1}{2pq}\ln\frac{1+(p+q)^2}{1+(p-q)^2}. \tag{19}$$

In atomic units, the length is measured in units of a_0 and the momentum space matrix elements t and V are also given in this unit. The wave number is in units of a_0^{-1}.

In order to perform a numerical calculation one has to decide on the number of integration mesh points, the constant c in transformation (15), and a choice for the function $\gamma(k,q)$. It would be better if the infinite integral in the T matrix equation can be truncated for a relatively small value of momentum. Motivated by this we consider

$$\gamma(k,q) = \left[\frac{k^2+\alpha^2}{q^2+\alpha^2}\right]^2, \tag{20}$$

for the exponential potential, and

$$\gamma(k,q) = \left[\frac{k^2+\alpha^2}{q^2+\alpha^2}\right], \tag{21}$$

for the Yukawa potential, where α is a constant which should be varied to obtain a rapid convergence of the iterative solution of Eq. (4). With these choices of the function γ, the leading asymptotic behavior, for $p,q \to \infty$, of the two terms in the kernel A, given by Eq. (3), cancels. In addition, we performed numerical calculation for $\gamma(k,q) = 1$. With this latter choice the integral equation (4) for the T matrix has convergent iterative solution for any local potential [29].

To start with we performed calculations for the choices (20) and (21) for $\gamma(k,q)$. In order to find a result precise to four or five significant figures a small value of the constant c (~ 1) and a relatively small number of Gauss-Legendre mesh points N ($\sim 20-30$) is needed. The constant c determines how far the integral extends in momentum space. But for obtaining accurate results, both c and N are to be increased. It is well known that the Yukawa potential is rapidly varying for small r compared to the smoothly varying exponential potential. In the momentum space the Yukawa potential extends far beyond the exponential potential as is clear from their asymptotic behaviors:

$$\lim_{p\to\infty} V(p,q) \sim [p^{-2}]^M, \tag{22}$$

where $M = 1$ for the Yukawa potential and $M = 2$ for the exponential potential. Consequently, in order to achieve the same degree of precision one needs a much larger N and c for the Yukawa potential compared to the exponential potential.

Numerical calculations were performed in double precision maintaining 16 significant digits. We found that $c = 20$ and $N = 128$ yielded results accurate to 1 in 10^{10} for the exponential potential. In order to obtain the same accuracy for the Yukawa potential one needs $c = 100$ and $N = 400$. These results were found to be stable when the number of mesh points N is increased. The use of almost any nonzero α in $\gamma(k,q)$ of Eqs. (20) and (21) for these c and N leads to the same stable converged result from the iterative series solution of the Γ matrix equation. However, the initial convergence depends on the value of α. After a small amount of experimentation we used $\alpha = 3.0$ for the exponential potential and $\alpha = 3.5$ for the Yukawa potential; these choices improve the lower order terms of the iterative solution.

The iterative series converged rapidly at all energies for both potentials. The iterative Neumann series based on the original Lippmann-Schwinger equation diverges in both cases. In the present study we report results for $k = 0$, 0.15 a.u., and 0.55 a.u. At zero energy the results are for the scattering length in atomic units and at other energies they are for the tangents of the phase shifts. The results are exhibited in Table 1. The entries in the table are the ratio of the result for a specific iteration n and the converged result. The converged results have been obtained by performing calculations with 1000 integration mesh points. In all cases the convergence is rapid and smooth. There are no oscillations around the converged value as the number of iterations is increased.

In the present method there is some arbitrariness in choosing the most desirable $\gamma(k,q)$. This arbitrariness is turned to good advantage -- the function $\gamma(k,q)$ has been chosen to obtain a rapid convergence of the iterative solution. However, the final converged result is independent of the specific choice of $\gamma(k,q)$. For the simplest choice, $\gamma(k,q) = 1$, the converged result is obtained after some 2 to 3 more iterations than in Table 1. This has been illustrated for the scattering length in Table 2 for the two potentials. In Table 2 we again show the ratio of the calculated results and the converged results. The $n = 1$ result in this case yielded accidentally very small (large) numbers for the Yukawa (exponential) potential. This means that in Eq. (8) the numerator or the denominator almost vanishes, respectively, for Yukawa or the exponential potentials. This is not of concern for results obtained with large n. The

vanishing of the denominator of Eq. (8) corresponds to true bound states [1], and this does not happen in the scattering region for a converged Γ. Also, for a converged Γ the numerator of Eq. (8) can not have spurious zero.

