PHYSICAL REVIEW A VOLUME 18, NUMBER 2 AUGUST 1978

Separable-expansion method for potential scattering and the off-shell T matrix

T. K. Lim and Judith Giannini
Department of Physics and Atmospheric Science, Drexel University, Philadelphia, Pennsylvania 19104
(Received 20 June 1977)

The closed-form, separable-expansion expression of Belyaev, Wrzecionko, and Irgaziev for the two-body T matrix is studied numerically for the case of a Yukawa potential. The method shows good convergence for the elastic scattering amplitude at intermediate energies, yielding results almost identical to Glauber's eikonal method.

I. INTRODUCTION

Traditionally, when solving the problem of nonrelativistic scattering of a particle by a fixed potential, physicists and chemists alike resort to the technique of expansion in partial waves.[1,2] In spite of the numerical difficulties attendant upon this method, the phase-shift analysis is not too involved at low particle energies.[1-3] At higher energies, this method, although still the most reliable, becomes an increasingly cumbersome tool because numerous partial waves are required. Consequently, in and beyond the intermediate energy range, it has become popular to avoid partial-wave expansion in calculating the scattering amplitude by using the second Born approximation[4] and other unexpanded or closed-form approximations such as the eikonal method of Glauber,[5] the impact-parameter method of Blankenbecler and Goldberger[6] and the Born-series method of Rabitz.[7] These methods have proved remarkably successful in the analysis of intermediate-energy atomic and hadronic collisions especially the eikonal method.[8,9]

Very recently, Belyaev, Wrzecionko, and Irgaziev[10] have proposed a new closed-form method which relies on a separable expansion for the interaction potential. The applicability of this approach was examined by Belyaev *et al.* only for the case of elastic scattering from a Gaussian potential. Because of its simple features, this separable-expansion (SE) method conceivably may have applications in atomic, nuclear, and high-energy collisions. At the same time, the method is also valid in the determination of the off-shell t matrix, the quantity of paramount importance in the Faddeev-equation treatment of three-particle scattering.[11] In view of these potential applications, it seems highly desirable to conduct other detailed tests on the SE method to ascertain its range of validity.

The present work is precisely an attempt to explore the method, to illustrate its simplicity, to write down the complete analytic expressions for the various integrals arising from its use on Gaussian, Yukawa, and exponential well shapes and finally to investigate its quantitative predictions for the case of elastic scattering from the Yukawa potential of Fanchiotti and Osborn,[12] where exact numerical results are available for comparison.

II. SEPARABLE-EXPANSION METHOD

If we use Dirac notation for the momentum-space matrix elements and take the states $|\vec{k}\rangle$ to be eigenstates of the unperturbed kinetic-energy operator, then the Lippmann-Schwinger equation for the nonrelativistic scattering of a spinless particle of mass m by a potential V can be written as

$$\langle \vec{k}'|t(K^2+i\epsilon)|\vec{k}\rangle = \langle \vec{k}'|V|\vec{k}\rangle + \int \langle \vec{k}'|V|\vec{k}''\rangle (K^2 - k''^2 + i\epsilon)^{-1} \langle \vec{k}''|t(K^2+i\epsilon)|\vec{k}\rangle\, d\vec{k}''. \quad (1)$$

Here, we denote by $\vec{k}$ and $\vec{k}'$ the initial and final wave vectors, units have been determined by choosing $2m/\hbar^2 = 1$ and $E = K^2$ is the energy of the particle.

In the SE method, Belyaev *et al.* introduce the plane waves

$$\vec{\chi}_i(\vec{r}) = (2\pi)^{-3/2} e^{i\vec{k}_i\cdot\vec{r}}, \quad (2)$$

so that

$$\langle \vec{k}|V|\vec{\chi}_i\rangle = (2\pi)^{-3} \int e^{-i\vec{k}\cdot\vec{r}}\, V(r)\, e^{i\vec{k}_i\cdot\vec{r}}\, d\vec{r} = \vec{\eta}_i(\vec{k}) \quad (3)$$

