Jost function for coupled partial waves of the Reid soft-core potential

T. Sasakawa
Department of Physics, Tohoku University, 980-Sendai, Japan

T. Sawada
Department of Applied Mathematics, Faculty of Engineering Science, Osaka University, 560-Toyonaka, Japan
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It is pointed out that the usual expression of the scattering amplitude of the Jost matrix can be used to the states coupled by the potential with $1/r$ singularity, as well as less singular couplings. The expression is useful for practical numerical calculations.

When the wave function of a scattering problem can be expressed in the form of a Fredholm integral equation, the Jost matrix method yields the most general and complete solution.[1,2] The denominator of the scattering amplitude, which is called the Jost function, is the Fredholm determinant. For the coupled states, if the coupling potential is well-behaved, the numerator and the denominator of the amplitude are obtained by the usual prescription. However, as pointed out by Newton,[3,4] if the coupling potential has $1/r$ singularity as in the Reid soft core potential (RSC),[5] the Jost matrix element [see, Eq. (17)] diverges since it contains overlap integrals of a regular solution of one orbital angular momentum l and an irregular solution of the higher one $l'=l+2$. A remedy to this difficulty for a regular solution has been proposed by Newton.[3,4] The aim of the present paper is to present a practical method of overcoming this difficulty by treating the $1/r$ coupling and less singular couplings on the same basis with a slight modification of the formula. This is done by inspecting the singular behavior near the origin of the irregular solutions. The present method provides a practical way of numerically solving the wave functions for coupled (and, of course, uncoupled) partial waves on the basis of the Jost matrix.

For completeness, first let us recapitulate the Jost matrix theory in a manner which has been presented before.[6] We use the following functions for the lth partial wave;

$$u_l(\rho)=\rho j_l(\rho), \quad v_l(\rho)=-\rho n_l(\rho) , \qquad w_l(\rho)=v_l(\rho)+iu_l(\rho) , \tag{1}$$

where $j_l(\rho)$ and $n_l(\rho)$ are the spherical Bessel and Neumann functions. To keep symmetry of the formula, we normalize the initial wave as $u_l(kr)/\sqrt{k}$. Let $|\psi\rangle$ and $|u\rangle$ stand for the matrices

$$|\psi\rangle=\begin{pmatrix}\psi_{ll} & \psi_{ll'}\\ \psi_{l'l} & \psi_{l'l'}\end{pmatrix}, \quad |u\rangle=(1/\sqrt{k})\begin{pmatrix}u_l & 0\\ 0 & u_{l'}\end{pmatrix}, \tag{2}$$

and G and V the matrices

$$G=\begin{pmatrix}G_l & 0\\ 0 & G_{l'}\end{pmatrix}, \qquad V=(2m/\hbar^2)\begin{pmatrix}V_{ll} & V_{ll'}\\ V_{l'l} & V_{l'l'}\end{pmatrix} , \tag{3}$$

where

$$G_l=-(1/k)w_l(kr_>)u(kr_<) . \tag{4}$$

Then, the regular solution of the Schrödinger equation for the coupled partial waves reads

$$|\psi\rangle=|u\rangle+GV|\psi\rangle . \tag{5}$$

In terms of the wave matrix Ω defined by

$$|\psi\rangle=\Omega|u\rangle , \tag{6}$$

Eq. (5) and the scattering amplitude read

$$\Omega|u\rangle=(1+GV\Omega)|u\rangle \qquad \text{(1: the unit matrix)} \tag{7}$$

and

$$\langle u|T|u\rangle=\langle u|V\Omega|u\rangle . \tag{8}$$

Using the step function $\theta(x)$ ($=1$ for $x>0$, $=0$ for $x<0$), we introduce another Green's function

$$g_l=-\frac{1}{k}[u_l(kr)v_l(kr') - v_l(kr)u_l(kr')]\theta(r'-r) . \tag{9}$$

The matrices $|v\rangle$ and $|w\rangle$ are defined in a similar manner as in Eq. (2). Then, the Green's function G is decomposed as

$$G=-|w\rangle\langle u|+g . \tag{10}$$

If we use a real matrix ω defined by

$$\omega=1+gV\omega \tag{11}$$

Eq. (7) is expressed as

$$\Omega|u\rangle=\omega(|u\rangle-|w\rangle\langle u|T|u\rangle) . \tag{12}$$

Noting that the function $v_l(\rho)$ behaves near the origin as

$$v_l(\rho) \underset{\rho\to 0}{\to} (2l-1)!!/\rho^l \quad , \tag{13}$$

we define the matrices R and C by

$$R=\begin{pmatrix}(kr)^l & 0\\ 0 & (kr)^{l'}\end{pmatrix} ,$$
$$C=\begin{pmatrix}(2l-1)!! & 0\\ 0 & (2l'-1)!!\end{pmatrix} . \tag{14}$$

When $gV\omega|w\rangle$ (or $gV\omega|u\rangle$) of Eq. (11) behaves near the origin as $|v\rangle$, we multiply R on both sides of Eq. (12), and take the limit $r\to 0$. Then, we obtain the formula

$$\lim_{r\to 0} R\omega|w\rangle\langle u|T|u\rangle = \lim_{r\to 0} R\omega|u\rangle \quad . \tag{15}$$

This is the usual expression of the scattering amplitude.[1,6]

On the other hand, we define the J matrix (the Jost matrix) by

$$J = V\omega \tag{16}$$

and operate V from the left of Eq. (12). Then, the T matrix elements are expressed in terms of the J-matrix elements as

$$(1+\langle u|J|w\rangle)\langle u|T|u\rangle = \langle u|J|u\rangle \quad . \tag{17}$$

A direct proof of equivalence of Eqs. (15) and (17) may be

$$\lim_{r\to 0} R\omega|w\rangle = \lim_{r\to 0} R(1+gV\omega)|w\rangle$$
$$= C(1+\langle u|V\omega|w\rangle) \quad , \tag{18}$$

where we have assumed the same singularity property near the origin for $gV\omega|w\rangle$ and $|v\rangle$. Equation (18) shows that this assumption is equivalent to the assumption of the existence of $\langle u|J|w\rangle$.

