Siegert pseudostate formulation of scattering theory: One-channel case

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Siegert pseudostates (SPSs) are defined as a finite basis representation of the outgoing wave solutions to the radial Schrödinger equation for cutoff potentials and the problem of their calculation is reduced to standard linear algebra easily implementable on computers. For a sufficiently large basis and the cutoff radius, the set of SPSs includes bound, weakly antibound, and narrow complex-energy resonance states of the system, i.e., all the physically meaningful states observable individually. Moreover, the set is shown to possess certain orthogonality and completeness properties that qualify it as a discrete basis suitable for expanding the continuum. We rederive many results of the theory of Siegert states in terms of SPSs and obtain some (to our knowledge) previously unknown relations. This not only makes the results practically applicable, but also sheds a new light on their mathematical nature. In particular, we show how the Mittag-Leffler expansions for the outgoing wave Green's function and the scattering matrix can be obtained on the basis of very simple algebraic relations, without assuming them to be meromorphic functions. Explicit construction of these two fundamental objects completes the SPS formulation of scattering theory for the one-channel case. The computational efficiency of this approach is illustrated by a number of numerical examples. [S1050-2947(98)05409-2]

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I. INTRODUCTION

In the nonrelativistic quantum theory of collisions between microscopic particles one works with Hamiltonians whose spectra consist of discrete and continuous parts; therefore expansions in terms of the complete set of eigenstates of such Hamiltonians contain summation over the former and integration over the latter. It is well known that the discrete part of the expansions is much easier to deal with than the continuous part, basically because summation is a natural operation to do on computers while integration is to be approximated by summation anyway. This difficulty keeps motivating one to seek a scheme to discretize the continuum; indeed, various such schemes have been proposed. Without the intention to overview all the literature, we mention only three major approaches in this direction. The first and the most developed one is the R-matrix method [1]. The basic idea here is to confine the system to a finite volume, with the asymptotic boundary conditions replaced by certain conditions on the boundary of the volume. The eigenstates of the Hamiltonian satisfying thus modified boundary conditions form a discrete set called the R-matrix basis. The second approach is to switch from the energy eigenstates to some kind of Sturmian eigenstates which are eigenfunctions of the same Hamiltonian but with a nonunity weight chosen in such a way that the Sturmian problem has a purely discrete spectrum [2]. A Sturmian basis can be defined by regarding some parameter of the potential energy, such as nuclear charge or angular momentum, as an eigenvalue instead of the energy. Each of these approaches enables one to replace integration over the continuum by summation over a discrete set of states; their performance depends on how close these states reproduce basic physical properties of the system. The third approach does not rely upon any specific set of states and consists in approximating the integral over the continuum by an appropriate quadrature [3]. Although this might seem to be purely mathematical, or one would say a numerical procedure, such methods may be extremely efficient in practical calculations [4], which eventually must have some physical interpretation.

The purpose of this paper is to promote Siegert *pseudostates* (SPSs) introduced in [5] as an appealing basis alternative to those mentioned above. The Siegert states (SSs) have long been known as a potentially powerful tool in the formal scattering theory. However, this power remained largely latent for the lack of an efficient method of their calculation, most of the applications to date being restricted to studying only individual resonances. In [5] we have proposed a method to implement this power in terms of SPSs. In this brief exposure of our basic idea many important details of the derivation were omitted and simple one-dimensional illustrative examples were skipped for the sake of more convincing demonstration of the method by calculations for realistic three-body Coulomb systems. The present paper is meant to fill this gap. Here we present a thorough discussion of the one-channel case; possible generalizations to a multichannel case go beyond the scope of this paper and will be touched upon only briefly [6].

The definition of SSs requires an extension of the real energy axis to complex energy ''plane,'' actually a multisheet Riemann surface. Although all the collision events can be described by the scattering matrix $S(E)$ taken at real energies E, the usefulness of considering complex energies was recognized long ago. As far as we know, the first person who employed complex energy in quantum mechanics was Gamow. In his famous paper on α decay of atomic nuclei [7] Gamow associated the lifetime of a resonance state with the imaginary part of the energy of the state. Later, Breit and Wigner [8] presented a formula describing a

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resonance profile in the scattering cross section in terms of the energy and the lifetime of the resonance state. In search of a formal derivation of the Breit-Wigner formula from the Schrödinger equation, Kapur and Peierls [9] introduced a discrete set of complex-energy eigenstates and showed that narrow resonances in scattering correspond to the states having a small imaginary part of the energy. However, the states considered by Kapur and Peierls were dependent on the scattering energy, which entered their formulation as an external parameter. A formulation that is free from any external parameters and therefore focuses on the intrinsic properties of the system was given by Siegert [10]. In this paper we restrict our treatment to the generic s-wave scattering problem defined by the radial Schrödinger equation

$$(H-E)\phi(r)=0, \quad H=-\frac{1}{2}\frac{d^2}{dr^2}+V(r), \tag{1a}$$

where the potential energy $V(r)$ is assumed to vanish sufficiently fast at $r\to\infty$. Then SSs are defined as the solutions to Eq. (1a) satisfying the regularity boundary condition at $r=0$,

$$\phi(0)=0, \tag{1b}$$

and the outgoing wave boundary condition at $r\to\infty$,

$$\left(\frac{d}{dr}-ik\right)\phi(r)\bigg|_{r\to\infty}=0, \tag{1c}$$

where the energy E and the momentum k are related by

$$E=\frac{1}{2}k^2. \tag{2}$$

Equations (1)–(2) can be satisfied simultaneously only for a discrete set of generally complex momenta k_n; thus one should consider them as an eigenvalue problem defining k_n and corresponding eigenfunctions $\phi_n(r)$. The eigenvalues k_n coincide with poles of the scattering matrix in the complex k plane. Those that lie on the positive imaginary semiaxis correspond to bound states of the system; those lying on the negative imaginary semiaxis correspond to antibound (or virtual) states; all the others occur in pairs k_n and $-k_n^*$ and lie in the lower half of the k plane. The bound states and the SSs with $\mathrm{Im}(k_n)<0$ lying close to the real axis, which manifest themselves as resonances in scattering at zero $[\mathrm{Re}(k_n)=0]$ or finite $[\mathrm{Re}(k_n)\neq 0]$ energies, individually represent some basic features of the system; the other SSs lying deeper in the lower half plane are not observable individually and are related to the background scattering. The distinction between the two groups is not mathematically rigorous, unless one rigorously defines what is a resonance, but it is well known to be physically meaningful. Note the important role played by relation (2): It specifies the structure of the Riemann surface of complex energy E for the present problem as having two sheets connected by the branching point at $E=0$ and establishes a uniformization mapping of this surface onto the plane of complex momentum k upon which the scattering matrix $S(k)$ becomes a single-valued function. Thus the momentum k takes the place of the energy E as a natural parameter of the problem. With the branching cut made along the positive real energy semiaxis, the upper/lower halves of the k plane map onto the so-called physical/unphysical energy sheets, respectively. Siegert eigenenergies are defined by $E_n=k_n^2/2$. Only the bound state poles may appear on the physical sheet; all the others are located on the unphysical sheet (see, e.g., Secs. 128, 133, and 134 in [11], Secs. 12.1 and 16.6 in [12], Sec. 2.2 in [13], and many other treatises on scattering theory).

There is a vast literature devoted to different aspects of the theory of SSs. We mention only several pioneering studies [14–35] containing results relevant to the present work; more references can be found in [12,13]. Hu [14] showed that the knowledge of only the SS eigenvalues k_n suffices to completely determine the scattering matrix $S(k)$ in the whole k plane and gave a formula for $S(k)$ in terms of k_n. Serdobol'skiĭ [18] derived an expansion for the continuous-energy wave function in terms of the SS eigenfunctions $\phi_n(r)$. More and Gerjuoy [28] presented a similar expansion for the outgoing wave Green's function. Many more subtle issues of the theory in which SSs differ from the usual energy eigenstates, such as the orthogonality and normalization condition [18,19,21–23,26–28,30,32], the completeness properties [22,23,28,29,32–34], and the perturbation theory [15,19,21,25,27,28], have also been clarified [36]. These results seem to suggest the foundation for a method capable of a unified treatment of bound states, resonances, and continuum, i.e., the whole spectrum of collision phenomena in terms of purely discrete set of SSs. However, no such method exists as far as computational implementations are concerned. The reason for this is rooted in the following practical difficulty: The momentum k appears in Eqs. (1) and (2) nonlinearly, which renders this eigenvalue problem tractable only by means of an iterative procedure. The iterations can be performed for one or a few SSs, provided that a good initial guess for their eigenvalues k_n is known, but iterative calculations of *many* SSs required for the results mentioned above to be practically useful become prohibitively difficult.

