

Unified treatment of bound-state and scattering problems

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The iteration-subtraction method for the unified treatment of bound-state and scattering problems is compared and contrasted with a similar method for the two-body bound-state problem via nonsingular scattering equations developed recently. We also compare another recent method for solving bound-state problems with the iteration-subtraction method.

I. INTRODUCTION

A recently proposed iteration-subtraction method¹⁻⁴ for the unified treatment of bound state and scattering problems in the momentum space suggests that solutions to both these problems can essentially be constructed using the iterative solution of an auxiliary integral equation of the Fredholm type. This auxiliary integral equation has a kernel which is free from singularities and is also sufficiently weak in order to allow a convergent iterative solution for a wide class of potentials. The solution of the original Lippmann-Schwinger scattering equation in the momentum space is then related to that of the auxiliary equation. At the bound state energy the solution of the auxiliary equation satisfies a certain condition which is used to pick up the binding energy, and the bound-state wave function is readily constructed using the solution of the auxiliary equation at this energy.

This method has been used to define³ a class of Jost-like functions and has been studied in the case of nonlocal potentials. This method has also been extended⁵ to the case of multichannel scattering problems and applied to three-body scattering problems. The approach has been demonstrated by Dzhubuti and Tsiklauri⁶ to be very useful to solve three- and four-body bound state problems using the hyperspherical harmonics method in momentum space. The method has easily been extended⁷ to study virtual states and resonances.

Sasakawa⁸ proposed an efficient method for computing phase shifts using a wave-function description of scattering. Later⁹ it was shown that the Sasakawa method can be reformulated to yield a practical method for computing half-on-shell t matrix elements using the momentum-space Lippmann-Schwinger equations. Also, a method by Kowalski and Noyes¹⁰ has the advantage of the methods of Refs. 1-7 in that it treats the scattering problem through the solution of an auxiliary equation. The above mentioned iteration-subtraction method¹⁻⁷ should be considered a generalization of methods of Refs. 8-10 to calculate fully-off-shell t matrix elements, binding energies, and bound state wave functions.

More recently, and specially after the completion of

the works of Refs. 1-7, Bartnik, Haberzettl, and Sandhas¹¹ proposed a method for two-body bound state problems via nonsingular scattering equations which has been claimed to have all the advantages of the method of Refs. 1-7, to be applicable to both local and nonlocal potentials, to yield a useful continuation of the momentum space representation of the Jost function, and to suggest an investigation of resonance phenomena (and virtual states). The striking similarity between these two approaches has led us to undertake the present study of comparing and contrasting the two methods—that of Refs. 1-7 on one hand and that of Ref. 11 on the other.

Also, after the completion of Ref. 2, Sasakawa and Ishikawa¹² proposed a method for the bound state problem, which transforms, as in Ref. 2, the homogeneous bound state equation to an inhomogeneous equation which is then solved by the method of continued fractions developed by Horáček and Sasakawa.¹³ We show that the method of Sasakawa and Ishikawa uses essentially the idea of Refs. 2 and 14 in order to transform the homogeneous bound state equation to an inhomogeneous equation and subsequently solve it.

It is also pointed out, as has been noted in Ref. 3, that special care is needed in order to extend the methods of Refs. 11-13 to the case of multichannel equations, which deal with essentially a nonlocal potential, because of the presence of spurious and continuum bound state solutions. Only for a local potential is the scattering formalism of Ref. 11 free of such spurious and continuum solutions.

The plan of the paper is as follows. In Sec. II we present a very brief review of our approach, which is appropriate for its comparison with the approach of Ref. 11. The actual comparison with the approach of Bartnik, Haberzettl, and Sandhas is presented in Sec. III. In Sec. IV we compare the bound state approaches of Refs. 2 and 12. Finally, in Sec. V, concluding remarks are given.

II. ITERATION-SUBTRACTION METHOD

In this section we present a brief summary of our approach. In order to be more objective, we consider only

the S -wave case, though generalization to other partial waves is straightforward. The S -wave Lippmann-Schwinger equation (in units of $\hbar=2m=1$) is written as¹⁻³

$$\begin{aligned} \langle p | t(E) | s \rangle &= \langle p | V | s \rangle \\ &+ \frac{2}{\pi} \int q^2 dq \langle p | V | q \rangle \\ &\times (k^2 - q^2 + i\epsilon)^{-1} \langle q | t(E) | s \rangle, \end{aligned} \quad (2.1)$$

where $k^2=E$ and E is the total center of mass energy.

