Wave function approach to reaction matrix theory. I*

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A wave function method for computing off-shell K matrix elements is presented. Certain computational advantages are derived thereby. The formalism developed is used to relate the K matrix elements for the exponential potential to tabulated functions.

[NUCLEAR REACTIONS Scattering theory, a wave function approach to K matrix theory.]

I. INTRODUCTION

In recent years a number of investigators[1] have used the reaction matrix (K matrix) as the basis for nuclear reaction calculations. These studies conclude that the K matrix formalism represents an effective way to evaluate the collision matrices for nuclear reactions. In a typical cross section calculation one usually computes the K matrix elements by means of an iterated version of the Shakin-Hufner-Lemmer method.[2] Keeping in mind the usefulness of K matrix elements in the studies of scattering reactions, the integral equation for the K operator has been studied in some detail by Tobocman and Nagarajan,[3] by Ernst *et al*,[4] and by Kouri and Levin.[5]

The integral equation for the K operator is given by

$$K(E)=V+V\,G_0^S(E)K(E), \tag{1}$$

with

$$G_0^{(S)}(E)=\frac{P}{E-H_0}=\frac{1}{2}\left(\frac{1}{E-H_0+i\epsilon}+\frac{1}{E-H_0-i\epsilon}\right),\quad \epsilon\to 0^+. \tag{2}$$

In Eqs. (1) and (2), V is the two-particle potential, E the energy parameter, and H_0 the kinetic energy operator.

It has been observed that the formal solutions of Eq. (1) are not given in any simple form containing $P/(E-H)$ since this operator does not have a Lippmann-Schwinger iteration.[6] Kouri and Levin have obtained the elements of the K operator in terms of an altered K matrix, which they denote by $\tilde{K}$. The Hermitian operator $\tilde{K}$ is defined by

$$\tilde{K}(E)=V+V\frac{P}{E-H}V=\operatorname{Re}T(E), \tag{3}$$

where

$$H=H_0+V. \tag{4}$$

In Eq. (3) Re $T(E)$ denotes the real part of the transition operator

$$T(E)=V+V(E-H_0+i\epsilon)^{-1}T(E). \tag{5}$$

The on-shell, half-off-shell, and off-shell matrix elements of $\tilde{K}$ are related[5] to those of K by

$$\operatorname{Re}\langle k|T_l(k^2)|k\rangle=\langle k|\tilde{K}_l(k^2)|k\rangle=\cos^2\delta_l(k)\langle k|K_l(k^2)|k\rangle, \tag{6}$$

$$\operatorname{Re}\langle p|T_l(k^2)|k\rangle=\langle p|\tilde{K}_l(k^2)|k\rangle=\cos^2\delta_l(k)\langle p|K_l(k^2)|k\rangle \tag{7}$$

and

$$\operatorname{Re}\langle p|T_l(k^2)|q\rangle=\langle p|\tilde{K}_l(k^2)|q\rangle=\langle p|K_l(k^2)|q\rangle+\frac{\pi k}{2\cos^2\delta_l(k)}\tan\delta_l(k)\langle p|\tilde{K}_l(k^2)|k\rangle\langle k|\tilde{K}_l(k^2)|q\rangle, \tag{8}$$

where $\delta_l(k)$ is the phase shift for the lth partial wave. We work with units in which $\hbar^2/2m$ is unity. Relations (6), (7), and (8) show that a determination of the matrix elements of $\tilde{K}$ together with the phase shift $\delta_l(k)$ leads to an evaluation of those of K itself. Thus in this approach one is not required to solve Eq. (1).

The present paper is directed towards the implementation of a wave function method for computing the K matrix, which might serve as an alternative to the integral equation method described above. The wave function approach of van Leeuwen and Reiner[7] has been found very useful to calculate the T matrix in closed form.[8] In their approach the

T matrix is obtained from the solution of an inhomogeneous Schrödinger-like equation which satisfies the outgoing wave boundary condition. It is, therefore, expected that the solution of such an inhomogeneous equation with a standing wave boundary condition could be employed to calculate the matrix element of the K operator.