In [5] we have proposed a method to overcome this difficulty. As a preliminary step of our formulation, the outgoing wave boundary condition (1c) should be applied at some finite point

$$\left(\frac{d}{dr}-ik\right)\phi(r)\bigg|_{r=a}=0. \tag{1c$'$}$$

This amounts to cutting off the tail of the potential $V(r)$ that extends beyond $r=a$. In the following, we shall call the solutions to Eqs. (1a), (1b), (1c$'$), and (2) Siegert states for cutoff potentials (SSCPs). In contrast to SSs, which depend on nothing but the potential energy $V(r)$ and certainly present a more general mathematical construction, SSCPs depend also on the cutoff radius a. For the special class of finite range potentials, when the function $V(r)$ identically vanishes outside some fixed radius, SSCPs coincide with SSs for a sufficiently large a; otherwise, the two sets are quite different and even in the limit $a\to\infty$ only a finite number of SSCPs may converge to SSs, as will be discussed below. Switching from Eq. (1c) to Eq. (1c$'$) drastically modifies the analytical structure of the problem, but it does not seem to introduce any restriction for our purposes. Indeed, we are

interested in developing a method that would make the basic results of the theory of SSs practically applicable. However, *all these results were rigorously derived only for finite range potentials*, i.e., actually in terms of SSCPs. Perhaps the results still hold for potentials decreasing faster than any exponential function, although even in this case a rigorous treatment is too complicated and definite statements are few [16]. For potentials decreasing slower than that, which includes exponentially decreasing potentials, the scattering matrix $S(k)$ besides the poles corresponding to SSs may also have so-called redundant poles, branching points, and any kind of singularity in the k plane, depending on the asymptotic behavior of $V(r)$ [17]. We believe that a physically sensible approach should not be sensitive to the extreme tail of the potential, provided that $V(r)$ vanishes sufficiently fast at $r\to\infty$. Accordingly, we shall treat the cutoff potential problem based on Eq. (1c′), with the understanding that the applicability of our method to infinite range potentials must be confirmed by demonstrating convergence with respect to the increase of the cutoff radius a. For the sake of historical accuracy it should be noted that in the original paper by Siegert [10] Eq. (1c′) rather than Eq. (1c) was used. The finiteness of the region to be considered allows us to apply an L^2 expansion technique. This leads to the definition of SPSs as a finite basis representation of SSCPs. In Sec. II we reduce the problem of constructing the complete set of SPSs to a linear algebraic eigenvalue problem and study its properties. This section provides an algebraic foundation for the rest of the paper. Next we rederive the basic results of Refs. [14,18,28] in terms of SPSs: In Sec. III we construct the outgoing wave Green's function and in Sec. IV we obtain the continuous-energy wave function and the scattering matrix. In Sec. V we consider the asymptotic distribution of the SSCP eigenvalues k_n for large n, needed for an understanding of the numerical results presented for a number of model potentials in Sec. VI. In Sec. VII we point out possible generalizations of the present approach and problems encountered therein. A summary of the results and a brief comparison of the SPS formulation with other computational methods in scattering theory conclude the paper in Sec. VIII.

II. SIEGERT PSEUDOSTATES AND THEIR PROPERTIES

A. Reduction to an algebraic form

We consider Eqs. (1a), (1b), (1c′), and (2) defining SSCPs. Having thus confined the problem to a finite interval, we expand the solutions in terms of some primitive square integrable basis, reducing the original differential equation to an algebraic form. Such a reduction is very convenient since it provides a practical recipe to implement our method. In addition, it renders the derivation of many basic equations of the theory simple and transparent. However, it also turns out to be essential, as will become clear later.

We employ a finite basis

$$\pi_i(r),\quad i=1,\ \ldots\ ,N, \tag{3}$$

which is assumed to be orthonormal on the interval $[0,a]$,

$$\int_0^a \pi_i(r)\,\pi_j(r)\,dr=\delta_{ij}\,. \tag{4}$$

Let us define the function

$$I_N(r,r')=\sum_{i=1}^{N}\pi_i(r)\,\pi_i(r'), \tag{5}$$

which is a representation of the unity operator within our basis. We assume that the basis (3) becomes complete in $L^2[0,a]$ when $N\to\infty$, i.e.,

$$I_N(r,r')|_{N\to\infty}=\delta(r-r'), \tag{6}$$

where the convergence is to be understood not pointwise, of course, but in the sense of generalized functions [37]. In order to satisfy Eq. (1b) we assume that $\pi_i(0)=0$, but no restriction on the behavior of $\pi_i(r)$ near $r=a$ is imposed, except that dictated by the condition of square integrability. Premultiplying Eq. (1a) by $\pi_i(r)$, integrating over $r\in[0,a]$, and using the boundary condition (1c′), we obtain

$$\frac{1}{2}\int_0^a \frac{d\pi_i(r)}{dr}\,\frac{d\phi(r)}{dr}\,dr-\frac{ik}{2}\,\pi_i(a)\,\phi(a)+\int_0^a \pi_i(r)[V(r)-E]\phi(r)\,dr=0. \tag{7}$$

Only the values of $\phi(r)$ for r within the interval $[0,a]$ appear in this equation. Hence we can expand $\phi(r)$ in Eq. (7) in terms of the basis (3),

$$\phi(r)=\sum_{j=1}^{N} c_j\pi_j(r),\quad 0\leqslant r\leqslant a. \tag{8}$$

Substituting this expansion into Eq. (7) and using the relation (2), we arrive at the algebraic equation

$$\left(\tilde{\mathbf{H}}-\frac{ik}{2}\mathbf{L}-\frac{k^2}{2}\mathbf{I}\right)c=0. \tag{9}$$

Let us comment on our notation. Here and further on, column vectors of the dimension N are denoted by lower case italic characters, e.g., c in Eq. (9) is a column vector composed of the coefficients c_j in Eq. (8); row vectors of the same dimension will be denoted as c^T, where T stands for transpose (we refrain from using Dirac's notation, because $\langle c|$ usually means transpose *and* complex conjugate of $|c\rangle$, while we shall almost never need complex conjugation); square matrices of the dimension $N\times N$ are denoted by upper case boldface characters and $\mathbf{I}$ is always the unit matrix. The matrices $\tilde{\mathbf{H}}$ and $\mathbf{L}$ in Eq. (9) are defined by their elements

$$\tilde{H}_{ij}=\frac{1}{2}\int_0^a \frac{d\pi_i(r)}{dr}\,\frac{d\pi_j(r)}{dr}\,dr+\int_0^a \pi_i(r)V(r)\pi_j(r)\,dr \tag{10}$$

and

$$L_{ij}=\pi_i(a)\,\pi_j(a). \tag{11}$$

Introducing the Bloch operator [38]

$$L=\frac{1}{2}\,\delta(r-a)\,\frac{d}{dr} \tag{12}$$

and the Hermitized Hamiltonian

$$\tilde{H}=H+L, \tag{13}$$

it can be seen that $\tilde{\mathbf{H}}$ is a matrix representation of $\tilde{H}$ within the basis (3). As follows from Eq. (1c′), the action of L on SSCPs is defined by

$$\int_0^a \pi_i(r)L\,\phi(r)dr=\frac{ik}{2}\pi_i(a)\,\phi(a); \tag{14}$$

thus $\mathbf{L}$ is proportional to a matrix representation of L for SSCPs. Note that for a real basis (3) the matrices $\tilde{\mathbf{H}}$ and $\mathbf{L}$ are real and symmetric. Also note, very importantly, that $\mathbf{L}$ is a projector-type matrix (see Appendix A) and has rank 1. It can be diagonalized by an orthogonal transformation of the basis (3) and its only nonzero eigenvalue is positive and coincides with the trace of $\mathbf{L}$ given by

$$\mathrm{tr}(\mathbf{L})=\sum_{i=1}^{N}\pi_i^2(a). \tag{15}$$

Equation (9) is a projection of Eqs. (1a), (1b), (1c′), and (2) onto an N-dimensional Hilbert space spanned by the basis (3). For any finite N, we shall call the solutions to Eq. (9) Siegert pseudostates. Because only the values of $\phi(r)$ for $r\in[0,a]$ were considered in the derivation of Eq. (9) and because the basis (3) is complete within this interval for infinite N, it is natural to expect by analogy with usual variational expansions (and this will be confirmed by numerical calculations) that the ''lower'' SPSs approximate some ''low-lying'' SSCPs, and that a better approximation for a larger number of SSCPs can be achieved by increasing N [39]. However, at this point it is not clear whether the ''higher'' SPSs represent anything but numerical rubbish. As will be shown below they do, although not individually but as essential members of a complete set. It is this property of SPSs that makes us distinguish them from SSCPs and justifies the introduction of the new term [40]. Accordingly, all the relations below will be derived for a finite N, i.e., in terms of SPSs, corresponding results in terms of SSCPs being recovered in the limit $N\to\infty$. Strictly speaking, we should assign the index N to all the quantities expressed in terms of SPSs. However, for the simplicity of notation we suppress such an index; moreover, we shall use the same notation for SPSs as for SSs and SSCPs, for it will always be clear which set is meant.

