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Potential separable expansion approach to scattering on Coulomb-like potentials

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An approximation method based on the separable expansion of the potential is described that can handle complicated local or nonlocal Coulomb-like potentials in scattering state calculations.

Almost all particles involved in nuclear physics are known to be composite, so they should be considered as clusters of more elementary particles. To avoid the incalculable N-body equations, it has been proposed to seriously consider them in a certain domain of physics to be pointlike particles and to put all information on their internal structure and on the Pauli principle into their effective interaction.[1] Such an effective interaction has a local part, which comes from the direct interaction of the constituents, and a nonlocal part, which comes from the Pauli exchange. The local potential is generally a long-range Coulomb-like potential, while the nonlocal potential is of short range because the exchange between the clusters takes place only when the clusters overlap. Moreover, these potentials might have an explicit energy and momentum dependence.

Handling a potential of this type is not trivial even in the case of two-body problems. The method, based on the direct numerical integration of the Schrödinger equation in coordinate representation can handle complicated long-ranged local plus nonlocal potentials,[2] but might become quite troublesome for momentum-dependent potentials. The momentum representation approach[3] is applicable to practically any potential. In a clever way it treats exactly the long-ranged Coulomb interaction, but the solution of the equation on a momentum space grid is a large numerical work.

A great simplification of the problem can be reached by the separable expansion of the potential. In this method the potential V, local or nonlocal, is approximated by a nonlocal separable finite-rank potential $V^N=\sum_{i,j=1}^N |\chi_i\rangle\lambda_{ij}\langle\chi_j|$, and so the solution of the Schrödinger equation is reduced to the solution of a system of linear algebraic equations. Here, N defines the rank of the expansion and $|\chi_i\rangle$ are the form factors. There are many ways of building up finite-rank approximations to a given potential. The form factors are generally chosen so as to minimize the rank of the expansion. Various sets of functions have been proposed and applied mainly to nucleon-nucleon potentials.[4]

A flexible and easy-to-apply variant of the above method can be gained by projecting the operator V on a finite subset of a Hilbert space basis $\{|i\rangle\}$

$$V\approx V^N=\sum_{i,j=1}^{N} |i\rangle\langle i|V|j\rangle\langle j| \ . \tag{1}$$

This also leads to a separable expansion to the potential, and here the basis can be chosen so that a large part of the work in the solution of the equations can be done analytically. The use of the harmonic-oscillator eigenstates as form factors was very successful in practical applications. The method was used, e.g., for looking for the bound-,[5] resonant-,[6] and scattering-state[7] solutions of a given potential. These applications proved that the method yields convergence at an acceptable small N for any physical quantities such as bound and resonant state energy, phase shift, wave function, etc. This is only possible if we use a special smoothing procedure, namely, instead of (1) we approximate V by

$$V\approx V^N=\sum_{i,j=1}^{N} |i\rangle\sigma_i^N\langle i|V|j\rangle\sigma_j^N\langle j| \ . \tag{2}$$

In the formulas the only modification implied is to replace $\langle i|V|j\rangle$ by $\sigma_i^N\langle i|V|j\rangle\sigma_j^N$. The choice of σ_i^N,

$$\sigma_i^N=\frac{1-\exp\{-[\alpha(i-N-1)/(N+1)]^2\}}{1-\exp(-\alpha^2)} \ , \tag{3}$$

with $\alpha\sim 6$ has proved to be very successful in practical applications.

The potential separable expansion (PSE) method, based on the harmonic-oscillator eigenstates, however, failed to cope with the long-ranged Coulomb potential in a similarly simple way. Therefore, another basis set, the complete set of Coulomb-Sturmian functions, was proposed and the method was applied in bound- and resonant-state calculations.[8] The aim of this paper is to extend it to scattering-state calculations and to demonstrate its power in a nontrivial example, in the fishbone optical model.[9] First we recall some results of Ref. 8, which form the background of this paper.

For the sake of simplicity we restrict ourselves to a given partial wave l. A long-ranged Coulomb-like potential V_l can be written in the form

$$V_l=V_C+V_{Sl} \ , \tag{4}$$

where $V_C=Z_1Z_2e^2/r$ is the pure Coulomb potential and V_{Sl} is a short-range potential. The radial wave function u_l of a bound or resonant state is the solution of the homogeneous Lippmann-Schwinger equation

$$|u_l\rangle=g_l^C(E)V_{Sl}|u_l\rangle \ , \tag{5}$$

where $g_l^C(E)=(E-H_{0l}-V_C)^{-1}$ is the Coulomb-Green operator and H_{0l} is the kinetic energy operator. This equation is solvable if and only if its Fredholm determinant $D_l(E)=\det[1-g_l^C(E)V_{Sl}]$ is equal to zero and these zeros give the bound- and resonant-states eigenvalues. If the potential V_{Sl} is approximated in the separable way (2), $D_l(E)$ boils down to a simple algebraic determinant

