PHYSICAL REVIEW C VOLUME 18, NUMBER 1 JULY 1978

Treatment of the Schrödinger equation with a nonlocal nonsymmetric potential*

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(Received 21 October 1977)

A method for expanding a nonlocal, nonsymmetric potential as the sum of separable terms is presented. The method of calculating the bound state and the scattering amplitude is described. A numerical example of the nonlocal potential related to *n-d* elastic scattering is given.

[NUCLEAR REACTIONS Method for calculating a nonlocal, nonsymmetric potential, with an example.]

I. INTRODUCTION

In the (energy independent) optical model,[1] in the resonating group model,[2,3] and in the elastic n-d scattering problem,[4] we meet with a nonlocal nonsymmetric potential. Although a method for solving the Schrödinger equation in such a potential has been proposed,[5] it has not been shown to be practical as yet.

Recently, we have suggested another method,[6] in which the nonlocal nonsymmetric potential $U(r, r')$ is divided into a real symmetric part and a real antisymmetric part which is equal to $i=\sqrt{-1}$ times a Hermitian part. The eigenfunctions for each part are defined, and $U(r, r')$ is expressed as the sum of separable potentials in terms of these functions. For a real symmetric kernel, the method of calculating the eigenfunctions has been well established. However, for a Hermitian kernel, the eigenfunctions have not been given much consideration in the literature. In Ref. 6, we have defined these functions and proposed a practical method of calculating them.

In the present paper, we present a more elegant way of computing the eigenfunctions and their eigenvalues for the Hermitian part of $U(r, r')$. In Sec. II, we describe the method of separable expansion. The real symmetric part is treated the same way as in Ref. 6. However, the treatment of the Hermitian part given here is new and has not been discussed anywhere else to the authors' knowledge. The separable expansion of $U(r, r')$ facilitates the calculations of various processes a great deal, if the number of separable terms is not too large. The best way, then, is to express the main part of $U(r, r')$ as the sum of a few separable terms, and treat the remaining part of $U(r, r')$ as perturbation. The process is explained in Sec. III for the calculations of bound states and scattering states. In order to demonstrate the feasibility of the method, in Sec. IV, we give as an example the approximation of the nonlocal potential that we encounter in the $n+d$ scattering problem in terms of a few separable terms.

II. SEPARABLE EXPANSION

Let the real, nonlocal, nonsymmetric potential $U(r, r')$ be divided into two parts,

$$U(r, r') = U_S(r, r') - iU_H(r, r') , \tag{1}$$

where the symmetric part $U_S(r, r')$ and the Hermitian part $U_H(r, r')$ are defined by

$$U_S(r, r') = \tfrac{1}{2}[U(r, r') + U(r', r)] \tag{2}$$

and

$$U_H(r, r') = \tfrac{1}{2}i[U(r, r') - U(r', r)] . \tag{3}$$

Since $U_S(r, r')$ is real symmetric, we can easily obtain the maximum eigenvalue $\lambda_{S,1}$ and its eigenfunction $\psi_{S,1}(r)$,

$$\int U_S(r, r')\psi_{S,1}(r')dr' = \lambda_{S,1}\psi_{S,1}(r) , \tag{4}$$

by Rayleigh's method.[7] We then construct the symmetric matrix

$$U_S^{(1)}(r, r') = U_S(r, r') - \lambda_{S,1}\psi_{S,1}(r)\psi_{S,1}(r') \tag{5}$$

and obtain the second eigenvalue and eigenfunctions, and so forth. Generally, from

$$U_S^{(N)}(r,r') = U_S(r,r') - \sum_{n=1}^{N} \lambda_{S,n}\psi_{S,n}(r)\psi_{S,n}(r') , \qquad (6)$$

we obtain $\lambda_{S,N+1}$ and $\psi_{S,N+1}(r)$ by solving the equation

$$\int U_S^{(N)}(r,r')\psi_{S,N+1}(r')dr' = \lambda_{S,N+1}\psi_{S,N+1}(r) . \qquad (7)$$

The calculation is done very easily. So far, the method is essentially the same as that described in Ref. 6. However, we note that the eigenfunctions used in Ref. 6 are the Sturm-Liouville functions,

$$G_0 U_S \hat{\psi}_{S,n} = \lambda_{S,n}\hat{\psi}_{S,n}, \quad \text{for negative energy.}$$