Note that for the present problem a representation of the R-matrix basis within our Hilbert space is defined by Eq. (9) with the $\mathbf{L}$ term dropped. This term originates from the Bloch operator and, as will be seen later, it plays a major part within the SPS formulation.

B. Linearization

Equation (9) can have a nontrivial solution only for a discrete set of $k=k_n$; thus it constitutes an algebraic eigenvalue problem defining k_n and corresponding eigenvectors $c^{(n)}$. Yet it is an unconventional eigenvalue problem since it is nonlinear with respect to k. This is a manifestation of the difficulty mentioned in the Introduction. This nonlinearity prohibits direct use of the standard methods of linear algebra. Fortunately, however, the nonlinearity is rather simple since k appears in Eq. (9) only *quadratically*. As is shown below, in this case the problem can be exactly *linearized* to a form of the usual eigenvalue problem, but with the dimension doubled.

Consider a quadratic algebraic eigenvalue problem

$$(\mathbf{A}+\lambda\mathbf{B}+\lambda^2\mathbf{I})c=0, \tag{16}$$

where $\mathbf{A}$ and $\mathbf{B}$ are some $N\times N$ matrices, $\mathbf{I}$ is the unit matrix, and λ and c are the eigenvalue and the eigenvector to be found, respectively. Here we have switched to new notation in order to emphasize the generality of the following discussion. The relation to Eq. (9) is obvious,

$$\lambda=ik,\quad \mathbf{A}=2\tilde{\mathbf{H}},\quad \mathbf{B}=-\mathbf{L}. \tag{17}$$

It is convenient to introduce the matrix

$$\mathbf{M}(\lambda)=\mathbf{A}+\lambda\mathbf{B}+\lambda^2\mathbf{I}, \tag{18}$$

which is called a quadratic matrix polynomial with respect to λ [41]. First, we observe that Eq. (16) has exactly $2N$ solutions, this number being the degree of the polynomial representing $\det[\mathbf{M}(\lambda)]$ as a function of λ. Thus, for a given N there are $2N$ SPSs. This gives a hint as how to linearize Eq. (16). With each eigenpair λ and c satisfying Eq. (16) we associate a column vector of doubled dimension,

$$\begin{pmatrix} c \\ \tilde{c} \end{pmatrix}=\begin{pmatrix} c \\ \lambda c \end{pmatrix}. \tag{19}$$

It is easy to see that this vector satisfies

$$\begin{pmatrix} \mathbf{0} & \mathbf{I} \\ -\mathbf{A} & -\mathbf{B} \end{pmatrix}\begin{pmatrix} c \\ \tilde{c} \end{pmatrix}=\lambda\begin{pmatrix} c \\ \tilde{c} \end{pmatrix}. \tag{20}$$

This is also an eigenvalue problem, but in contrast to Eq. (16) this is a *linear* one and can be dealt with routinely. Equation (20) defines $2N$ eigenvalues λ_n, which coincide with the eigenvalues of Eq. (16), and $2N$ eigenvectors

$$\begin{pmatrix} c^{(n)} \\ \tilde{c}^{(n)} \end{pmatrix}=\begin{pmatrix} c^{(n)} \\ \lambda_n c^{(n)} \end{pmatrix},\quad n=1,\ \ldots\ ,2N, \tag{21}$$

from which the eigenvectors $c^{(n)}$ of Eq. (16) can be found. Thus Eqs. (16) and (20) are equivalent. Such linearization of the problem by means of doubling its dimension is a discrete analog of the well-known procedure of reducing a second-order differential equation to a set of two first-order equations. Obviously, this technique can be extended to a polynomial eigenvalue problem of an arbitrary order [41].

Premultiplying Eq. (20) by the matrix

$$\begin{pmatrix} \mathbf{B} & \mathbf{I} \\ \mathbf{I} & \mathbf{0} \end{pmatrix} \tag{22}$$

it can be reduced to a symmetric form

$$\begin{pmatrix} -\mathbf{A} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \begin{pmatrix} c \\ \tilde{c} \end{pmatrix} = \lambda \begin{pmatrix} \mathbf{B} & \mathbf{I} \\ \mathbf{I} & \mathbf{0} \end{pmatrix} \begin{pmatrix} c \\ \tilde{c} \end{pmatrix}. \tag{23}$$

This is a generalized algebraic eigenvalue problem with the weight matrix given by Eq. (22). If **A** and **B** are symmetric, then the matrices in Eq. (23) are also symmetric. Equation (23) is more convenient than Eq. (20) for deriving some general relations and it may be found advantageous also for numerical solution.

From here on we assume that the matrices **A** and **B** are real and symmetric, as is the case for Eq. (9). From this some properties of the SPS eigenvalues k_n can be deduced. First, if the pair λ and c is a solution of Eq. (16), then the complex conjugate pair λ^* and c^* also is a solution. This means that k_n are either pure imaginary (bound and antibound states), or occur in pairs k_n and $-k_n^*$. Second, using Eq. (16) it can be shown that

$$\mathrm{Im}(\lambda)[c^{*T}\mathbf{B}c + 2\,\mathrm{Re}(\lambda)c^{*T}c] = 0. \tag{24}$$

If $\mathrm{Im}(\lambda) \neq 0$ then, recalling that the only nonzero eigenvalue of **B** ($=-\mathbf{L}$) is negative, from Eq. (24) we have $\mathrm{Re}(\lambda) \geqslant 0$. Thus complex k_n with $\mathrm{Re}(k_n) \neq 0$ may appear only in the lower half of the k plane. These properties coincide with the well-known properties of Siegert eigenvalues; however, in the present formulation we have derived them not from the analytical dependence of the solutions to Eq. (1a) on E, as it is usually done [12], but from the properties of the matrices **A** and **B**. Note an interesting possibility allowed by Eq. (24): $\mathrm{Im}(\lambda) \neq 0$ when $c^{*T}\mathbf{B}c = 0$ and $\mathrm{Re}(\lambda) = 0$. This would correspond to a discrete state embedded in the continuum, in which case $\mathrm{Im}(k_n) = 0$ while $\mathrm{Re}(k_n) \neq 0$.