$$D_l^N(E)=\det\{\underline{1}-\underline{g}_l^C\underline{V}_{Sl}\}\ , \tag{6}$$

where

$$(\underline{g}_l^C)_{ij}=\langle i\,|\,g_l^C\,|\,j\rangle$$

and

$$(\underline{V}_{Sl})_{ij}=\sigma_i^N\langle i\,|\,V_{Sl}\,|\,j\rangle\sigma_j^N$$

are the Green and smoothed potential matrices, respectively.

In the calculation of $D_l^N(E)$ the most crucial point is the calculation of the matrix elements of the Coulomb-Green operator. To make this analytically possible we choose the set of Coulomb-Sturmian functions[10] and perform a transformation on the Eq. (5). The Coulomb-Sturmian functions are the Sturm-Liouville solutions of the hydrogen problem. In coordinate representation the bound-state Coulomb-Sturmian functions have the form

$$\langle r\,|\,nl\,\rangle=S_{nl}(r)=[n!/(n+2l+1)!]^{1/2}(2br)^{l+1}\times\exp(-br)L_n^{2l+1}(2br)\ , \tag{7}$$

where L is the Laguerre polynomial and b is a scaling parameter which is connected to the energy in the Sturm-Liouville equation. These functions are orthogonal and form a complete set with respect to the weight function $1/r$, so the set $\{\,|\widetilde{nl}\rangle\}=\{\Delta^{1/2}\,|\,nl\,\rangle\}$, where $\langle r\,|\,\Delta\,|\,r'\rangle=\delta(r-r')/r$, is orthonormal and complete in the conventional sense. With $|\,\tilde{u}_l\rangle=\Delta^{1/2}\,|\,u_l\rangle$, $\tilde{g}_l^C=\Delta^{1/2}g_l^C\Delta^{1/2}$, and $\tilde{V}_{Sl}=\Delta^{-1/2}V_{Sl}\Delta^{-1/2}$ we have

$$|\,\tilde{u}_l\,\rangle=\tilde{g}_l^C\tilde{V}_{Sl}\,|\,\tilde{u}_l\,\rangle\ . \tag{8}$$

It is easy to show that the transformation leaves the Fredholm determinant unchanged.

To construct the Fredholm determinant, we need the potential matrix, which, in general, can only be calculated numerically. It is possible, however, to set up a three term recurrence relation between the matrix elements of the Coulomb-Green operator

$$\langle\widetilde{n'l}\,|\,\tilde{g}_l^C\,|\,\widetilde{n+1l}\,\rangle=\left[\frac{(n+l+1)(4mE-2\hbar^2b^2)-4mbZ_1Z_2e^2}{2mE+\hbar^2b^2}\langle\widetilde{n'l}\,|\,g_l^C\,|\,\widetilde{nl}\,\rangle-[n(n+2l+1)]^{1/2}\langle\widetilde{n'l}\,|\,\tilde{g}_l^C\,|\,\widetilde{n-1l}\,\rangle-\delta_{nn'}\frac{4mb}{2mE+\hbar^2b^2}\right][(n+1)(n+2l+2)]^{-1/2}\ , \tag{9}$$

which makes the calculation of every matrix element possible if $\underline{\tilde{g}}_{00}^{Cl}=\langle\widetilde{0l}\,|\,\tilde{g}_l^C\,|\,\widetilde{0l}\,\rangle$ is at our disposal. This matrix element also can be given in a closed form,

$$\underline{\tilde{g}}_{00}^{Cl}=-\frac{m}{\hbar^2b}\left[\frac{2ib/k}{1+ib/k}\right]^2\frac{1}{l+i\eta+1}\,{}_2F_1\left[-l+i\eta,1;l+i\eta+2;\left[\frac{1-ib/k}{1+ib/k}\right]^2\right]\ , \tag{10}$$

where $k=(2mE/\hbar^2)^{1/2}$ is the wave number, $\eta=Z_1Z_2e^2/k$, and ${}_2F_1$ is the hypergeometric function. Upon deriving (10), we have assumed that k lies in a restricted area of the complex k plane, but the result is more general because it can be continued analytically to the whole complex k plane, except for a branch cut from 0 to $-\infty$.