For positive energy, we must use $\mathcal{P}G_0$ ($\mathcal{P}$: the principal value of Cauchy) in place of G_0. The function $\hat{\psi}_{S,n}(r)$ thus depends on energy, while the function $\psi_{S,n}(r)$ does not. This is one of the advantages of the present paper compared with Ref. 6. The functions $\hat{\psi}_{S,n}$ are normalized as

$$\int\int \hat{\psi}_{S,n}(r)U_S(r,r')\hat{\psi}_{S,m}(r')drdr' = \delta_{nm} ,$$

while the functions $\psi_{S,n}(r)$ are orthonormalized as

$$\int \psi_{S,n}(r)\psi_{S,m}(r)dr = \delta_{nm} .$$

Thus the calculation of $\psi_{S,n}(r)$ [Eq. (7)] and its normalization are more easily done than for $\hat{\psi}_{S,n}(r)$. This is another advantage.

For handling the Hermitian part, we proceed as follows, making use of the special properties of $U_H(r,r')$. (This part is new, and has not been described in Ref. 6.)

To the Hermitian matrix $U_H(r,r')$, there exists[6] a set of real eigenvalues $\{\lambda_{H,m}\}$ and (complex) eigenfunctions $\{\phi_{H,m}\}$,

$$U_H\phi_{H,m} = \lambda_{H,m}\phi_{H,m} . \qquad (8)$$

Then

$$U_H{}^2\phi_{H,m} = \lambda_{H,m}^2\phi_{H,m} , \qquad (9)$$

where $U_H{}^2$ is defined by

$$U_H{}^2(r,r') \equiv \int U_H(r,r'')U_H(r'',r')dr'' . \qquad (10)$$

Since $U_H{}^2$ is a real symmetric matrix, it has real positive eigenvalues $\{\lambda_{H,m}{}^2\}$ which we can obtain numerically. Once we obtain $\{\lambda_{H,m}{}^2\}$, the eigenvalues $\{\lambda_{H,m}\}$ of $U_H(r,r')$, and $\{\phi_{H,m}\}$ of Eq. (8) can be found.

Now, if $\{\phi_{H,m}\}$ is the set of eigenfunctions belonging to the eigenvalues $\{\lambda_{H,m}\}$, the set $\{\phi_{H,m}^*\}$ belongs to the eigenvalues $\{-\lambda_{H,m}\}$ satisfying

$$U_H\phi_{H,m}^* = -\lambda_{H,m}\phi_{H,m}^* . \qquad (11)$$

Equation (11) is obtained from Eqs. (3) and (8). The function $\phi_{H,n}(r)$ is orthonormalized as

$$\int \phi_{H,n}^*(r)\phi_{H,m}(r)dr = \delta_{nm} .$$

Further, the identity

$$\int \phi_{H,n}(r)\phi_{H,m}(r)dr = 0$$

holds for all n and m.

Finally, making use of the above properties, we see that $U_H(r,r')$ can be expanded as

$$\begin{aligned} U_H(r,r') &= \sum_m \lambda_{H,m}[\phi_{H,m}(r)\phi_{H,m}^*(r') \\ &\quad - \phi_{H,m}^*(r)\phi_{H,m}(r')] \\ &= 2i\sum_m \lambda_{H,m}\{\mathrm{Im}[\phi_{H,m}(r)]\,\mathrm{Re}[\phi_{H,m}(r')] \\ &\quad - \mathrm{Re}[\phi_{H,m}(r)]\,\mathrm{Im}[\phi_{H,m}(r')]\} \end{aligned} \qquad (12)$$

(Re: the real part; Im: the imaginary part.) Therefore Eq. (1) is expanded into the sum of separable terms

$$\begin{aligned} U_{NM}(r,r') &= \sum_{n=1}^{N} \lambda_{S,n}\psi_{S,n}(r)\psi_{S,n}(r') \\ &\quad + 2\sum_{m=1}^{M} \lambda_{H,m}\{\mathrm{Im}[\phi_{H,m}(r)]\,\mathrm{Re}[\phi_{H,m}(r')] \\ &\quad - \mathrm{Re}[\phi_{H,m}(r)]\,\mathrm{Im}[\phi_{H,m}(r')]\} . \end{aligned} \qquad (13)$$

In Eq. (13), we have stopped the sum over n and m at suitable numbers N and M. We treat the rest,

$$V(r,r') \equiv U(r,r') - U_{NM}(r,r') , \qquad (14)$$

as perturbation. N and M must be so chosen that the perturbative calculation may converge. In concluding this section, we note that all quantities in Eq. (13) are real. This property facilitates further calculations.