C. Orthogonality and normalization condition

Assuming that all the eigenvalues λ_n are distinct, it can be shown that the eigenvectors of Eq. (23) are orthogonal with respect to the following inner product

$$(c^{(n)T}\tilde{c}^{(n)T}) \begin{pmatrix} \mathbf{B} & \mathbf{I} \\ \mathbf{I} & \mathbf{0} \end{pmatrix} \begin{pmatrix} c^{(m)} \\ \tilde{c}^{(m)} \end{pmatrix} = 2\lambda_n \delta_{nm}, \tag{25}$$

where the choice of the normalization factor on the right-hand side will become clear shortly. Using Eq. (21), this condition can be rewritten as

$$c^{(n)T}c^{(m)} + \frac{c^{(n)T}\mathbf{B}c^{(m)}}{\lambda_n + \lambda_m} = \delta_{nm}. \tag{26}$$

In the coordinate representation, the SPS eigenfunctions are given by

$$\phi_n(r) = \sum_{j=1}^{N} c_j^{(n)} \pi_j(r), \quad 0 \leqslant r \leqslant a, \tag{27}$$

and Eq. (26) takes the form

$$\int_0^a \phi_n(r)\phi_m(r)dr + i\frac{\phi_n(a)\phi_m(a)}{k_n + k_m} = \delta_{nm}. \tag{28}$$

The function (27) can be smoothly continued beyond $r = a$ by

$$\phi_n(r) = C_n e^{ik_n r}, \quad r \geqslant a, \tag{29}$$

where C_n is a constant. For bound states $k_n = i\kappa_n$, where κ_n is real and positive. In this case, the function (29) exponentially decays at $r \to \infty$ and it is easy to see that Eq. (28) coincides with the ordinary orthogonality and normalization condition for bound states

$$\int_0^\infty \phi_n(r)\phi_m(r)dr = \delta_{nm}. \tag{30}$$

This explains the choice of the normalization factor in Eq. (25). For all the other SPSs the function (29) exponentially grows at $r \to \infty$, since $\mathrm{Im}(k_n) < 0$, and the condition (28) differs from the conventional one (30). The normalization condition for SSCPs is obtained from Eq. (26) in the limit $N \to \infty$; in coordinate representation it is given by the same equation (28). The expression on the left-hand side of this equation for $n = m$ has appeared already in [10]; its relation to the norm of SSCPs was first realized in [18] and in the present form Eq. (28) was first given in [23]. In the latter paper it was interpreted as an analytical continuation of Eq. (30). The unconventional normalization of SSCPs was a big obstacle on the way of incorporating these states into the apparatus of scattering theory. This problem has been addressed by many authors [19,21,23,26–28] who employed different arguments and regularization techniques. Within the SPS formulation this matter becomes very simple: The eigenvectors (21) are orthonormal in the usual sense of the word, but in the space of doubled dimension and with a nonunit weight [see Eq. (25)], and the condition (26) [or (28)] results from the reduction of Eq. (25) to the original Hilbert space. Note the absence of complex conjugation in Eqs. (26) and (28), which is a characteristic feature of all theories of SSs.

D. Completeness relations

The eigenvectors (21), being linearly independent, form a complete set in the space of doubled dimension. This fact is expressed by

$$\sum_{n=1}^{2N} \frac{1}{2\lambda_n} \begin{pmatrix} c^{(n)} \\ \lambda_n c^{(n)} \end{pmatrix} (c^{(n)T}\lambda_n c^{(n)T}) = \begin{pmatrix} \mathbf{B} & \mathbf{I} \\ \mathbf{I} & \mathbf{0} \end{pmatrix}^{-1} = \begin{pmatrix} \mathbf{0} & \mathbf{I} \\ \mathbf{I} & -\mathbf{B} \end{pmatrix} \tag{31}$$

or, equivalently, by

$$\sum_{n=1}^{2N} \frac{1}{\lambda_n} c^{(n)}c^{(n)T} = \mathbf{0}, \tag{32a}$$

$$\sum_{n=1}^{2N} c^{(n)}c^{(n)T} = 2\mathbf{I}, \tag{32b}$$

$$\sum_{n=1}^{2N} \lambda_n c^{(n)}c^{(n)T} = -2\mathbf{B}. \tag{32c}$$

In the coordinate representation, these equations read

$$\sum_{n=1}^{2N} \frac{1}{ik_n}\phi_n(r)\phi_n(r')=0, \tag{33a}$$

$$\sum_{n=1}^{2N} \phi_n(r)\phi_n(r')=2I_N(r,r'), \tag{33b}$$

$$\sum_{n=1}^{2N} ik_n\phi_n(r)\phi_n(r')=2I_N(r,a)I_N(r',a), \tag{33c}$$

where both r and r' lie within the interval $[0,a]$. These equations express important properties of SPSs that hold for any N. In the limit $N\to\infty$, using Eq. (6), we obtain the corresponding properties of SSCPs:

$$\sum_{n=1}^{\infty} \frac{1}{ik_n}\phi_n(r)\phi_n(r')=0, \tag{34a}$$

$$\sum_{n=1}^{\infty} \phi_n(r)\phi_n(r')=2\delta(r-r'), \tag{34b}$$

$$\sum_{n=1}^{\infty} ik_n\phi_n(r)\phi_n(r')=2\delta(r-a)\delta(r'-a). \tag{34c}$$

Equations (34a) and (34b) were first given in [29]. Equation (34b) shows that the set of SSCPs is complete in $L^2[0,a]$, while Eq. (34a) indicates that the set is actually overcomplete, giving a linear combination of the functions $\phi_n(r)$ that turns zero identically. The overcompleteness of SSCPs was another big obstacle for the theory. It renders the question of convergence of the expansions in terms of SSCPs a nontrivial one, namely, convergence is not guaranteed by simply increacing the number of terms. There is no such problem for the expansions in terms of SPSs, provided that *all* $2N$ SPSs are included and convergence is understood with respect to the increase of N. This follows from Eqs. (33b) and (6), which ensure that the set of $2N$ SPSs becomes complete in $L^2[0,a]$ when $N\to\infty$. In other words, taking the limit $N\to\infty$ *within* the SPS formulation provides a control over the overcompleteness. Some authors [28,32,35,13] related the overcompleteness of SSCPs to the factor 2 in Eq. (34b). Such an interpretation is hardly acceptable since this factor can be easily removed by a mere renormalization of $\phi_n(r)$. The SPS formulation also sheds some light on the nature of the overcompleteness: The set of the eigenvectors (21) is complete in the space of doubled dimension, but reduction to the original Hilbert space results in the overcompleteness.

Relation (32c) and its coordinate representations Eqs. (33c) and (34c) have not been given previously, as far as we know. In fact, there is an infinite sequence of such relations that can be generated by the following procedure [42]. Let $\mathbf{Q}_p$ be defined by

$$\mathbf{Q}_p=\sum_{n=1}^{2N} \lambda_n^p c^{(n)}c^{(n)T}. \tag{35}$$

From Eqs. (32a)–(32c) we have $\mathbf{Q}_{-1}=\mathbf{0}$, $\mathbf{Q}_0=2\mathbf{I}$, and $\mathbf{Q}_1=-2\mathbf{B}$. Using Eq. (16) we obtain

$$\mathbf{A}\mathbf{Q}_{p-1}+\mathbf{B}\mathbf{Q}_p+\mathbf{Q}_{p+1}=\mathbf{0}, \tag{36}$$

which provides a three-term recurrence for generating $\mathbf{Q}_p$ for $p\leqslant -2$ and/or $p\geqslant 2$. For example,

$$\mathbf{Q}_{-2}=\sum_{n=1}^{2N} \frac{1}{\lambda_n^2}c^{(n)}c^{(n)T}=-2\mathbf{A}^{-1} \tag{37}$$

and

$$\mathbf{Q}_2=\sum_{n=1}^{2N} \lambda_n^2 c^{(n)}c^{(n)T}=2(\mathbf{B}^2-\mathbf{A}). \tag{38}$$

We do not write down expressions for the higher $\mathbf{Q}_p$ in coordinate representation; just note that the larger positive p, the more diverging at $r=a$ they are when $N\to\infty$.

E. Spectral resolutions of a quadratic matrix polynomial and its inverse

Having found all the eigenvalues λ_n and the eigenvectors $c^{(n)}$ of Eq. (16), one should be able to construct spectral resolutions of the matrix (18) and its inverse. $\mathbf{M}(\lambda)$ can be expressed in terms of λ_n and $c^{(n)}$ using Eqs. (32b), (32c), and (38). The result is quite different from the well-known spectral resolution of a linear matrix polynomial. We give it only for the case when $\mathbf{B}$ is a projector-type matrix (see Appendix A). Using the property (A1) we obtain

$$\mathbf{M}(\lambda)=\frac{1}{2}\sum_{n=1}^{2N} [\lambda^2-\lambda\lambda_n-\lambda_n^2-\mathrm{tr}(\mathbf{B})\lambda_n]c^{(n)}c^{(n)T}, \tag{39}$$

where $\mathrm{tr}(\mathbf{B})$ can be expressed in terms of λ_n and $c^{(n)}$ using Eq. (32c). A similar expansion for the inverse of $\mathbf{M}(\lambda)$ turns out to be simpler. Without assuming any particular structure of $\mathbf{B}$, using Eqs. (32a) and (32b) it can be easily shown that

$$\mathbf{M}^{-1}(\lambda)=\sum_{n=1}^{2N} \frac{c^{(n)}c^{(n)T}}{2\lambda_n(\lambda-\lambda_n)}. \tag{40}$$

This formula will be used in Sec. III for constructing the Green's function.