and construct the approximate two-body potential

$$\langle \vec{k}'|\tilde{V}|\vec{k}\rangle = \sum_{i,j=1}^{N} \langle \vec{k}'|V|\vec{\chi}_i\rangle [d^{-1}]_{ij} \langle \vec{\chi}_j|V|\vec{k}\rangle$$

$$= \sum_{i,j=1}^{N} \vec{\eta}_i(\vec{k}')[d^{-1}]_{ij}\vec{\eta}_j(\vec{k}), \tag{4}$$

where

$$d_{ij} = \langle \vec{\chi}_i|V|\vec{\chi}_j\rangle . \tag{5}$$

This SE form of the potential coincides with the exact one if at least one of the two vectors $\vec{k}$ or $\vec{k}'$ matches one of the vectors $\vec{k}_i$ and represents the three-dimensional generalization of the Bateman expansion.[13] It is well known that a separable potential leads to a separable t matrix.[14] Here, it is a simple matter to show that the SE method produces the approximate t matrix

$$\langle \vec{k}'|\tilde{t}(K^2+i\epsilon)|\vec{k}\rangle = \sum_{i,j=1}^{N} \vec{\eta}_i(\vec{k}')[\Delta^{-1}(K^2+i\epsilon)]_{ij}\vec{\eta}_j(\vec{k}), \tag{6}$$

where the tilde over t indicates that the operator $\tilde{t}$ is not the exact one but that yielded by the approximate potential and

$$\Delta_{ij}(K^2+i\epsilon) = d_{ij} + \int \vec{\eta}_i(\vec{k}'')(K^2-k''^2+i\epsilon)^{-1}\vec{\eta}_j(\vec{k}'')\,d\vec{k}''. \tag{7}$$

From Adhikari and Sloan's work,[14] we find the separable expansion in Eq. (6) to be formally equivalent to calculations based on the Schwinger variational principle which connection would seem to assure good convergence for the SE method. For any rank N, $\tilde{t}$ automatically satisfies exact unitarity and time-reversal symmetry since it is obtained from a Hermitian symmetric potential.[14]

The expressions for $\vec{\eta}_i(\vec{k})$ and $\Delta_{ij}(K^2+i\epsilon)$ are those required and determined in second Born approximation[4,7,15] and explicitly analytic forms can be found for familiar potential shapes such as the Gaussian, the Yukawa, and exponential wells. For completeness, we list these here (a) Gaussian potential, $V(r) = V_0 e^{-\mu r^2}$:

$$\vec{\eta}_i^{G}(\vec{k}) = \tfrac{1}{8} V_0(\pi\mu)^{-3/2} e^{-|\vec{k}-\vec{k}_i|^2/4\mu}, \tag{8}$$

$$\Delta_{ij}^{G}(K^2+i\epsilon) = \tfrac{1}{8} V_0(\pi\mu)^{-3/2} e^{-|\vec{k}_i-\vec{k}_j|^2/4\mu} + (\tfrac{1}{8}V_0)^2 2\pi^{-1}\mu^{-2} i\,|\vec{k}_i+\vec{k}_j|^{-1} e^{|\vec{k}_i-\vec{k}_j|^2/8\mu}$$
$$\times\{W[(2\mu)^{-1/2}K + \tfrac{1}{2}(2\mu)^{-1/2}|\vec{k}_i+\vec{k}_j|] - W[(2\mu)^{-1/2}K - \tfrac{1}{2}(2\mu)^{-1/2}|\vec{k}_i+\vec{k}_j|]\}, \tag{9}$$

where $W(x) = e^{-x^2}\operatorname{erfc}(-ix)$ and the limit $\epsilon\to 0$ is taken after the required integral has been performed. (b) Yukawa potential, $V(r) = V_0(e^{-\mu r}/r)$:

$$\vec{\eta}_i^{Y}(\vec{k}) = (V_0/2\pi^2)(\mu^2 + |\vec{k}-\vec{k}_i|^2)^{-1}, \tag{10}$$

$$\Delta_{ij}^{Y}(K^2+i\epsilon) = (V_0/2\pi^2)(\mu^2+|\vec{k}_i-\vec{k}_j|^2)^{-1} + (V_0/2\pi^2)^2 I(1,\mu,\vec{k}_i,1,\mu,\vec{k}_j), \tag{11}$$