III. PERTURBATIVE CALCULATIONS OF BINDING ENERGY AND SCATTERING AMPLITUDE

We express Eq. (13) simply as

$$U_{NM} = \sum_i \lambda_i |\,\xi_i\rangle\langle\eta_i\,| . \qquad (15)$$

For negative energies, we solve the bound-state problem

$$\psi = G_0 U \psi \ . \tag{16}$$

By Eqs. (14) and (15), Eq. (16) reads

$$\psi = G_0 \sum_i \lambda_i \, | \, \xi_i \rangle \langle \eta_i \, | \, \psi \rangle + G_0 V \psi \ . \tag{17}$$

Treating $G_0 V$ as a perturbation, Eq. (17) is expressed as

$$\psi = \frac{1}{1 - G_0 V} G_0 \sum_i \lambda_i \, | \, \xi_i \rangle \langle \eta_i \, | \, \psi \rangle \ . \tag{18}$$

Here the operator $(1 - G_0 V)^{-1}$ must be calculated by the expansion

$$\frac{1}{1 - G_0 V} = 1 + G_0 V + G_0 V G_0 V + \cdots \ . \tag{19}$$

The binding energy is calculated by solving the equation

$$\langle \eta_i \, | \, \psi \rangle = \sum_j M_{ij} \lambda_j \langle \eta_j \, | \, \psi \rangle \ , \tag{20}$$

where

$$M_{ij} = \langle \eta_i \, | \frac{1}{1 - G_0 V} G_0 \, | \, \xi_j \rangle = \sum_{n=0} M_{ij}^{(n)} \ , \tag{21}$$

$$M_{ij}^{(n)} = \langle \eta_i \, | \, (G_0 V)^n \, G_0 \, | \, \xi_j \rangle \ . \tag{22}$$

Once the binding energy is obtained from Eq. (20), we can find the vectors $\langle \eta_i \, | \, \psi \rangle$ also from Eq. (20). These vectors are used in Eq. (18) to obtain the wave function of the bound state.

For positive energies, if we let the initial state be ϕ, the Schrödinger equation reads

$$\psi = \phi + G_0 U \psi$$

$$= \phi + G_0 \sum_i \lambda_i \, | \, \xi_i \rangle \langle \eta_i \, | \, \psi \rangle + G_0 V \psi \ . \tag{23}$$

For simplicity, we restrict ourselves to s wave. (The generalization to other partial waves is straightforward.) The scattering amplitude is given by

$$T = - \frac{1}{k} \langle \sin kr \, | \, U \, | \, \psi \rangle \ . \tag{24}$$

From Eq. (23), we have

$$\psi = \frac{1}{1 - G_0 V} \left(\phi + G_0 \sum_i \lambda_i \, | \, \xi_i \rangle \langle \eta_i \, | \, \psi \rangle \right) . \tag{25}$$

First we should find $\langle \eta_i \, | \, \psi \rangle$ solving the set of linear algebraic equations

$$\langle \eta_i \, | \, \psi \rangle - \sum_j \lambda_j M_{ij} \langle \eta_j \, | \, \psi \rangle = \left\langle \eta_i \, | \frac{1}{1 - G_0 V} | \, \phi \right\rangle . \tag{26}$$

We put $\langle \eta_i \, | \, \psi \rangle$, found by solving Eq. (26), into Eq. (25) and then ψ into Eq. (24) to obtain the amplitude.