F. Miscellaneous properties

To conclude this algebraic section, we consider one more property of SPSs needed for the discussion below. From Eq. (18) we have

$$\mathbf{M}(\lambda)-\mathbf{M}(-\lambda)=2\lambda\mathbf{B}, \tag{41}$$

which can be put in the equivalent form

$$\mathbf{I}-2\lambda\mathbf{B}\mathbf{M}^{-1}(\lambda)=\mathbf{M}(-\lambda)\mathbf{M}^{-1}(\lambda). \tag{42}$$

This implies equality of the determinants of the matrices on each side of the equation. The determinant of $\mathbf{M}(\lambda)$ is given by

$$\det[\mathbf{M}(\lambda)]=\prod_{n=1}^{2N} (\lambda-\lambda_n). \tag{43}$$

Again using the fact that **B**, and hence also $\mathbf{BM}^{-1}(\lambda)$, is a projector-type matrix (see Appendix A), from the property (A2) and Eq. (43) we obtain

$$1-2\lambda\ \mathrm{tr}[\mathbf{BM}^{-1}(\lambda)]=\prod_{n=1}^{2N}\frac{\lambda+\lambda_n}{\lambda-\lambda_n}. \tag{44}$$

Taking the residue of both sides at $\lambda\to\lambda_m$ and using Eq. (40) we have

$$c^{(m)T}\mathbf{B}c^{(m)}=-2\lambda_m\prod_{n\neq m}^{2N}\frac{\lambda_m+\lambda_n}{\lambda_m-\lambda_n}. \tag{45}$$

In a coordinate representation these relations read

$$1+ik\sum_{n=1}^{2N}\frac{[\phi_n(a)]^2}{k_n(k_n-k)}=\prod_{n=1}^{2N}\frac{k_n+k}{k_n-k} \tag{46}$$

and

$$[\phi_m(a)]^2=2ik_m\prod_{n\neq m}^{2N}\frac{k_m+k_n}{k_m-k_n}. \tag{47}$$

Equation (46) is essential for expressing the scattering matrix in terms of only the SPS eigenvalues k_n; see Sec. IV. Equation (47) defines the boundary contribution to the SPS norm in Eq. (28), the coefficient C_n in Eq. (29), and the residues of the scattering matrix at its poles given by Eq. (60) below. By taking the limit $N\to\infty$ in Eqs. (46) and (47), one obtains the corresponding properties of SSCPs. To our knowledge, these properties have never been presented in the literature.

III. OUTGOING WAVE GREEN'S FUNCTION

We proceed to rederive the basic results of the theory of SSs in terms of SPSs. Here we construct the outgoing wave Green's function $G(r,r';k)$. For the cutoff potential problem it is defined by the equation

$$(H-E)G(r,r';k)=\delta(r-r') \tag{48a}$$

and the boundary conditions

$$G(0,r';k)=0, \tag{48b}$$

$$\left(\frac{d}{dr}-ik\right)G(r,r';k)\bigg|_{r=a}=0, \tag{48c}$$

where both r and r' lie within the interval $[0,a]$ and we recall the relation (2). We seek the solution in the form

$$G(r,r';k)=\sum_{i,j=1}^{N}G_{ij}(k)\pi_i(r)\pi_j(r'),\quad 0\leqslant r,\ r'\leqslant a. \tag{49}$$

Then for the matrix $\mathbf{G}(k)$ composed of the coefficients $G_{ij}(k)$ we obtain

$$\left(\tilde{\mathbf{H}}-\frac{ik}{2}\mathbf{L}-\frac{k^2}{2}\mathbf{I}\right)\mathbf{G}(k)=\mathbf{I}. \tag{50}$$

Using Eq. (40), the solution to this equation is given by

$$\mathbf{G}(k)=\sum_{n=1}^{2N}\frac{c^{(n)}c^{(n)T}}{k_n(k_n-k)}. \tag{51}$$

In the coordinate representation we have

$$G(r,r';k)=\sum_{n=1}^{2N}\frac{\phi_n(r)\phi_n(r')}{k_n(k_n-k)},\quad 0\leqslant r,r'\leqslant a. \tag{52}$$

This is the SPS expansion of the Green's function. The derivation presented is based on Eqs. (32a) and (32b) or, equivalently, on Eqs. (33a) and (33b), which due to Eq. (6) ensure the δ function on the right-hand side of Eq. (48a) in the limit $N\to\infty$. The SSCP expansion of $G(r,r';k)$ obtained from Eq. (52) in this limit was anticipated in [24,27] and in the present form it was first given in [28]. In its derivation these and subsequent authors [29,31,32] essentially followed the same logical route: Certain analytical properties of $G(r,r';k)$ in the complex k plane were assumed [$G(r,r';k)$ is a meromorphic function of k], which allowed one to apply the Mittag-Leffler expansion theorem [a meromorphic function can be expanded in terms of its poles]. In the SPS formulation, Eq. (52) follows from Eqs. (32a) and (32b), which in turn are rather simple algebraic relations.

Following [29,32], we note that once the SSCP expansion of $G(r,r';k)$, i.e., Eq. (52) in the limit $N\to\infty$, is established, relations (34a) and (34b) follow from the formula

$$G(r,r';k)\big|_{|k|\to\infty}=-\frac{2}{k^2}\delta(r-r')+O(k^{-3}), \tag{53}$$

which is an obvious consequence of Eq. (48a).

IV. CONTINUOUS-ENERGY WAVE FUNCTION AND THE SCATTERING MATRIX

The knowledge of the outgoing wave Green's function $G(r,r';k)$ amounts to a complete solution of the Schrödinger equation. Having expanded $G(r,r';k)$ in terms of SPSs [see Eq. (52)], we are in a position to derive similar expansions for other quantities of interest. In particular, here we consider a continuous-energy wave function $\psi(r;k)$ and the scattering matrix $S(k)$. For the s-wave scattering by a cutoff potential they are defined by

$$(H-E)\psi(r;k)=0, \tag{54a}$$

$$\psi(0;k)=0, \tag{54b}$$

$$\psi(r;k)\big|_{r\geqslant a}=e^{-ikr}-S(k)e^{ikr}. \tag{54c}$$

The solution $\psi(r;k)$ to this one-dimensional equation is related to the Green's function $G(r,r';k)$ by

$$G(r,r';k)=\frac{i}{k}\psi(r_<;k)e^{ikr_>},\quad r_>\geqslant a, \tag{55}$$

where $r_<$ ($r_>$) is the smaller (the larger) of r and r'. Setting $r'=a$, we obtain

$$\psi(r;k)=-ike^{-ika}G(r,a;k),\quad r\leqslant a. \tag{56}$$

Substituting here Eq. (52), we get an expansion for $\psi(r;k)$ in terms of SPSs:

$$\psi(r;k)=-ike^{-ika}\sum_{n=1}^{2N}\frac{\phi_n(r)\phi_n(a)}{k_n(k_n-k)},\quad r\leqslant a. \tag{57}$$

From the condition that Eqs. (54c) and (56) must coincide at $r=a$ we have [38]

$$S(k)=e^{-2ika}[1+ikG(a,a;k)]. \tag{58}$$

Again using Eq. (52), we obtain an expansion for $S(k)$:

$$S(k)=e^{-2ika}\left[1+ik\sum_{n=1}^{2N}\frac{[\phi_n(a)]^2}{k_n(k_n-k)}\right]. \tag{59}$$