In Sec. II we derive the formal method for computing the off-shell K matrix by the wave function approach. The results outlined in Sec. II are applied in Sec. III to obtain a closed form expression for the fully off-shell K matrix for the exponential potential. In Sec. IV we summarize our outlook on such a calculation.

II. OFF-SHELL K MATRIX

Following van Leeuwen and Reiner we define a wave operator

$$\Omega(E) = 1 + G_0^S(E)K(E). \tag{9}$$

Combining Eqs. (1) and (9) and neglecting squares and higher powers of ϵ we obtain

$$K(E) = V\Omega(E) \tag{10}$$

and

$$(E - H_0 - V)\Omega(E) = E - H_0. \tag{11}$$

In a mixed representation Eq. (11) reads

$$[E - \nabla^2 - v(r)]\langle \vec{r}\,|\,\Omega(E)\,|\,qlm\rangle = (E - q^2)\langle \vec{r}\,|\,qlm\rangle, \tag{12}$$

where

$$\langle \vec{r}\,|\,qlm\rangle = \left(\frac{2}{\pi}\right)^{1/2} j_l(qr)y_{lm}(\hat{r}). \tag{13}$$

The objects $j_l(qr)$ and $y_{lm}(\hat{r})$ represent the usual spherical Bessel function and spherical harmonic. It may be noted that Efimov and Schulz[9] have recently computed the off-shell K matrix for a Jastrow-type potential by imposing certain boundary conditions on the solutions of Eq. (12).

The boundary conditions for large r on the solution of Eq. (12) are obtained from Eq. (9). We have

$$\langle \vec{r}\,|\,\Omega(E)\,|\,qlm\rangle = \left(\frac{2}{\pi}\right)^{1/2} j_l(qr)y_{lm}(\hat{r}) + \int \langle \vec{r}\,|\,G_0^S(E)\,|\,\vec{r}'\rangle d\vec{r}'\langle \vec{r}'\,|K(E)\,|\,qlm\rangle. \tag{14}$$

In Eq. (14) we now insert the representation for the standing wave Green's function

$$\langle \vec{r}\,|\,G_0^S\,|\,\vec{r}'\rangle = -k\sum_{lm} j_l(kr_<)\eta_l(kr_>)y_{lm}(\hat{r})y_{lm}^*(\hat{r}') \tag{15}$$

and let r become large. We thus find

$$\langle \vec{r}\,|\,\Omega(E)\,|\,qlm\rangle \underset{r\to\infty}{\sim} \left(\frac{2}{\pi}\right)^{1/2} y_{lm}(\hat{r})(qr)^{-1}[\sin(qr - \tfrac{1}{2}l\pi) - \tfrac{1}{2}\pi q\langle klm\,|K(E)\,|\,qlm\rangle\cos(kr - \tfrac{1}{2}l\pi)]. \tag{16}$$

In Eq. (16) $\langle klm\,|K(E)\,|\,qlm\rangle$ represents the half-off-shell K matrix elements. By comparing the on-shell version ($q = k$) of Eq. (16) with the asymptotic solution[10]

$$\psi(r) \underset{r\to\infty}{\sim} \left(\frac{2}{\pi}\right)^{1/2} y_{lm}(\hat{r})(kr)^{-1}[\sin(kr - \tfrac{1}{2}l\pi) + \tan\delta_l \cos(kr - \tfrac{1}{2}l\pi)] \tag{17}$$

of the Schrödinger equation with standing wave boundary condition, we see that the on-shell K matrix elements have the normalization

$$\langle klm\,|K(E)\,|\,klm\rangle = -\frac{2}{\pi k}\tan\delta_l(k). \tag{18}$$