For positive energies G_0 is complex, which may be expressed as

$$G_0 = - \frac{i}{k} \, | \sin kr \rangle \langle \sin kr' \, | + \mathcal{P} G_0 \tag{27}$$

with

$$\mathcal{P} G_0 = - \frac{1}{k} \cos kr_> \sin kr_< \ . \tag{28}$$

The operator

$$G \equiv \frac{1}{1 - G_0 V} G_0 = G_0 + G_0 V G \tag{29}$$

that appears in M_{ij} of Eq. (26) is calculated in the following manner:

We assume that the potential V defined by Eq. (14) is sufficiently weak so that the perturbative series

$$\frac{1}{1 - \mathcal{P} G_0 V} \equiv 1 + \mathcal{P} G_0 V + \mathcal{P} G_0 V \mathcal{P} G_0 V + \cdots \tag{30}$$

converges. We use Eq. (27) into Eq. (29) to obtain

$$G = \frac{1}{1 - \mathcal{P} G_0 V} \left(G_0 - \frac{i}{k} \, | \sin kr \rangle \langle \sin kr \, | \, V G \right) \ . \tag{31}$$

Multiplying by $\langle \sin kr \, | \, V$ on both sides of Eq. (31), we find

$$\langle \sin kr \, | \, V G = \frac{1}{1 + (i/k) \langle \sin kr \, | \, V [1/(1 - \mathcal{P} G_0 V)] \sin kr \rangle}$$

$$\times \langle \sin kr \, | \, V \frac{1}{1 - \mathcal{P} G_0 V} G_0 \ . \tag{32}$$

Putting Eq. (32) into Eq. (31), we obtain

$$G = \left(1 - \frac{i}{k} \frac{1}{1 - \mathcal{P} G_0 V} | \sin kr \rangle \right.$$

$$\times \frac{1}{1 + (i/k) \langle \sin kr \, | \, V [1/(1 - \mathcal{P} G_0 V)] \, | \sin kr \rangle}$$

$$\left. \times \langle \sin kr \, | \, V \right) \frac{1}{1 - G_0 V} G_0 \ . \tag{33}$$

This expression may be used for calculations of M_{ij} [Eq. (21)] in Eq. (26).

IV. EXAMPLE

In this section, we shall examine the convergence of the series (21) for negative energies and that of the series

$$M_{ij}^{(+)} \equiv \langle \eta_i | \frac{1}{1-\Phi G_0 V} \Phi G_0 | \xi_j \rangle = \sum_{n=0} M_{ij}^{(+)}(n) \tag{34}$$

involved in M_{ij} [Eq. (21)] of Eq. (26) for positive energies.

As an example, we shall take a nonlocal potential that appears in the n-d scattering [see Eq. (171) of Ref. 4.],

$$U(y_1, y_2) = \frac{8\pi}{3} \int_{4/3|y_2-(1/2)y_1|}^{4/3[y_2+(1/2y_1)]} x_1 dx_1 \phi(x_1) V(x_1) \phi\{[\,|x_1^2 + \tfrac{4}{3}(y_1^2 - y_2^2)|\,]^{1/2}\}\,, \tag{35}$$

where $\phi(x)$ denotes the wave function of the deuteron, and $V(x)$ denotes the phenomenological nucleon-nucleon potential. Here, we take the potential fitted to the $^3S_1$ data,[8]

$$V(x) = \hbar c[-p_1 \exp(-p_2 x) + p_3 \exp(-2p_2 x) + (p_1 - p_3)\exp(-5p_2 x)]/x\,,$$

with

$$\hbar c = 197 \text{ MeV fm}, \quad p_1 = 3.1344, \quad p_2 = 1.5502 \text{ fm}^{-1}$$
$$p_3 = 7.4616. \tag{36}$$

The function $x\phi(x)V(x)$ is large only at the region near $x=0$. As a result, the main contribution comes from the lower limit of the integral (35), and especially from a small region where $y_2 \approx \frac{1}{2}Y_1$. There is no other competing restriction. Since the deuteron wave function extends to a large distance, the function $\phi\{[|x_1^2 + \frac{4}{3}(y_1^2 - y_2^2)|]^{1/2}\}$ in Eq. (35) vanishes very slowly along $y_2 = \frac{1}{2}y_1$. Therefore, (A) the potential is very long ranged. For a set of points $(y_2+\epsilon,\ y_1-2\epsilon)$ and $(y_2-\epsilon,\ y_1+2\epsilon)$, the lower limit of integration is $|y_2 - \frac{1}{2}y_1 + 2\epsilon|$ and $|y_2 - \frac{1}{2}y_1 - 2\epsilon|$, respectively. Therefore, (B) the potential is almost symmetric along the line of $y_2 = \frac{1}{2}y_1$. The nonlocal potential (35) is shown in Fig. 1, which represents the above properties (A) and (B). To perform the calculation effectively, we make use of the fact that the potential (35) is al-