We can calculate that matrix elements of the Green operator nearly on the whole complex k plane including the real k axis, so we have several ways to use our method in scattering-state calculations. We could calculate the S matrix directly from the Fredholm determinant (see p. 522 in Ref. 11), or we could start from the inhomogeneous Lippmann-Schwinger equation for the wave function. Instead, we have chosen a more straightforward approach which will be easy to generalize to multichannel problems.

The scattering amplitude of a Coulomb-like potential can be written in the form $A(\mathbf{k},\mathbf{k}')=A^C(\mathbf{k},\mathbf{k}')+A'(\mathbf{k},\mathbf{k}')$, where A^C is the pure Coulomb, and A' is the Coulomb-modified nuclear scattering amplitude. The amplitude A' can be expanded into a fast converging partial-wave series, and the partial-wave scattering amplitude a_l' is proportional to the on-shell matrix elements of the Coulomb-modified transition operator t_{Sl}^C between Coulomb scattering states (p. 430 in Ref. 11)

$$a_l'=\frac{1}{k}e^{i(2\sigma_l+\delta_l)}\sin\delta_l=-\frac{2m}{\hbar^2k^2}\langle k_l^C-\,|\,t_{Sl}^C(k+i0)\,|\,k_l^C+\rangle\ , \tag{11}$$

where σ_l is the Coulomb phase shift, δ_l is the Coulomb-modified nuclear phase shift, and $\langle r\,|\,k_l^C\pm\rangle=\psi_l^{C\pm}(k,r)$ are the radial Coulomb wave functions. The operator t_{Sl}^C is connected to the potential V_{Sl} via the Lippmann-Schwinger–type equation

$$t_{Sl}^C=V_{Sl}+V_{Sl}g_l^Ct_{Sl}^C\ . \tag{12}$$

To make use of our formulas (9) and (10) we transform our quantities according to Eq. (8). The operator

$$\tilde{t}_{Sl}^C=\Delta^{-1/2}t_{Sl}^C\Delta^{-1/2} \tag{13}$$

also satisfies the Lippmann-Schwinger–type equation

$$\tilde{t}_{Sl}^C=\tilde{V}_{Sl}+\tilde{V}_{Sl}\tilde{g}_l^C\tilde{t}_{Sl}^C\ . \tag{14}$$

If the potential $\widetilde{V}_{Sl}$ is expanded in the Coulomb-Sturmian basis $|\widetilde{nl}\rangle$, the operator $\widetilde{t}^{C}_{Sl}$ has a similar separable expansion,

$$\underline{\widetilde{t}}^{C}_{Sl} \approx \widetilde{t}^{CN}_{Sl} = \sum_{n,n'=0}^{N} |\widetilde{nl}\rangle \widetilde{t}^{C}_{Sl} \langle \widetilde{n'l}| \; , \tag{15}$$

and for its matrix we get

$$\underline{\widetilde{t}}^{C}_{Sl} = [[\underline{\widetilde{V}}_{Sl}]^{-1} - \underline{\widetilde{g}}^{C}_{l}]^{-1} \; . \tag{16}$$

So, for the partial-wave scattering amplitude we arrive at

$$a_l'(k) = -\frac{2m}{\hbar^2 k^2} \sum_{n,n'=0}^{N} \langle k_l^C - |\Delta| nl\rangle \times [\underline{\widetilde{t}}^{C}_{Sl}]_{nn'} \langle n'l |\Delta| k_l^C + \rangle \; . \tag{17}$$

We can immediately notice that everything, needed for calculating $a_l'(k)$ is already at our disposal, except for the matrix elements $\langle k_l^C \pm |\Delta| nl\rangle$. This can also be given in a closed form via the three-term recurrence relation

$$\langle k_l^C \pm |\Delta| n+1l\rangle = \left[\frac{(n+l+1)(4mE - 2\hbar^2 b^2) - 4mbZ_1Z_2e^2}{2mE + \hbar^2 b^2} \langle k_l^C \pm |\Delta| nl\rangle - [n(n+2l+1)]^{1/2} \langle k_l^C \pm |\Delta| n-1l\rangle \right] [(n+1)(n+2l+2)]^{-1/2} \; , \tag{18}$$

with starting values

$$\langle k_l^C \pm |\Delta| 0l\rangle = \exp[\pm i\sigma_l + 2\eta \arctan(k/b)] \left[\frac{2\pi\eta}{\exp(2\pi\eta) - 1} \right]^{1/2} \left[\frac{2k/b}{1+(k/b)^2} \right]^{l+1} \prod_{j=1}^{l} \left[\frac{\eta^2 + j^2}{j(j+\frac{1}{2})} \right]^{1/2} \; . \tag{19}$$