We shall call this the ''sum'' formula for the scattering matrix. It shows that $S(k)$ has simple poles at $k=k_n$ with the residues

$$(k-k_n)S(k)|_{k=k_n}=-ie^{-2ik_na}[\phi_n(a)]^2. \tag{60}$$

Using Eq. (46), we obtain an alternative expression for $S(k)$:

$$S(k)=e^{-2ika}\prod_{n=1}^{2N}\frac{k_n+k}{k_n-k}. \tag{61}$$

This will be called the ''product'' formula. Taking into account the properties of the SPS eigenvalues k_n, the product formula explicitly ensures unitarity of the scattering matrix which for real k reads

$$S(k)S^*(k)=S(k)S(-k)=1. \tag{62}$$

In the limit $N\to\infty$, Eqs. (57), (59), and (61) become expressed in terms of SSCPs. The SSCP expansion of the continuous-energy wave function following from Eq. (57) was first given in [18]; see also [30,32]. The product representation of the scattering matrix in terms of SSCPs following from Eq. (61) was first given in [14] and later derived rigorously for finite range potentials in [16]. The situation in the literature regarding the SSCP analog of Eq. (59) is less certain. Although similar expansions have been discussed by many authors [15,20,31,32,35], they always contain some undefined quantities such as an entire function, some residues, or matrix elements (see, e.g., Sec. 12.1 in the standard textbook [12]), which make them actually useless for practical applications. To our knowledege, in that simple form that follows from Eq. (59) in the limit $N\to\infty$, the sum formula for the scattering matrix has not been given previously. Similarly to the case of Green's function, all previous authors following Ref. [15] based their derivations of the scattering matrix on the Mittag-Leffler expansion theorem; this was the source of appearance of some undefined entire function in the resulting formulas. (''The relation between $P(k)$ [*the entire function*] and the poles of S is hard to disentangle, and no simple expression is known.'' See p. 366 in [12]). Within the SPS formulation this matter also gets clarified and Eqs. (59) and (61) do not involve any undefined quantities. Moreover, now we can see a relation between them, namely, formulas (59) and (61) are algebraically equivalent, as follows from the results of Sec. II F. However, they were derived under different assumptions regarding the matrix **B** in Eq. (16): Eq. (59) holds for an arbitrary symmetric **B**, while Eq. (61) requires **B** to be a projector-type matrix (see Appendix A), which is actually the case because **B** represents the Bloch operator (11). This circumstance becomes somehow hidden when the limit $N\to\infty$ is taken. Note that, as follows from Eq. (24), if a discrete state embedded in the continuum exists, it must satisfy $\phi_n(a)=0$; hence the residue (60) vanishes, i.e., such a state is not visible in the scattering.

V. ASYMPTOTIC DISTRIBUTION OF SIEGERT EIGENVALUES FOR CUTOFF POTENTIALS

Prior to discussing the numerical illustrations, here we investigate asymptotic distribution of the SSCP eigenvalues k_n defined by Eqs. (1a), (1b), (1c′), and (2) for $n\to\infty$. This will prove to be helpful for understanding general features of the distributions of SPS eigenvalues presented in Sec. VI.

We shall consider only the eigenvalues k_n lying in the fourth quadrant of the k plane; those lying in the third quadrant are their mirror images with respect to the imaginary axis and there may exist only a finite number of the eigenvalues in the upper half plane. An expansion of k_n for large n was first discussed in [15]. The well-known result reads (see, e.g., [12])

$$k_na|_{n\to\infty}=\pi n-i\left(1+\frac{1}{2}\sigma\right)\ln n+O(1), \tag{63}$$

where σ is defined by

$$V(r)|_{r\to a-0}\propto(a-r)^{\sigma}. \tag{64}$$

Equation (63) gives too rough an approximation: Its first neglected term does not decay with the increase of n, which makes a comparison with the calculated results difficult and ambiguous. We are not aware whether the higher terms in the expansion (63) have ever been treated in the literature; probably, for the lack of an efficient method of calculating k_n, this was considered to be of no practical use, which is not the case in the present work.

Let us consider the case $\sigma=0$, i.e., $V(a)\neq 0$, which is of main interest for the cutoff potential problem. As can be seen from Eq. (63), $|k_n|\sim n$ for $n\to\infty$, so the expansion (63) can be developed further by constructing the Born series for the solutions to Eq. (1a). This approach was actually used in [15,18,16] to derive Eq. (63); however, it becomes too awkward for treating the higher terms. For this purpose, it is very convenient to use a version of the phase-amplitude method proposed in [43]. In this method, the solution to Eq. (1a) satisfying the first boundary condition (1b) is presented in the form

$$\phi(r)=\frac{\mathcal{A}(r)}{\sqrt{k(r)}}\sin[s(r)+\theta(r)]. \tag{65}$$

Here $\mathcal{A}(r)$ and $\theta(r)$ are the amplitude and the phase functions, respectively, and $k(r)$ and $s(r)$ are the classical momentum and action conventionally defined by

$$k(r)=\sqrt{k^2-2V(r)}, \quad s(r)=\int_0^r k(r')dr'. \tag{66}$$

In order to determine the two unknown functions $\mathcal{A}(r)$ and $\theta(r)$ an additional relation between them is needed. This is fixed by

$$\phi'(r)=\sqrt{k(r)}\mathcal{A}(r)\cos[s(r)+\theta(r)]. \tag{67}$$

Then for the phase $\theta(r)$ one obtains the equation

$$\theta'(r)=\frac{k'(r)}{2k(r)}\sin[2s(r)+2\theta(r)], \tag{68a}$$

$$\theta(0)=0 \tag{68b}$$

and the amplitude $\mathcal{A}(r)$ can be found by a straightforward integration, provided that $\theta(r)$ is known [43]. The second boundary condition (1c′) leads to the dispersion relation defining the eigenvalue k:

$$k(a)\cot[s(a)+\theta(a)]=ik, \tag{69}$$

which can be cast in the equivalent form

$$s(a)+\theta(a)=\pi n-\frac{i}{2}\ln\frac{k+k(a)}{k-k(a)}. \tag{70}$$

This equation can be solved iteratively, starting with the approximation provided by Eq. (63); the details are given in Appendix B and the result reads

$$k_n a|_{n\to\infty}=\pi n-i\ln n+\alpha_0+\alpha_1\frac{\ln n}{n}+\alpha_2\frac{1}{n}+\alpha_3\left(\frac{\ln n}{n}\right)^2+O\left(\frac{\ln n}{n^2}\right), \tag{71a}$$

where

$$\alpha_0=-\frac{i}{2}\ln\frac{2\pi^2}{a^2V(a)}, \tag{71b}$$

$$\alpha_1=-\frac{1}{\pi}, \tag{71c}$$

$$\alpha_2=\frac{a}{\pi}\int_0^a V(r)dr-\frac{aV'(a)}{4\pi V(a)}-\frac{1}{2\pi}\ln\frac{2\pi^2}{a^2V(a)}, \tag{71d}$$

$$\alpha_3=-\frac{i}{2\pi^2}. \tag{71e}$$

The branch of the logarithm function for the case $V(a)<0$ should be determined by the substitution $V\to V-i0$, and we have assumed that the integral of $V(r)$ over $r\in[0,a]$ and the derivative $V'(a)$ exist. Note that the terms involving these quantities are the only ones that make Eq. (71) different from the corresponding result for a rectangular potential of the value $V(a)$.

Equation (71) defines an asymptotic string of SSCP eigenvalues that goes to infinity in the fourth quadrant of the k plane. For a more general class of potentials having discontinuities in one of the derivatives somewhere inside the interval $[0,a]$, each discontinuity produces such an asymptotic string [33]. From the presence of the cutoff radius a in Eq. (71) it is clear that this equation describes the *cutoff* SSCPs, which are something like ''particle-in-a-box'' states, but satisfying the outgoing wave boundary condition (1c′). These SSCPs are only weakly affected by the presence of the potential; the individuality of the system is represented by a finite group of SSCPs whose eigenvalues lie in the vicinity of the origin $k=0$. For infinite range potentials, only this finite group can converge to SSs in the limit $a\to\infty$; the cutoff SSCPs never converge, as can be seen from Eq. (71). This indicates that in addition to being incomplete (there generally are branching cuts to be taken into account), SSs are pathologically sensitive to the asymptotic tail of the potential. Cutting off this tail, whatever physically and numerically negligible effect it might seem to produce, drastically modifies the distribution of higher SS eigenvalues. This feature was first realized by Ma [44] for the special case of an exponential potential and later analyzed by Ferreira and Teixeira [45] for the Coulomb potential.

The leading term of the $n\to\infty$ asymptotic for the normalized SSCP wave function is given by

$$\phi_n(r)\approx\sqrt{\frac{2}{a}}\sin(k_n r)\approx\frac{1}{i\sqrt{2a}}\exp(ik_n r). \tag{72}$$

The latter equality holds for all r except for a small vicinity of $r=0$, where the boundary condition (1b) is to be satisfied.