In the case of RSC, the matrix element $\langle u|J|w\rangle$ is infinite. Also $gV\omega|w\rangle$ (or $gV\omega|u\rangle$) of Eq. (11) does not behave near the origin as $|v\rangle$. Indeed, we find that one set of the irregular solutions of coupled partial waves l and $l'=l+2$ for RSC behaves near the origin as

$$\xi_l=\sum_{n=0}^{\infty} A_n r^{n-l-1} + \ln r \sum_{n=0}^{\infty} C_n r^{n-1} + (\ln r)^2 \sum_{n=0}^{\infty} E_n r^{n+l+1} + (\ln r)^3 \sum_{n=0}^{\infty} G_n r^{n+l+4} \quad , \tag{19}$$

$$\xi_{l'}=\sum_{n=0}^{\infty} B_n r^{n-l-2} + \ln r \sum_{n=0}^{\infty} D_n r^{n-l+1} + (\ln r)^2 \sum_{n=0}^{\infty} F_n r^{n+l+2} + (\ln r)^3 \sum_{n=0}^{\infty} H_n r^{n+l+3} \quad . \tag{20}$$

The remaining three linearly independent sets of solutions are obtained from Eqs. (19) and (20): To obtain another set of irregular solutions, we put all A_n and B_n equal to zero, and reduce one power of $\ln r$. A regular solution is obtained by further putting all C_n and D_n equal to zero and reducing one power of $\ln r$. Another regular solution is simply given by the series with G_n and H_n without $\ln r$ factor. For each set, H_0 alone is free, other coefficients being determined by recurrence relations, except for F_1, D_{2l+2}, and B_{2l+5} which can be set equal to zero. Hence, if we modify the matrix R of Eq. (14) to

$$R=\begin{pmatrix}(kr)^{l+1} & 0\\ 0 & (kr)^{l+2}\end{pmatrix} \tag{21}$$

we can also use Eq. (15) as the formula of the scattering amplitude for RSC.

Equation (15) is very useful in practice: To calculate $R\omega|w\rangle$ (or $R\omega|u\rangle$), we take $1|w\rangle$ (or $1|u\rangle$) as the starting function at a large distance from the origin, and simply proceed with inward integration. Near the origin, the wave function so obtained is smoothly joined to a linear combination of the four sets of solutions.

As an example, the T matrix for the ${}^3S_1+{}^3D_1$ states for RSC at $k=0.538\ \mathrm{fm}^{-1}$ ($E_{\mathrm{lab}}=24$ MeV) is given below. The calculation is done on an NEAC 2200-700 with the Runge-Kutta method using the x mesh 0(0.001)0.012(0.01)0.112(0.05)1.112(0.1) 2.112(0.2)8.112, where x is the distance in units of pion Compton wavelength:

$$T=\mathcal{T}^{-1}\mathrm{Im}\,\mathcal{T}=\begin{pmatrix}0.142\,63+0.978\,17i, & -0.006\,16-0.031\,21i\\ -0.006\,16-0.031\,22i, & 0.049\,64-0.003\,49i\end{pmatrix} , \tag{22}$$

where

$$\mathcal{T}=\lim_{r\to 0} R\omega|w\rangle$$
$$=\begin{pmatrix} 1.381\,376\,467\,68\times 10^{6}+1.557\,839\,544\,05\times 10^{7}i, & -1.134\,304\,136\,81\times 10^{8}-5.171\,193\,600\,60\times 10^{6}i \\ -1.030\,800\,037\,06\times 10^{5}-1.162\,478\,964\,60\times 10^{6}i, & 8.464\,316\,465\,89\times 10^{6}+3.858\,808\,029\,99\times 10^{5}i \end{pmatrix}. \tag{23}$$

These values give the nuclear bar phase shifts $\delta_0=1.4259$, $\delta_2=-0.0493$, and the mixing parameter $\rho_1=0.0636$ in agreement with Reid.[5] Notice the very severe cancellation that occurs in getting T from $\mathcal{T}$. This is due to rather singular nature of the solution near the origin. Other uncoupled and coupled partial waves are also treated by this method, and are found to yield phase shifts and mixing parameters in agreement with Reid,[5] e.g. $\delta(^3P_2)=0.0377$, $\delta(^3F_2)=0.0016$, $\rho_2=-0.0262$ for $E_{\text{lab}}=24$ MeV with the above mesh. Bound states can also be obtained by setting the determinant of $\lim_{r\to 0}R\omega|w\rangle$ equal to zero. We have found the deuteron binding energy at $|E|=2.231$ MeV for RSC. In conclusion, we see thus the Jost matrix method is not only formally complete but also numerically practicable for a realistic potential such as RSC.

[1]R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966).
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[3]See Ref. 1, p. 464.
[4]R. G. Newton, Phys. Rev. 100, 412 (1955).
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