where

$$I(m,\lambda,\vec{k}_i,n,\alpha,\vec{k}_j) = \lim_{\epsilon\to 0}\int(\lambda^2+|\vec{k}_i-\vec{k}''|^2)^{-m}(K^2-k''^2+i\epsilon)^{-1}(\alpha^2+|\vec{k}_j-\vec{k}''|^2)^{-n}\,d\vec{k}''$$

$$= \frac{(-)^{m+n}}{(m-1)!\,(n-1)!}\,\frac{\partial^{m-1}}{\partial(\lambda^2)^{m-1}}\,\frac{\partial^{n-1}}{\partial(\alpha^2)^{n-1}}\,I(1,\lambda,\vec{k}_i,1,\alpha,\vec{k}_j) \tag{12}$$

and

$$I(1,\lambda,\vec{k}_i,1,\alpha,\vec{k}_j) = -\pi^2(\beta^2-\rho\gamma)^{-1/2}\ln\frac{\beta+(\beta^2-\rho\gamma)^{1/2}}{\beta-(\beta^2-\rho\gamma)^{1/2}}, \tag{13}$$

$$\rho = -iK[(\lambda+\alpha)^2 + |\vec{k}_i-\vec{k}_j|^2] + \alpha(\lambda^2-K^2+k_i^2) + \lambda(\alpha^2-K^2+k_j^2), \tag{14}$$

$$\rho\gamma = [(\lambda+\alpha)^2+|\vec{k}_i-\vec{k}_j|^2][(\lambda-iK)^2+k_i^2][(\alpha-iK)^2+k_j^2]. \tag{15}$$

In particular, when $\lambda=\alpha=\nu$ and $|\vec{k}_i| = |\vec{k}_j| = K$

$$I(1,\nu,\vec{k}_i,1,\nu,\vec{k}_j) = -2\pi^2\left\{\frac{1}{2KA\sin\frac{1}{2}\phi}\left[\tan^{-1}\left(\frac{\nu K\sin\frac{1}{2}\phi}{A}\right) + \frac{i}{2}\ln\left(\frac{A+2K^2\sin\frac{1}{2}\phi}{A-2K^2\sin\frac{1}{2}\phi}\right)\right]\right\}, \tag{16}$$

$$A^2 = \nu^4 + 4\nu^2K^2 + 4K^4\sin^2\tfrac{1}{2}\phi, \tag{17}$$

and ϕ is the angle between $\vec{k}_i$ and $\vec{k}_j$. (c) Exponential potential, $V(r) = V_0 e^{-\mu r}$:

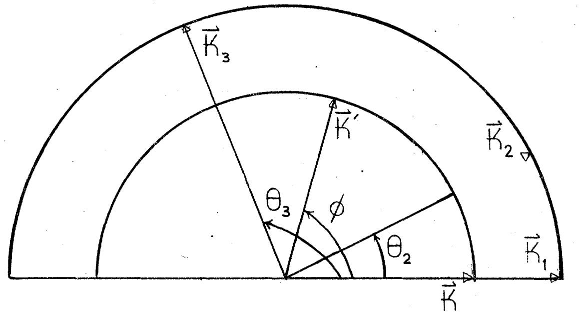

FIG. 1. Plot of the SE parameters $\vec{k}_i$ in the scattering plane.

$$\vec{\eta}_i^E(\vec{k}) = -(\partial/\partial\mu)\vec{\eta}_i^Y(\vec{k}) = (V_0\mu/\pi^2)(\mu^2 + |\vec{k} - \vec{k}_i|^2)^{-2}, \quad (18)$$

$$\Delta_{ij}^E(K^2+i\epsilon) = (V_0\mu/\pi^2)(\mu^2 + |\vec{k}_i - \vec{k}_j|^2)^{-2} + (V_0\mu/\pi^2)^2 I(2, \mu, \vec{k}_i, 2, \mu, \vec{k}_j). \quad (19)$$

The SE approach is applicable to both elastic and inelastic scattering and to the determination of the off-shell two-body t matrix. No partial-wave decomposition is used while the analytic forms of $\vec{\eta}_i(\vec{k})$ and $\Delta_{ij}(K^2+i\epsilon)$ indicate that only one numerical operation is required, viz., the inversion of an $N\times N$ complex matrix.