Since the potential in Eq. (12) is central we can write

$$\langle \vec{r}\,|\,\Omega(E)\,|\,qlm\rangle = \left(\frac{2}{\pi}\right)^{1/2}(qr)^{-1}\phi_l(k,q,r)y_{lm}(\hat{r}). \tag{19}$$

Substitution of Eq. (19) into Eq. (12) yields

$$\left[k^2 + \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - V(r)\right]\phi_l(k,q,r) = (k^2 - q^2)u_l(qr), \tag{20}$$

where $u_l(qr)$ is the Ricatti-Bessel function.[11] The solutions of Eq. (12) have been shown to be related[12] to the solutions of the equation

$$\left[k^2 + \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - V(r)\right]f_l(k,q,r) = (k^2 - q^2)e^{il\pi/2}\omega_l^+(qr), \tag{21}$$

where $\omega_l^+(qr)$ is the Ricatti-Hankel function of the first kind. The solution of Eq. (21) which is of interest has the asymptotic normalization

$$f_l(k,q,r) \underset{r\to\infty}{\sim} e^{iqr}. \tag{22}$$

From Eqs. (21) and (22) we see that when $q=\pm k$ this function goes over to the Jost solution[13]

$$f_l(\pm k,r)=f_l(k,\pm k,r). \tag{23}$$

Using Eqs. (19), (22), and (23) in (16), it is easy to see that for finite r the object $\phi_l(k,q,r)$ is given by

$$\phi_l(k,q,r)=-\tfrac{1}{4}\pi q\langle k|K_l(E)|q\rangle[e^{-il\pi/2}f_l(k,r)+e^{il\pi/2}f_l(-k,r)]+(1/2i)[e^{-il\pi/2}f_l(k,q,r)-e^{il\pi/2}f_l(k,-q,r)], \tag{24}$$

where

$$\langle k|K_l(E)|q\rangle=\langle klm|K(E)|qlm\rangle. \tag{25}$$

We note that $\phi_l(k,q,r)$ represents the off-shell wave function[14] regular at the origin. The behavior of $\phi_l(k,q,r)$ for small r will determine the half-off-shell K matrix elements. We have

$$\langle k|K_l(E)|q\rangle=\left(\frac{k}{q}\right)^l\frac{2\,\mathrm{Im}f_l(k,q)}{\pi q|f_l(k)|\cos\delta_l(k)}. \tag{26}$$

In deducing Eq. (26) we have used the following definition for the off-shell Jost function[12]:

$$f_l(k,q)=\frac{q^l e^{-il\pi/2}(2l+1)}{(2l+1)!!}\lim_{r\to 0} r^l f_l(k,q,r). \tag{27}$$

We have also used

$$f_l(k,-q,r)=f_l^*(k,q,r) \tag{28a}$$

and

$$f_l(k,q)=f_l^*(k,-q). \tag{28b}$$

In Eq. (26) $\delta_l(k)$ is the negative of the phase of the Jost function $f_l(k)$ which by definition is the phase shift.[6]

The off-shell K matrix can be obtained by combining the relations (10), (13), and (19). We have

$$\langle p|K_l(k^2)|q\rangle=\frac{2}{\pi pq}\int_0^\infty u_l(pr)v(r)\phi_l(k,q,r)dr. \tag{29}$$

With the help of Eq. (24), Eq. (29) reduces to

$$\langle p|K_l(k^2)|q\rangle=\frac{2}{\pi pq}\left\{\int_0^\infty dr\,u_l(pr)V(r)\left[\beta_l(r)-\left(\frac{k}{q}\right)^l\frac{\mathrm{Im}f_l(k,q)}{|f_l(k)|\cos\delta_l}\alpha_l(r)\right]\right\}, \tag{30}$$

where

$$\alpha_l(r)=\cos\tfrac{1}{2}l\pi\,\mathrm{Re}f_l(k,r)+\sin\tfrac{1}{2}l\pi\,\mathrm{Im}f_l(k,r), \tag{31a}$$