The entries 1.0 in Tables 1 and 2 denotes that the result has converged to the desired precision. The small deviation from 1.0 in some of the converged results in Tables 1 and 2 does not indicate a defect of the iterative scheme but simply means that the number and/or distribution of mesh points employed is not enough to obtain the desired accuracy. Also, compared to the numerical solutions obtained by the variational methods for the same potentials [10–12, 15, 27, 28], the present method yields vastly superior results.

Though we have illustrated the present method here for two simple potentials, it is applicable in more complex situations, for example, in solving multi-channel problems. Also, it can be used for the calculation of the off-shell K (or the t) matrix elements $k(p,q;k^2)$ where $p \neq k \neq q$. We have indeed calculated these elements and found that they converge equally rapidly. Essentially, the same method can be used for the calculation of the binding energy and the bound state wave function [26]. The present iterative method, which involves only several matrix vector multiplications, is also numerically much more economic than a direct solution by matrix inversion, specially when the dimension of the matrix is large. The Γ matrix is real for each order of iteration and the solution for each iteration obeys the constraints of unitarity. The multi-channel version of the present method[22–24] has been used in solving electron-hydrogen[30] and positron-alkali atom[31] scattering using the close-coupling approach. However, in these applications the Γ matrix equation was solved by matrix inversion and not by iteration. Preliminary model calculations in nuclear physics produced good convergence for the iterative solution of the multi-channel neutron-deuteron scattering Γ matrix equations [23]. In view of the rapid convergence obtained in the present iterative study, it will be interesting to try an iterative solution of the Γ matrix equation in multi-channel problems.

The work has been supported in part by the Conselho Nacional de Desenvolvimento Cientifico e Tecnológico, Fundação de Amparo à Pesquisa do Estado de São Paulo, and Financiadora de Estudos e Projetos of Brazil.

REFERENCES

[1] S. K. Adhikari and K. L. Kowalski, Dynamical Collision Theory and its Applications, Academic Press, Boston, 1991.
[2] J. Schwinger, Phys. Rev. 72 (1947) 742.
[3] W. Kohn, Phys. Rev. 74 (1948) 1763.
[4] L. Hulthen, K. Fysiogr. Sallsk. Lund. Foerh. 14 (1944) 257.
[5] I. H. Sloan and T. J. Brady, Phys. Rev. C 6 (1972) 701.
[6] R. G. Newton, Scattering Theory of Particles and Waves, Second Edition, Springer-Verlag, 1982.
[7] S. K. Adhikari and L. Tomio, Phys. Rev. C 36 (1987) 1275.
[8] K. Takatsuka, R. R. Lucchese, and V. McKoy, Phys. Rev. A 24 (1981) 1812.
[9] K. Takatsuka and V. McKoy, Phys. Rev. A 23 (1981) 2352.
[10] C. Schwartz, Phys. Rev. 124 (1961) 1468.
[11] G. Staszewska and D. G. Truhlar, J. Chem. Phys. 86 (1987) 2793.
[12] J. Callaway, Phys. Lett. 77A (1980) 137.
[13] G. Staszewska and D. G. Truhlar, Chem. Phys. Lett. 130 (1986) 311.
[14] Y. Mito and M. Kamimura, Prog. Theor. Phys. 56 (1976) 583.
[15] W. H. Miller and B. M. D. D. Jansen op de Haar, J. Chem. Phys. 86 (1987) 6213.
[16] T. N. Rescigno and B. I. Schneider, Phys. Rev. A 36 (1987) 2061.
[17] R. R. Lucchese, Phys. Rev. A 40 (1989) 6879.
[18] S. K. Adhikari, Chem. Phys. Lett. 181 (1991) 435.
[19] S. K. Adhikari, Chem. Phys. Lett. 189 (1992) 340.
[20] B. Apagyi, P. Lévai, and K. Ladányi, Phys. Rev. A 37 (1988) 4577.
[21] L. Tomio and S. K. Adhikari, Phys. Rev. C 22 (1980) 28.
[22] S. K. Adhikari, Phys. Rev. C 19 (1979) 1789.
[23] L. Tomio and S. K. Adhikari, Phys.Rev.C 22 (1980) 2359.
[24] K. L. Kowalski, Nucl. Phys. A190 (1972) 645.
[25] K. L. Kowalski, Phys. Rev. Lett. 15 (1965) 798.
[26] S. K. Adhikari and L. Tomio, Phys.Rev.C 24 (1981) 1186.
[27] F. E. Harris, Phys. Rev. Lett. 19 (1967) 173.
[28] D. Thirumalai and D. G. Truhlar, Chem. Phys. Lett. 70 (1980) 330.
[29] F. Coester, Phys. Rev. C 3 (1971) 525.
[30] B. H. Bransden, C. J. Noble, and R. N. Hewitt, J. Phys. B 26 (1993) 2487.
[31] S. K. Adhikari, A. S. Ghosh, and H. Ray, Chem. Phys. Lett. 222 (1994) 302.