In Eq. (2.1) and throughout the rest of the paper the momentum space integration limits are from 0 to ∞ . The solution of Eq. (2.1) is conveniently expressed in terms of the solution of the following auxiliary equation:

$$\begin{aligned} \langle p | \Gamma(E) | s \rangle &= \langle p | V | s \rangle \\ &+ \frac{2}{\pi} \int q^2 dq \langle p | A(E) | q \rangle \\ &\times (k^2 - q^2 + i\epsilon)^{-1} \langle q | \Gamma(E) | s \rangle, \end{aligned} \quad (2.2)$$

by

$$\langle p | t(E) | s \rangle = \frac{\langle p | \Gamma(E) | k_1 \rangle}{\langle k_1 | \Gamma(E) | k_1 \rangle} t(k_1) \frac{\langle s | \Gamma(E) | k_1 \rangle}{\langle k_1 | \Gamma(E) | k_1 \rangle} + \left[\langle p | \Gamma(E) | s \rangle - \frac{\langle p | \Gamma(E) | k_1 \rangle \langle k_1 | \Gamma(E) | s \rangle}{\langle k_1 | \Gamma(E) | k_1 \rangle} \right], \quad (2.3)$$

where

$$t(k_1) \equiv \langle k_1 | t(E) | k_1 \rangle = \frac{\langle k_1 | \Gamma(E) | k_1 \rangle}{1 - \frac{2}{\pi} \int q^2 dq (k^2 - q^2 + i\epsilon)^{-1} \gamma(k_1, q) \langle q | \Gamma(E) | k_1 \rangle}. \quad (2.4)$$

Here,

$$\langle p | A(E) | q \rangle = [\langle p | V | q \rangle - \langle p | V | k_1 \rangle \gamma(k_1, q)], \quad (2.5)$$

where $\gamma(k_1, q)$ is an arbitrary function of the yet arbitrary momentum k_1 . At positive energies we take $k_1=k$, the on-shell momentum, and the property

$$\gamma(k, k) = 1, \quad (2.6)$$

which has the advantage of making the kernel of Eq. (2.2) nonsingular. At negative energies the momentum variable k_1 can be left arbitrary as in Refs. 2 and 3 and no special condition, such as (2.6), on γ is necessary, though such a condition can be maintained. It has been shown that at the zero of the denominator of Eq. (2.4), given by

$$\begin{aligned} F(k^2) &\equiv 1 - \frac{2}{\pi} \int q^2 dq (k^2 - q^2 + i\epsilon)^{-1} \\ &\times \gamma(k_1, q) \langle q | \Gamma(E) | k_1 \rangle = 0, \end{aligned} \quad (2.7)$$

one has a bound state, and the bound state wave function is given by³

$$\Psi_{|k^2|}(q) = -(|k^2| + q^2)^{-1} \langle q | \Gamma(E) | k_1 \rangle. \quad (2.8)$$

It is to be noted that k^2 in Eq. (2.8) is negative and $|k^2|$ is the binding energy. The bound state wave function $\Psi(q)$ of (2.8) is independent of the subtraction point k_1 . Thus one can generate the solution of bound-state and scattering problems essentially via the solution of the auxiliary equation (2.2). It has been stressed^{3,9} that

if $\gamma(k_1, q)=1$ and $k_1=k$, the on-shell momentum, the function $F(k^2)$ defined by (2.7) is identically equal to the Jost function¹⁵—both for local and nonlocal potentials. It has been pointed out³ that if we maintain $k_1=k$ and use a restricted class of $\gamma(k_1, q)$, Eq. (2.7) defines a wide class of functions $F(k^2)$ with all the properties of the Jost function. This class of Jost-like functions may have spurious poles for certain real k^2 —both for local and nonlocal potentials. Such spurious poles were known to appear¹⁵ in the case of nonlocal potentials and were considered peculiar to such problems. The generalization of Ref. 3 of the Jost function makes the appearance of such poles for nonlocal potentials much less anomalous. It has been pointed out that such poles appear at discrete real energies and correspond to solutions of the homogeneous version of Eq. (2.2). The appearance of such poles may render the method numerically inapplicable at and near certain discrete real energies where Γ tends to infinity. The presence of these poles has been demonstrated^{3,15} in the case of a simple separable (nonlocal) interaction.