$$\beta_l(r)=\cos\tfrac{1}{2}l\pi\,\mathrm{Im}f_l(k,q,r)-\sin\tfrac{1}{2}l\pi\,\mathrm{Re}f_l(k,q,r), \tag{31b}$$

and

$$\nu_l(r)=\cos\tfrac{1}{2}l\pi\,\mathrm{Im}f_l(k,r)-\sin\tfrac{1}{2}l\pi\,\mathrm{Re}f_l(k,r). \tag{31c}$$

Equation (30) represents the basic equation for computing the off-shell K matrix by the wave function method. A useful check on the validity of this equation is that one can relate Eq. (30) with the real part of the T matrix given by Fuda and Whiting [Eqs. (2.18) and (2.30) of Ref. 12] to obtain the relations (6), (7), and (8) between K and $\tilde{K}$.

III. EXPONENTIAL POTENTIAL–AN EXAMPLE

For the exponential potential

$$V(r)=-\frac{z_0^2}{4a^2}e^{-r/a}, \tag{32a}$$

the s-wave part of Eq. (23) is given by

$$\left[k^2+\frac{d^2}{dr^2}+\frac{z_0^2}{4a^2}e^{-r/a}\right]f(k,q,r)=(k^2-q^2)e^{iqr}. \tag{32b}$$

In writing out Eq. (32b) we omitted the subscript $l=0$. We now change the variable by substituting $z=z_0e^{-r/2a}$ and arrive at the equation

$$\left[\frac{d^2}{dz^2}+\frac{1}{z}\frac{d}{dz}+(1-\nu^2/z^2)\right]f(k,q,z)=4a^2(k^2-q^2)z_0^{2iaq}z^{-2-2iaq}. \tag{33}$$

The particular solution of Eq. (33) is given by[15]

$$f(k,q,z)=4a^2(k^2-q^2)z_0^{2iqa}s_{\mu\nu}, \tag{34}$$

where $s_{\mu\nu}$ is the Lommel function written as

$$s_{\mu\nu}(z)=\frac{z^{\mu+1}}{(\mu+\nu+1)(\mu-\nu+1)}\times{}_1F_2(\tfrac{1}{2}\mu-\tfrac{1}{2}\nu+\tfrac{3}{2}\,,\ \tfrac{1}{2}\mu+\tfrac{1}{2}\nu+\tfrac{3}{2}\,|-\tfrac{1}{4}Z^2)\ , \quad (35)$$

with

$$\mu=-1-2iqa\ ,\quad \nu=2ika\ . \quad (35')$$

The function ${}_1F_2(:::|x)$ is a special case of the generalized hypergeometric function defined by Luke.[16] Inserting Eq. (35) in Eq. (34) we have

$$f(k,q,z)=z_0^{\,2iqa}z^{-2iqa}\,{}_1F_2\begin{pmatrix}1\\1-ika-iqa,\ \ 1+ika-iqa\end{pmatrix}\left|-\tfrac{1}{4}z^2\right.\Big)\ . \quad (36)$$

It can be easily shown that in the asymptotic limit

$$f(k,q,z)\underset{r\to\infty}{\sim}e^{iqr}\ . \quad (37)$$

Equation (37) represents the correct asymptotic limit prescribed for the off-shell Jost solution. The on-shell Jost solution $f(k,z)$ is given by

$$f(k,z)=\lim_{q\to k}f(k,q,z)=(\tfrac{1}{2}z_0)^{2ika}\Gamma(1-2ika)J_{-2ika}(z)\ . \quad (38)$$

In writing Eq. (38) we have used

$$\Gamma(\alpha+1)\left(\frac{z}{2}\right)^{-\alpha}J_\alpha(z)={}_0F_1(\alpha+1;-\tfrac{1}{4}z^2)\ . \quad (39)$$