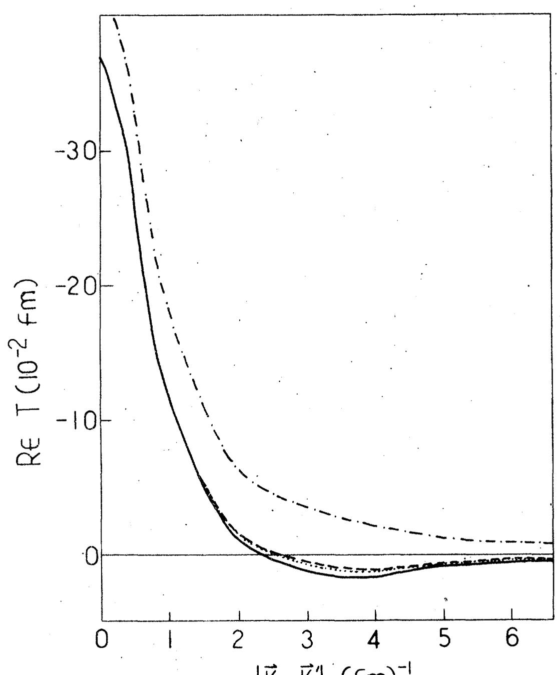

FIG. 2. Real part of the elastic scattering amplitude for the Yukawa potential at $k=4.0$ fm^{-1}. The solid curve shows the exact result, the dashed curve the SE result, the dotted curve the Glauber eikonal result and the dash-dotted curve is the Born approximation.

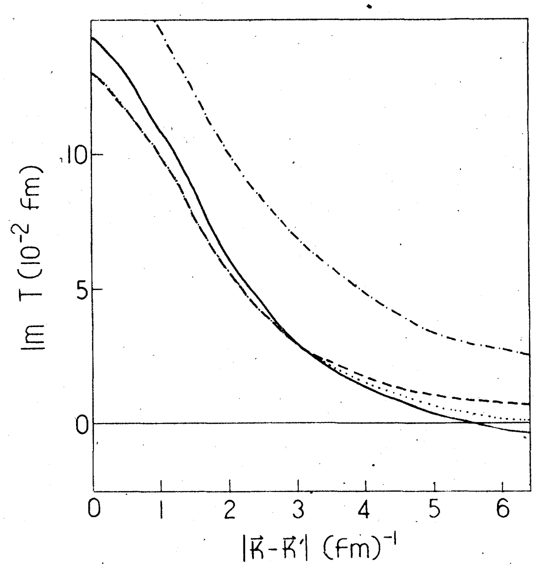

FIG. 3. Imaginary part of the elastic scattering amplitude with the same identification as in Fig. 2.

III. NUMERICAL RESULTS AND DISCUSSION

In our numerical work, we have confined our attention to the Yukawa potential of Fanchiotti and Osborn,[12] with $V_0 = -6.5$ fm^{-1} and $\mu = 1/1.17$ fm^{-1}.

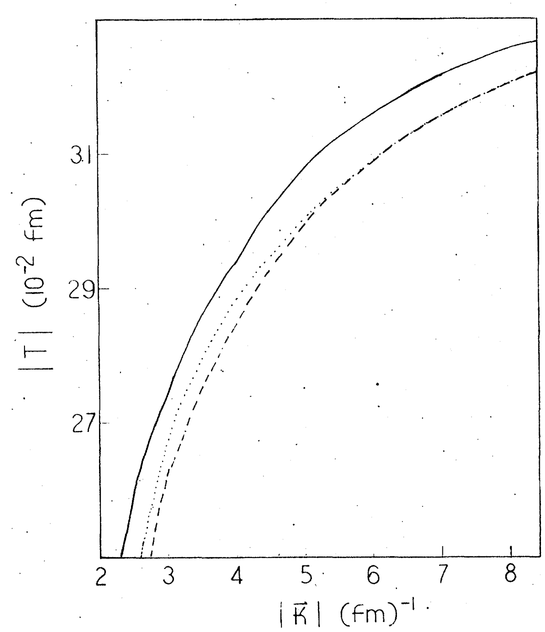

FIG. 4. Modulus of the elastic scattering amplitude with the momentum transfer held at 0.5 fm^{-1}. The same identification is used as in Fig. 2 except that the Born result, constant at 33.5×10^{-2} fm, lies outside the figure and is not shown.