It has also been noted³ that if k_1 is taken to be the on-shell momentum at negative energies, then k_1 becomes imaginary and, because of the left-hand cut, intrinsic to many potentials, the function $F(k^2)$ of Eq. (2.7) can only be calculated up to certain negative energy $E = -E_0$. Hence, for this choice of k_1 , binding energy and bound state wave functions cannot be calculated if the energy of the bound state is smaller than $-E_0$. Also, negative energy t matrix elements cannot be calculated using (2.3) for $E < -E_0$ if k_1 is chosen to be k . This difficulty, however, can be avoided, as has been done in finding binding energies and bound state wave

functions numerically in Refs. 2 and 6—by taking k_1 to be a real momentum variable at negative energies. However, with this choice no meaningful Jost function can be defined using Eq. (2.7).

III. COMPARISON WITH THE METHOD OF BARTNIK, HABERZETTL, AND SANDHAS

Now it is easy to compare our approach presented in Sec. II with the approach of Bartnik, Haberzettl, and Sandhas¹¹ (BHS hereafter) presented recently. Though BHS have claimed in the text of Ref. 11 that their method is original in treating the bound state problem via an inhomogeneous integral equation, they have kindly admitted in their “note added in proof” that their bound state technique is similar to that of Ref. 2, with a special choice of the function $\gamma(k_1, q)$, which provides the connection to the well-known coordinate space results and which, in particular, leads to an important generalization of the Jost function. BHS, however, failed to realize that their off-shell t matrix given by Eq. (42) of Ref. 11 is the same as (2.3) with a special choice of $\gamma(k_1, q)$. The choice of γ of Ref. 2 resulted after an extensive study¹ aimed at obtaining a rapid convergence of the iterative solution of Eq. (2.2). We also considered other choices of γ , especially that suggested by BHS, both numerically and formally in Refs. 1 and 3. In fact, it is easy to realize that the approach of BHS is the same as that of Refs. 1–7, briefly summarized here in Sec. II, where at positive energies $k_1 = k$ and $\gamma(k, q) = 1$, and at negative energies k_1 is taken to be arbitrary together with $\gamma(k_1, q) = 1$. (Remember that we are considering only the S wave analysis of BHS.) With this particular choice of γ and k_1 , BHS claim that their approach (a) is, of course, valid irrespective of whether the potential is local or not, (b) leads, in particular, to an important generalization of the Jost function, and (c) is valid for resonance phenomena.

Substantial work is needed, as has been shown in Ref. 3, in order to incorporate nonlocal potentials in this approach. The statement of BHS, namely that the approach is valid for nonlocal potentials, does not and cannot replace a proof or demonstration of the type presented in Ref. 3 to that effect. BHS did not worry about the possible spurious and continuum states of the nonlocal potential that make the development of any approach for this potential very subtle and delicate.³ As pointed out in Sec. II and in Ref. 3, the spurious states are solutions of the homogeneous version of Eq. (2.2) that make Γ infinite at certain discrete energies. For $k_1 = k$ and $\gamma(k, q) = 1$ such states do not appear in the approach of BHS at positive energies for local potentials, but they may appear, in general, at negative energies—both for local and nonlocal potentials if k_1 is arbitrary. Such states may also appear at discrete positive energies for nonlocal potentials in the approach of BHS. It has been pointed out in Ref. 3 that extreme care is needed in extending this method to the case of nonlocal potentials or multichannel scattering.

BHS also suggest an “important generalization” of the Jost function which is given essentially by $F(k^2)$ of (2.7)

with their choice of $\gamma(k_1, q)$ and k_1 , namely at positive energies $k_1 = k$, $\gamma(k_1, q) = 1$, and at negative energies k_1 is arbitrary and $\gamma(k_1, q) = 1$. Jost function¹⁵ is a mathematical function with desired analytic properties in the entire complex k plane as has been detailed in Refs. 3 and 15. As BHS do not define their important generalization of the Jost function in the entire complex k plane, it will not be appropriate to call their “Jost function” a function in the usual mathematical sense. Their important generalization of the Jost function serves as an impetus for solving the bound state and scattering problem on the real energy axis rather than defining a mathematical function in the sense used in the original definition of the Jost function. This is because it will be extremely difficult, if not impossible, to define a continuous analytic function in the complex k plane using the recipe of BHS, who leave the parameter k_1 arbitrary for negative energies. Unless the parameter k_1 is defined in the complex energy plane, it is not clear how the method of BHS can be extended to study resonance phenomena, because one needs to define k_1 in the complex energy plane in order to define a continuous Jost function with desirable analytic properties. Their procedure may work in calculating a resonance state, but certainly will not lead to a mathematically meaningful Jost function. Also, it is worth mentioning that the procedure of BHS, which leaves k_1 arbitrary, was already suggested and used before.^{1–3,6}