VI. ILLUSTRATIVE EXAMPLES

Numerical calculations of Siegert states apparently were initiated by Nussenzweig [46], who studied the motion of Siegert eigenvalues for a rectangular potential as its strength varies [47]. This work was followed by many others where Siegert states were studied for various one-dimensional potentials [29,32,35,45,48–81] both analytically and numerically. This includes simple models for which the analytical solution is available [46,45,48–51,29,54,32,35,65,73,74], calculations using different variants of the complex rotation method [52,53,55,56,58,59,63,65,70,74], variational calculations with the outgoing wave function explicitly included into the basis [57,60,64,72], calculations using Weyl's theory [61,67,69], Milne's differential equation [66,68], absorbing potentials [75–77], semiclassical approximations [62,66,70], and other methods [71,78–81]. We refer only to those methods that are capable of calculating complex-energy resonance states directly. This does not include, for example, scattering calculations and the stabilization method; even then, the list is inevitably incomplete. Most of these studies focused on one or a few Siegert eigenvalues corresponding to the states visible as distinct resonances in the scattering cross section. Only few of them attempted application of the theory of SSs to calculations of the scattering matrix $S(k)$ [32,35,65,71,73].

In this section we consider several representative potentials for which the numerical calculations have been carried

out in order to demonstrate the computational efficiency of the present approach. The selected examples illustrate some general observations drawn from the calculations for a wider class of potentials and parameters than that reported here. These observations will be formulated and numbered by Roman numerals throughout this section, summarizing our numerical results. We believe that they all apply generally, i.e., for an arbitrary reasonably well behaving potential $V(r)$ vanishing sufficiently fast at $r\to\infty$.

Details of the present numerical procedure are given in Appendix C. In all the cases, SPSs were calculated by solving Eq. (20). Thus, for a given potential $V(r)$, the cutoff radius a, and the number of basis functions N, the computational labor involved for constructing the whole set of $2N$ SPSs amounts to a single diagonalization of a real matrix of the dimension $2N\times 2N$. There are two sources of the numerical errors: the inaccuracy of our potential matrix [we are using an N-point Gauss-Jacobi quadrature (C8)] and the roudoff errors. The former is not intrinsic to our method and can be avoided by using a better integration scheme; the latter seems to be unavoidable. In each case, the accuracy of the presented results will be specified separately.

In the following discussion, instead of the scattering matrix $S(k)$ we often consider the phase shift $\delta(k)$ or the scattering cross section $\sigma(k)$. These quantities are defined by

$$S(k)=\exp[2i\,\delta(k)],\quad \sigma(k)=\frac{4\pi}{k^2}\sin^2\,\delta(k). \tag{73}$$

A. Rectangular potential: General features

We start with the rectangular potential

$$V(r)=\begin{cases} V_0, & r\leqslant a \\ 0, & r>a, \end{cases} \tag{74}$$

which is the simplest example of a cutoff potential. SSCPs in this case were studied in [46,49,50,32,35,73]. The values of the parameters $a=1$ and $V_0=-112.5$ used here are the same as in [73].

It is convenient to order SPSs in accordance with the increase of $|k_n|$. This specifies the meaning of the terms ''lower'' and ''higher'' used in the previous sections. The first feature to be observed is the following.

(i) For a given potential $V(r)$ and the cutoff radius a, each SPS eigenvalue k_n converges when N grows and the lower k_n converge faster. Those k_n that are not affected by a further increase of N within a specified accuracy we shall call basis-independent or N-converged eigenvalues; all the others depend on the basis (3). In the situations where independent calculations of SSCP eigenvalues for the same $V(r)$ and a are available, we confirmed that SPSs converge to SSCPs.

For the potential (74), 50 SSCPs have been tabulated in [73], including 5 bound, 4 antibound, and 41 lowest complex eigenvalues lying in the fourth quadrant of the k plane. Our calculations with the minimum $N=90$ reproduce all of them within the six-digit accuracy quoted in [73]. Together with 41 mirror images lying in the third quadrant, this makes 91 N-converged, within six digits, SPS eigenvalues, which is about a half of the total number $2N=180$ of SPSs in this case. The other half, i.e., the basis-dependent SPSs, differ from their SSCP counterparts more considerably and the difference rapidly grows for higher SPSs. These features are illustrated in Figs. 1 and 2. Figure 1(a) shows the potential function (74) together with the energy positions of the bound and antibound states superimposed on it. Figures 1(b) and 1(c) present distributions of some low-lying SPS eigenvalues in the complex k and E planes, respectively. Figure 2(a) shows a larger portion of the SPS eigenvalues in the k plane and Fig. 2(b) depicts the complete set. Figures 1(b), 1(c), and 2(a) present also the results obtained from the SSCP

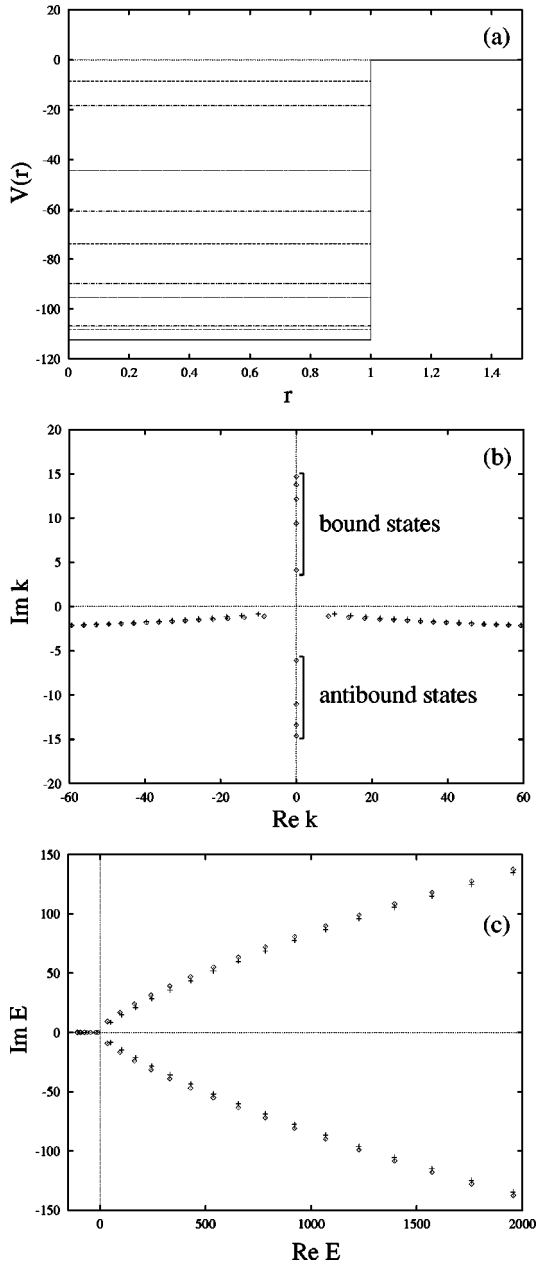

FIG. 1. SPS eigenvalues for the rectangular potential (74) with the parameters $V_0=-112.5$ and $a=1$ calculated using $N=90$ basis functions. (a) Solid line, the potential energy; dashed (dash-dotted) lines, energies of the bound (antibound) states. (b) Diamonds, low-lying SPS eigenvalues in the complex k plane; pluses, the results obtained from the SSCP asymptotic formula (71) shown for $n\geqslant 5$. (c) Same as in (b), but in the complex E plane. All the eigenvalues shown are N-converged within the scale of the figure.

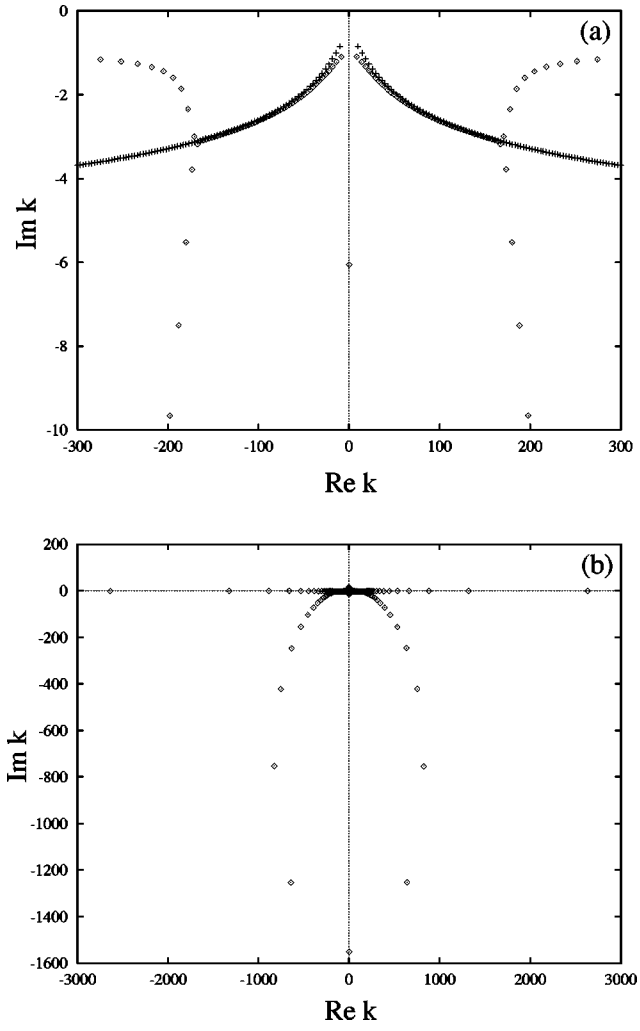

FIG. 2. (a) Same as in Fig. 1(b), but on a larger scale. (b) An even larger scale, which enables one to see the distribution of all $2N=180$ SPS eigenvalues k_n for this case.