This potential has two bound states in the s-wave channel and a p-wave resonance at 0.5 fm^{-1}. We chose $\vec{k}_i$ to be in the scattering plane so that $\vec{k}_i = (p, \theta_i)$ (see Fig. 1). A comparative examination of the SE, exact, Glauber, and Born-approximation results for elastic scattering at one fixed medium energy, $K = 4.0$ fm^{-1}, are illustrated in Figs. 2 and 3. The SE results, at virtually every momentum transfer, lie almost on top of the Glauber results and are clearly superior to Born approximation although achieved with comparable machinery. Our results, obtained with $p = K$ and $N = 12$, are a good facsimile of the exact results calculated by Fanchiotti and Osborn. From Fig. 4, we see that the SE method yields particularly accurate results above $K = 3.0$ fm^{-1}. We note here a point of technical significance. To prevent the matrix Δ^{-1} from becoming too singular, we had to choose $\vec{k}_i$ such that the θ_i are unevenly spaced over 0°–180°. Problems with inversion occur whenever the matrix elements of Δ are almost equal in value, i.e., for evenly spaced θ_i. Provided this precaution is observed, we derive results which are relatively insensitive to the rank N and values of θ_i; equally accurate magnitudes were achieved with $N = 6$. Although we also varied p, the best results were realized at $p = K$.

The example we have probed in detail in this work certainly does not constitute a complete analysis or test of the SE method. Nevertheless, this study does indicate evidence that Belyaev *et al.* have indeed devised a convenient and accurate approximation for the two-body t matrix on and perhaps off the energy shell. We cannot ignore an important drawback; some definitive criteria must be developed for the choice of the parameters $\vec{k}_i$. Studies should also be performed for cases where the interaction potential possesses a repulsive core. We intend to continue our investigations in those directions.

[1]T. R. Mongan, Nuovo Cimento B 63, 539 (1969).

[2]M. S. Stern, J. Phys. A 5, 426 (1972).

[3]I. H. Sloan and T. J. Brady, Phys. Rev. C 6, 701 (1972).

[4]A. R. Holt and B. L. Moiseiwitsch, in *Advances in Atomic and Molecular Physics*, edited by D. R. Bates and I. Estermann (Academic, New York, 1968), Vol. 4; J. Phys. B 1, 36 (1968).

[5]R. J. Glauber, in *High Energy Collision Theory*, edited by W. E. Brittin (Interscience, New York, 1959).

[6]R. Blankenbecler and M. L. Goldberger, Phys. Rev. 126, 766 (1962).

[7]H. Rabitz, Phys. Rev. A 5, 620 (1972).

[8]R. J. Glauber, in *High Energy Physics and Nuclear Structure*, edited by S. Devons (Plenum, New York, 1970).

[9]E. Gerjuoy and B. K. Thomas, Rep. Prog. Phys. 37, 1345 (1974).

[10]V. B. Belyaev, E. Wrzecionko, and B. F. Irgaziev, Sov. J. Nucl. Phys. 20, 664 (1975).

[11]L. D. Faddeev, Sov. Phys. JETP 12, 1014 (1961); Sov. Phys. Doklady 6, 384 (1961); Sov. Phys. Doklady 7, 600 (1963).

[12]H. Fanchiotti and T. A. Osborn, Nucl. Phys. A 177, 273 (1971).

[13]L. V. Kantorovich and V. I. Krylov, *Approximate Methods of Higher Analysis* (Interscience, New York, 1958).

[14]S. K. Adhikari and I. H. Sloan, Phys. Rev. C 11, 1133 (1975).

[15]R. H. Dalitz, Proc. R. Soc. Lond. A 206, 509 (1951); R. R. Lewis, Jr., Phys. Rev. 102, 537 (1956).