From Eqs. (36) and (38) the off-shell and on-shell Jost functions are obtained in the forms

$$f(k,q)={}_1F_2\begin{pmatrix}1\\1-ika-iqa,\ \ 1+ika-iqa\end{pmatrix}\left|-\tfrac{1}{4}z_0^2\right.\Big) \quad (40)$$

and

$$f(k)=(\tfrac{1}{2}z_0)^{2ika}\Gamma(1-2ika)J_{-2ika}(z_0)\ . \quad (41)$$

In terms of the Jost solutions and Jost function, the off-shell wave function $\phi(k,q,r)$ regular at the origin can be written as

$$\phi(k,q,r)=A(k,q)[c(k)J_{-2iak}(z)+c^*(k)J_{2iak}(z)]+B(k,q)[z_0^{\,2iqa}s_{-1-2iqa,2ika}(z)-z_0^{-2iqa}s_{-1+2iqa,2ika}(z)]\ , \quad (42)$$

where

$$A(k,q)=-\tfrac{1}{4}\pi q\langle k|K|q\rangle\ , \quad (43a)$$

$$c(k)=(\tfrac{1}{2}z_0)^{2ika}\Gamma(1-2ika)\ ,\qquad c^*(k)=(\tfrac{1}{2}z_0)^{-2ika}\Gamma(1+2ika)\ , \quad (43b)$$

and

$$B(k,q)=-2ia^2(k^2-q^2)\ , \quad (43c)$$

with

$$\langle k|K|q\rangle=\frac{8a^2(k^2-q^2)[z_0^{\,2iqa}s_{-1-2iqa,2ika}(z_0)-z_0^{-2iqa}s_{-1+2iqa,2ika}(z_0)]}{i\pi q[c(k)J_{-2ika}(z_0)+c^*(k)J_{2ika}(z_0)]}\ . \quad (44)$$

With the help of Eqs. (29), (32a), and (42), the s-wave part of the off-shell K matrix is obtained in the form

$$\langle p|K|q\rangle=\frac{z_0}{2i\pi apq}[A(k,q)I_1+B(k,q)I_2]\ , \quad (45)$$

where

$$I_1=\int_0^{z_0}[(z/z_0)^{1+2iap}-(z/z_0)^{1-2iap}][c(k)J_{-2ika}(z)+c^*(k)J_{-2ika}(z)]dz \quad (46)$$

and

$$I_2=\int_0^{z_0}[(z/z_0)^{1+2iap}-(z/z_0)^{1-2iap}][z_0^{\,2iqa}s_{-1-2iqa,2ika}(z)-z_0^{-2iqa}s_{-1+2iqa,2ika}(z)]dz\ . \quad (47)$$

Fortunately, the integrals in Eqs. (46) and (47) can be related to the tabulated integrals[17] given by

$$y(p,k)=\int_0^{z_0}(z/z_0)^{1+\lambda}J_{-\nu}(z)\frac{dz}{z_0}=\frac{(2/z_0)^\nu}{(\lambda-\nu+2)\Gamma(1-\nu)}\,{}_1F_2\begin{pmatrix}\tfrac{1}{2}(\lambda-\nu+2)\\1-\nu\ \ ,\tfrac{1}{2}(\lambda-v+4)\end{pmatrix}\left|\tfrac{1}{4}z_0^2\right.\Big) \quad (48)$$

and

$$x(p,q,k)=\int_0^{z_1} z^{2\alpha-\mu}s_{\mu,\nu}(z)dz$$
$$=\frac{1}{2}\frac{z_0^{2(\alpha+1)}\Gamma(1+\alpha)}{(\mu-\nu+1)(\mu+\nu+1)\Gamma(\alpha+2)}\,{}_2F_3\left(\begin{matrix}1, & 1+\alpha & \\ \frac{1}{2}(\mu-\nu+3), & \frac{1}{2}(\mu+\nu+3), & \alpha+2\end{matrix}\middle|-\tfrac{1}{4}z_0^2\right), \tag{49}$$

with $\lambda=2ipa$, $\alpha=ia(p-q)$, and μ and ν given by Eq. (35′).