TABLE I. The matrix elements (41). The energy used is $(3\hbar^2/4m)k^2 = -(6-2.229)$ MeV, where 2.229 MeV is the binding energy of deuteron.

N	M_{11}^N	N	M_{11}^N
0	−0.3604	7	−1.1721
1	−0.8061	8	−1.1746
2	−0.9985	9	−1.1759
3	−1.0899	10	−1.1765
4	−1.1343	11	−1.1768
5	−1.1561	12	−1.1770
6	−1.1668	13	−1.1771

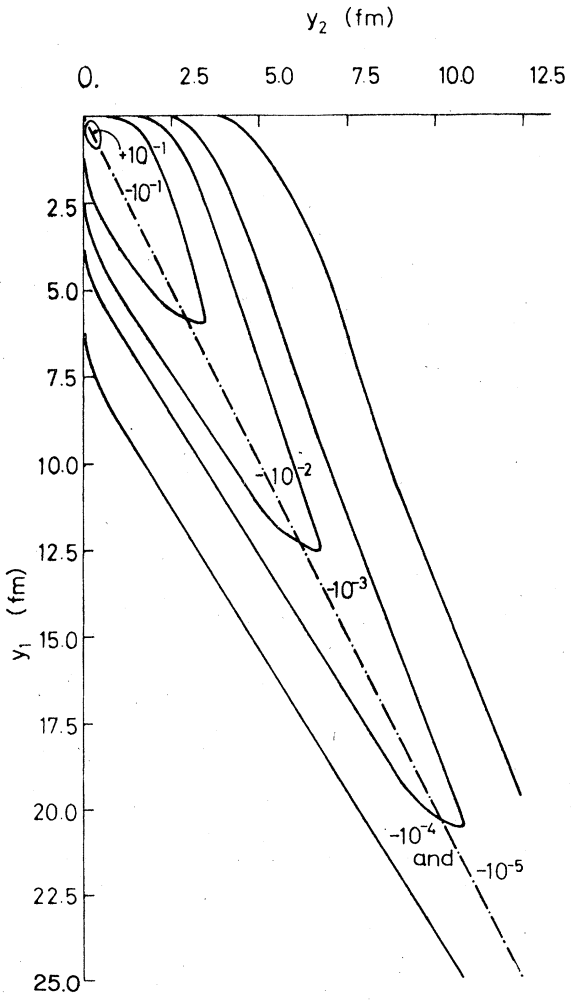

FIG. 1. The nonlocal potential (35). The dash-dot line shows the line of $y_2 = (\frac{1}{2})y_1$.