We can also calculate the phase shift δ_l from the relation

$$\delta_l = \log[2ika_l'(k)\exp(-2i\sigma_l) + 1]/2i \; . \tag{20}$$

We show now the power of the method in the example of the two-cluster fishbone optical model.[9] This model can be considered as a Pauli-correct optical model of the interaction of composite particles. Its basis equation looks like a Schrödinger equation with the Hamiltonian

$$H_l^{FB} = H_{0l} + V_l^{\mathrm{opt}} - \sum_{i,j} |u_{li}\rangle \langle u_{li} | H_{0l} + V_l^{\mathrm{opt}} - \epsilon_i | u_{lj}\rangle \overline{M}^{\,l}_{ij} \langle u_{lj}| \; . \tag{21}$$

Here H_{0l} is the kinetic energy operator and V_l^{opt} is a real or complex local potential. The third term, to be interpreted as a nonlocal potential, represents the Pauli effects. It is given in terms of the norm kernal eigenstates $|u_{li}\rangle$ of the two-cluster system. The Pauli principle enters through the symmetric matrix $\overline{M}^{\,l}$, whose elements are equal to 1, whenever i or j refers to a fully Pauli-forbidden state, and are equal to $1-[(1-\eta_i)/(1-\eta_j)]^{1/2}$ otherwise, where η_i are the normal kernal eigenvalues and $i \leq j$. The fully Pauli-forbidden states are removed from the physical part of the spectrum by choosing the energy ϵ_i to be very high. We present the example of the $\alpha - \mathrm{O}^{16}$ scattering with a potential

$$V_l^{\mathrm{opt}} = V_0(1 + V_1 r^2)\exp(-\beta_1 r^2) + V_2 \exp(-\beta_2 r^2) + 16e^2 \mathrm{erf}(\beta_3 r)/r \; , \tag{22}$$

where $V_0 = -139.16$ MeV, $V_1 = 0.041\,11$ fm^{-2} $\beta_1 = 0.134\,28$ fm^{-2}, $V_2 = -1.677\,09$ MeV, $\beta_2 = 0.189\,63$ fm^{-2}, $\beta_3 = 0.435\,46$ fm^{-1}, and $\epsilon_i = 300$ MeV. The eigenstates of the norm kernel operator are harmonic oscillator states of width parameter $a = 0.512$ fm^{-2}, and the eigenvalues are taken from Ref. 12. In Fig. 1 the line represents the phase shift δ_l at $l = 3$ and $E = 12$ MeV as a function of N with smoothing parameter $\alpha = 6$ while the arrow shows the result of direct numerical integration.[2] The values without smoothing differ so much that they cannot be displayed on this figure.

In this Brief Report the potential separable expansion method based on Coulomb-Sturmian functions has been presented for single-channel two-body scattering states. The method treats exactly the part of the Hamiltonian which has an effect on the asymptotic motion, viz. the kinetic energy operator and the Coulomb potential. We have demonstrated that the short-range interaction is well represented by our separable form if we use the σ_i^N

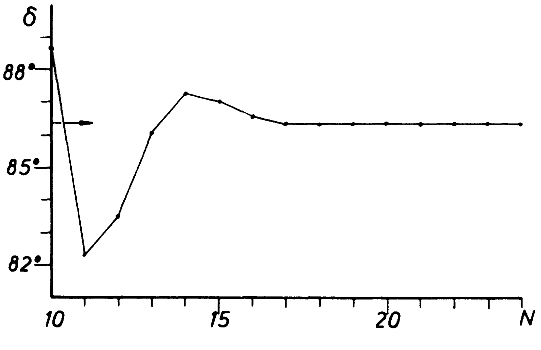

FIG. 1. The convergence of the phase shift δ of the $\alpha - \mathrm{O}^{16}$ scattering calculated by the fishbone optical model in Coulomb-Sturmian basis.

smoothing factors. The rate of convergence is rather stable against any reasonable variation of the smoothing parameter α and of the Coulomb-Sturmian parameter b. The best choice for α is $\alpha \sim 6$ while the best b depends on the range of the potential. The method is as accurate and fast as the other well-known standard numerical methods.

The main advantage of our method lies in its generality. Any short-range potential, which has some relevance to nuclear physics, can be treated in the same way, and the solution of the Lippmann-Schwinger equation is reduced to the solution of some matrix equation. Moreover all matrix elements, except for the potential matrix, have been calculated analytically. The method can also easily be extended to two-body multichannel problems. The channel-coupling interactions are generally of short-range type and they can be approximated by separable forms. The multichannel Green operator is block-diagonal in channel space and the blocks are our single-channel Green matrices. So, everything that we need for the matrix of the t-matrix operator is practically at our disposal.

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