Combining Eqs. (45), (46), (47), (48), and (49) we obtain the expression for the s-wave part of the exponential potential K matrix in the form

$$\langle p|K|q\rangle=\frac{z_0}{2i\pi apq}\Big(A(k,q)z_0\{c(k)[y(p,-k)-y(-p,-k)] + c^*(k)[y(p,k)-y(-p,k)]\}+B(k,q)\{x(p,q,k) - x(p,-q,k)-x(-p,q,k)+x(-p,-q,k)\}\Big). \tag{50}$$

IV. CONCLUSION

Based on the van Leeuwen-Reiner approach to off-shell scattering we have presented a straightforward method to compute the matrix elements of the K operator. We have expressed the K matrix elements as a single quadrature over the potential sandwiched between a plane wave and an appropriate off-shell wave function. It is seen that the results for the off-shell K matrix element for the exponential potential can be expressed in closed form involving functions whose series representations have infinite radii of convergence. It should therefore be possible to sum the series on a computer and use it as a check on programs which evaluate K matrix elements by numerical methods.

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[1]C. Block and V. Gillett, Phys. Lett. 16, 62 (1965); W. M. MacDonald and A. Makjian, Phys. Rev. 160, 730 (1967); F. Schmittroth and W. Tobocman, Phys. Rev. C 3, 1010 (1971); D. Rodijak, W. Tobocman, and D. K. Tandon, Phys. Rev. C 6, 1192 (1972).

[2]J. Hufner and R. H. Lemmer, Phys. Rev. 175, 1394 (1968); J. Hufner and C. M. Shakin, *ibid*. 175, 1350 (1968).

[3]W. Tobocman and M. A. Nagarajan, Phys. Rev. 163, 1011 (1967).

[4]D. J. Ernst, C. M. Shakin, R. M. Thaler, and D. L. Weiss (unpublished); Phys. Rev. C 8, 2056 (1973).

[5]D. J. Kouri and F. S. Levin, Phys. Lett. 48B, 203 (1974); Ann. Phys. (N.Y.) 83, 316, 326 (1974); Phys. Rev. C 10, 2096 (1974).

[6]R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966).

[7]J. M. J. Van Leeuwen and A. S. Reiner, Physica (The Hague) 27, 99 (1961).

[8]M. G. Fuda, J. Math. Phys. 12, 1163 (1971); B. Talukdar, M. N. Sinha Roy, N. Mallick, and D. K. Nayek, Phys. Rev. C 12, 370 (1975); M. N. Sinha Roy, B. Talukdar, and D. Chatterji, J. Math. Phys. (to be published).

[9]V. N. Efimov and H. Schulz, Nucl. Phys. A235, 436 (1974).

[10]T. Wu and T. Ohmura, *Quantum Theory of Scattering* (Prentice-Hall, New Jersey, 1962).

[11]A. Messiah, *Quantum Mechanics* (Wiley-Interscience, New York, 1961, 1962), Vols. 1 and 2.

[12]M. G. Fuda and J. S. Whiting, Phys. Rev. C 8, 1255 (1973).

[13]R. Jost, Helv. Phys. Acta 20, 256 (1974).

[14]O. P. Bahethi and M. G. Fuda, J. Math. Phys. 12, 2076 (1971).

[15]A. W. Babister, *Transcendental Functions Satisfying Nonhomogeneous Linear Differential Equations* (MacMillan, New York, 1967).

[16]Y. L. Luke, *The Special Functions and Their Approximations* (Academic, New York, London, 1969), Vol. 1.

[17]I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series and Products*, translated by A. Jaffrey (Academic, New York, 1965).