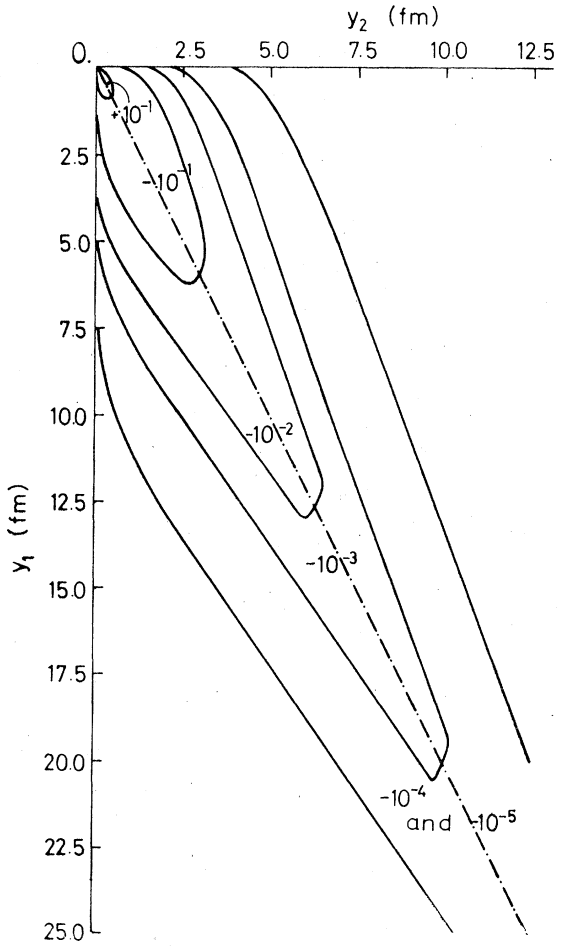

FIG. 2. The potential $U_{S,2m,n}$ of Eq. (38).

most symmetric with respect to $y_2 = \frac{1}{2}y_1$. First, we decide the mesh points such that $(y_1, y_2) = (2m, n)$ in units of length a, where m and n are some integers. Then we define the potential matrix $U_{2m,n}$ consisting of these points and divide it into two parts:

$$U_{2m,n} = U_{S,2m,n} - iU_{H,2m,n} , \tag{37}$$

where U_S is a real symmetric matrix and U_H is a Hermitian matrix defined by

$$\begin{aligned} U_{S,2m,n} &= \tfrac{1}{2}(U_{2m,n} + U_{2n,m}) , \\ U_{H,2m,n} &= \tfrac{1}{2}i(U_{2m,n} - U_{2n,m}) . \end{aligned} \tag{38}$$

Figure 2 shows the potential $U_{S,2m,n}$. The comparison of Fig. 2 with Fig. 1 shows that $U_{S,2m,n}$ almost exhausts the potential U. The eigenvalues and eigenfunctions of $U_{S,2m,n}$ are calculated by Eqs. (4) and (7). For the matrix $U_{S,2m,n}$, the maximum eigenvalues is found to be $\lambda_{S,1} = -0.6260$, which is not large. For the Hermitian matrix, the maximum eigenvalue of $U_{H,2m,n}{}^2$ is found to be 0.03283, thus the maximum eigenvalue of $U_{H,2m,n}$ is 0.1812. Since the contribution from the Hermitian part is rather small, we do not include it in the approximate potential, but we approximate $U_{2m,n}$ by

$$U_{2m,n}^{\text{Approx}} = \lambda_{S,1} |\psi_{S,1}(2m)\rangle\langle\psi_{S,1}(n)| . \tag{39}$$

The approximate value of $U_{2m+1,n}$ is so far unknown. Calculating $|\psi_{S,i}(2m+1)\rangle$ by a numerical (four point) interpolation from $|\psi_{S,i}(2m)\rangle$, we obtain

$$U(y_1, y_2)^{\text{Approx}} = \lambda_{S,1} |\psi_{S,1}(y_1)\rangle\langle\psi_{S,1}(y_2)| . \tag{40}$$

This is to be used as $U_{N,M}(r, r')$ of Eq. (14). For an example, at negative energies, the matrix elements

$$M_{ij}^{N} = \sum_{n=0}^{N} M_{ij}^{(n)} \quad (i=j=1) , \tag{41}$$

where $M_{ij}^{(n)}$ is given by Eq. (22), are given in Table I for $(3\hbar^2/4m)k^2 = -(6 - 2.229)$ MeV. For example, at positive energies, the matrix elements

$$M_{ij}^{(+)N} = \sum_{n=0}^{N} M_{ij}^{(+)(n)} \quad (i=j=1) , \tag{42}$$

where $M_{ij}^{(+)(n)}$ are given by Eq. (34), are given in Table II for $(3\hbar^2/4m)k^2 = 26$ MeV. In both cases, we see that the perturbative calculations of M_{ij} and $M_{ij}^{(+)}$ converge. This example shows that the proposed method is very practical in handling nonlocal potentials.

TABLE II. The matrix elements (42). The energy used is $(3\hbar^2/4m)k^2 = 26$ MeV.

N	$M_{11}^{(+)N}$
0	1.8136
1	1.7228
2	1.7230
3	1.7224
4	1.7223
5	1.7222

*Work supported in part by the Japan Society for Promotion of Science under Grant No. 6R-036.

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