TABLE 1. Scattering lengths and phase shifts obtained from the iterative solution of the Γ matrix equation for the exponential and the Yukawa potentials for k=0, 0.15 a.u., and 0.55 a.u., with $\gamma(k,q)$ given by Eqs. (20) and (21). The ratios of the calculated result for a particular iteration n to the converged exact result are shown in each case. At $k = 0$ the exact scattering lengths are 8.693254332 a.u. (exponential) and 7.911380206 a.u. (Yukawa). The exact results at k= 0.15 a.u. are $\tan\delta$ = −1.744939321 (exponential), −1.386339121 (Yukawa); and at k=0.55 a.u. are $\tan\delta$ = 2.200382707 (exponential), 5.797211392 (Yukawa).

n =	Yukawa ($k = 0$)	Exponential ($k = 0$)	Yukawa ($k = 0.15$)	Exponential ($k = 0.15$)	Yukawa ($k = 0.55$)	Exponential ($k = 0.55$)
0	0.4550407017	0.5889624075	2.4070888958	1.9537093230	−0.581089599	0.6875213332
1	1.0628835422	1.1094969597	0.9508377182	0.8898028226	0.8505445555	0.9543748521
2	1.0009906100	1.0013279806	0.9991722408	0.9972672993	0.9953429156	1.0035508106
3	1.0000400237	0.9999635234	0.9999916475	1.0000133976	0.9994524687	1.0001518592
4	1.0000019050	0 9999946001	1.0000023971	1.0000067319	0.9999328458	1.0000019555
5	1.0000000823	0.9999997030	1.0000004774	1.0000004479	0.9999916278	0.9999997597
6	1.0000000013	0.9999999926	1.0000000709	1.0000000150	0 9999989473	0.9999999776
7	0.9999999996	1.0000000002	1.0000000098	1.0000000000	0.9999998667	0.9999999989
8	1.0000000000	1.0000000000	1.0000000014	1.0000000001	0.9999999826	0.9999999999
9	1.0000000000	1.0000000000	1.0000000003	1.0000000002	0.9999999973	0.9999999999
≥10	1.0000000000	1.0000000000	1.0000000001	1.0000000002	0.9999999994	0.9999999999

TABLE 2. Scattering lengths obtained from the iterative solution of the Γ matrix equation for the exponential and the Yukawa potentials for $\gamma(k,q) = 1$. For other details see Table 1.

n =	Yukawa ($k = 0$)	Exponential ($k = 0$)
0	0.2528003898	0.4601268808
1	0.0000000000	99999999.002
2	0.7111651786	0.9394257325
3	1.0595716354	1.0051581219
4	0.9957968559	0.9997361315
5	1.0002435433	1.0000100510
6	0.9999891830	0.9999997065
7	1.0000003827	1.0000000068
8	0.9999999890	0.9999999999
9	1.0000000003	1.0000000000
≥10	1.0000000000	1.0000000000