IV. COMPARISON WITH THE BOUND STATE APPROACH OF SASAKAWA AND ISHIKAWA

Now it is easy to compare the bound state methods of Ref. 2 and of Sasakawa and Ishikawa¹² (SI hereafter) suggested recently. For this comparison we briefly state our approach in operator notation. The Schrödinger equation for the bound state,

$$|\Psi\rangle = G_0 V |\Psi\rangle, \quad (4.1)$$

together with the normalization condition,²

$$\langle \gamma | \Psi \rangle = 1, \quad (4.2)$$

for the wave function, is rewritten as²

$$|\Psi\rangle = G_0 V |k_1\rangle + G_0 V_1 |\Psi\rangle, \quad (4.3)$$

where

$$V_1 = V - V |k_1\rangle \langle \gamma|. \quad (4.4)$$

Here, $G_0 = (E + i\epsilon - H_0)^{-1}$ is the free Green's function, and γ is an arbitrary function such that

$$\langle \gamma | q \rangle = \gamma(k_1, q), \quad (4.5)$$

where $\gamma(k_1, q)$ is essentially the same function defined in Eqs. (2.2)–(2.5), and k_1 is an arbitrary momentum variable. So one can solve Eq. (4.3) with a given $\langle \gamma |$ and test whether Eq. (4.2) is satisfied. If Eq. (4.2) is satisfied, one has an eigenfunction of Eq. (4.1). Equation (4.3) is usually solved by iteration.^{2,6} In practice, the energy parameter E is varied, and when Eq. (4.2) is satisfied one simultaneously has the eigenfunction and eigenvalue.

This method is the same as that presented in Sec. II, because condition (4.2) is, in an explicit momentum representation, essentially given by (2.7) with $|\Psi\rangle$ defined by (2.8).

The method of SI follows from Eqs. (4.1)–(4.5) if one takes

$$\langle \gamma | = \frac{\langle f | V}{\langle f | V | F_0 \rangle} \quad (4.6)$$

and replaces $|k_1\rangle$ by the function $|F_0\rangle$. Then Eqs. (4.2) and (4.3) become

$$|\Psi\rangle = G_0 V |F_0\rangle + G_0 V_1 |\Psi\rangle \quad (4.7)$$

and

$$\langle f | V |\Psi\rangle - \langle f | V |F_0\rangle = 0. \quad (4.8)$$

Equations (4.7) and (4.8) are identical to Eqs. (15) and (14) of SI, respectively. Then SI suggest Eq. (4.7) be solved by the method of continued fractions,¹³ whereas we solve it by iteration.^{1,2} The fact that the method of continued fractions does not lead to special advantages over the iterative method has already been emphasized in Ref. 16. Though SI and the author of Ref. 2 do not treat the same numerical problem, it is easily realized that the rate of convergence of Ref. 2 is superior to that obtained by SI in their Table 2 if we recall¹⁶ that the rank m of SI is to be multiplied by 2 before comparing it with rank N of Ref. 2. Hence the method of SI essen-

tially uses the same idea to transform the homogeneous Schrödinger equation to an inhomogeneous integral equation.

Of course, other choices of $\langle \gamma |$ are possible in Eq. (4.4). The last term of Eq. (4.4) can be substituted for by any separable representation of the potential.

V. CONCLUSIONS

A simple connection is established between a recently proposed approach¹¹ to the bound state problem via nonsingular integral equations and a formerly developed approach^{1–3} to the same problem. It is realized that the recently proposed method is just a special case of the method developed previously by us. Also, the claims¹¹ about most of the advantages in this special case are not well founded, as we have seen in Sec. III.

It is also pointed out that another recently proposed method¹² for solution of the bound state problem uses the same idea as a formerly developed approach^{2,14} to the same problem does in transforming the homogeneous integral equation to an inhomogeneous integral equation. There is no apparent advantage in the recently proposed version¹² of this method over the version developed previously by us,² as we have seen in Sec. IV.

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