asymptotic formula (71). The N-converged SPS eigenvalues, such as those shown in Figs. 1(b) and 1(c), first approach the asymptotic results as n increases. However, as can be seen from Fig. 2(a), this tendency holds only up to some maximum n after which the basis-dependent SPSs quickly diverge from the SSCP asymptotic string, forming quite a different pattern shown in Fig. 2(b).

Next we discuss calculations of the scattering matrix. The convergence of the results obtained from the product formula (61) in terms of SSCPs for the potential (74) was analyzed in [32,35,73]. Korsch *et al.* [73] calculated the elastic phase shift $\delta(k)$ at $k=20$ using different numbers of SSCP eigenvalues in Eq. (61). As follows from their Table 2, the convergence is very poor. For example, with 491 SSCPs (this corresponds to the last entry in the table and includes 241 mirror images lying in the third quadrant) for the phase shift they got -10.7750 against the analytical result -10.6816, as quoted in [73]. Our calculations by Eq. (61) with only $2N=38$ SPSs reproduce six digits of the analytical result and with $2N=50$ we obtain correct twelve digits $-10.681\,639\,621\,0(1)$, which is the best we can do using the double precision arithmetics. The sum formula (59), although it was shown to be algebraically equivalent to Eq. (61), is quite different in implementation and, due to the numerical errors, it yields somewhat different results. For the potential (74), the phase shifts obtained from Eqs. (59) and (61) using the present numerical scheme coincide with each other within at least twelve digits.

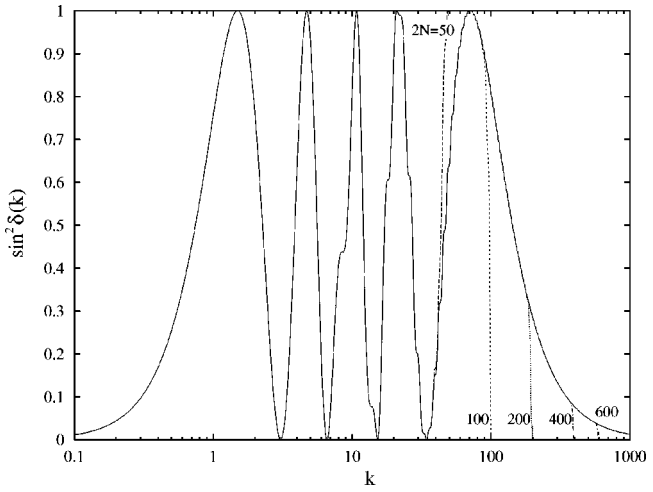

FIG. 3. Function characterizing the phase shift $\delta(k)$ produced by the potential (74). Solid curve, the exact analytical result; broken curves, the results obtained from Eqs. (59) and (61) (indistinguishable in the figure) for different numbers $2N$ of SPSs. At smaller k, all the curves coincide within the scale of the figure. For each value of $2N$, there is a breakdown value of k starting from which the corresponding broken curve diverges from the solid one. Only the initial stages of this divergence are shown; this is followed by violent oscillations of the broken curves at larger k.

Now we make a very important observation regarding the SPS expansions (59) and (61) for the scattering matrix.

(ii) To achieve fast convergence with the increase of N *all* $2N$ SPSs must be included into Eqs. (59) and (61); skipping even one of them, either N-converged or basis-dependent, may make the result completely wrong. Such a behavior is quite different from what one would expect since the higher SPSs certainly do not have any physical meaning individually. However, it has a simple explanation: Our derivation of Eqs. (59) and (61) was essentially based on the completeness relations (32a) and (32b) [or (33a) and (33b)], which are valid only upon inclusion of all $2N$ SPSs.

The following observation concerns the rate of the convergence as a function of k.

(iii) With the increase of N, the upper boundary of the interval of k where the SPS expansions (59) and (61) yield the converged results moves towards the larger k.

This is illustrated in Fig. 3, which shows the function $\sin^2\delta(k)$ calculated using Eqs. (59) and (61) for different values of $2N$. For each $2N$, there is a breakdown value of k up to which the calculated results are indistinguishable in Fig. 3 from the analytical ones and above which they rapidly diverge. As one can see, the convergence with the increase of N is very fast. For example, for $2N=100$ Eqs. (59) and (61) work well up to $k\approx 100$, i.e., up to the energy $E=k^2/2\approx 5000$, which is about 50 times larger than the depth of the potential (74). Remarkably, scattering in this wide energy range is described by the information obtained from diagonalization of only a 100×100 matrix. Note that the convergence is uniform with respect to k: Even tiny diffraction

wavelets seen in Fig. 3 are excellently reproduced by Eqs. (59) and (61). Fast convergence of the SPS expansions (59) and (61) for the scattering matrix demonstrated above constitutes an important advantage of the SPS formulation over all previous theories of SSs.

B. Potential with a barrier: Complex-energy resonance states

The rectangular potential is a bit too special case; the realistic potentials of interest in the collision theory usually have infinite range. In this section we discuss convergence of the results obtained within the SPS formulation with respect to the increase of the cutoff radius a. We consider the potential

$$V(r)=7.5r^2\ \exp(-r), \tag{75}$$

which has a barrier with a maximum height of ≈ 4.06 at $r=2$ [see Fig. 4(a)]. This potential is known to produce a distinct resonance in the scattering cross section at the energy indicated in Fig. 4(a), which has been a testing ground for numerous schemes of resonance calculations [52,53,57,60,62,64,66,70,72,74,76–81].

Figures 4(b) and 4(c) show distributions of some low-lying N-converged SPS eigenvalues calculated for the cutoff radius $a=10$, together with the results obtained from the SSCP asymptotic formula (71). A few lowest SS eigenvalues for the potential (75) have been calculated in [66,77,81]; three of them are also shown in the figures. The general structure of these distributions is similar to that shown in Figs. 1(b), 1(c), and 2 on a larger scale. The only different feature is the appearance of one (apart from its mirror image) separately standing complex eigenvalue indicated as ''resonance.'' Its position coincides within the scale of the figures with that of the lowest SS. The convergence of this eigenvalue with the increase of N and a is illustrated in Table I. Our final results for the position $E_{\rm res}$ and width Γ of this resonance state obtained with the minimum parameters $(a,N)=(30,60)$, i.e., by diagonalizing a 120×120 matrix, are in excellent agreement with and even provide an additional digit in Γ as compared to the best available results of Ref. [77]. Note that in [77] a larger basis of 300 functions and a more accurate scheme of calculating the potential matrix was used; most of the other calculations cited above are restricted to a much lower accuracy. In order to see what happens when the resonance becomes broader, we performed similar calculations with the coefficient 7.5 in Eq. (75) replaced by 2.5. The converged results for the resonance state in this case obtained with the minimum parameters $(a,N)=(35,60)$ are $E_{\rm res}=1.477\,948\,257(1)$ and $\Gamma/2=0.159\,117\,864(1)$. The convergence is achieved at larger a, which is understandable because this resonance is about 10 times broader, and fewer digits get stabilized. These results illustrate the following observation.

(iv) For infinite range potentials, some of the SPS eigenvalues k_n converge within a specified accuracy with the increase of both the number of basis functions N and the cutoff radius a; the others never do. The converging SPSs correspond to bound, weakly antibound, and narrow complex-energy resonance states of the system. In the situations where independent calculations of SS eigenvalues for the same potential are available, we confirmed that these SPSs converge to SSs.

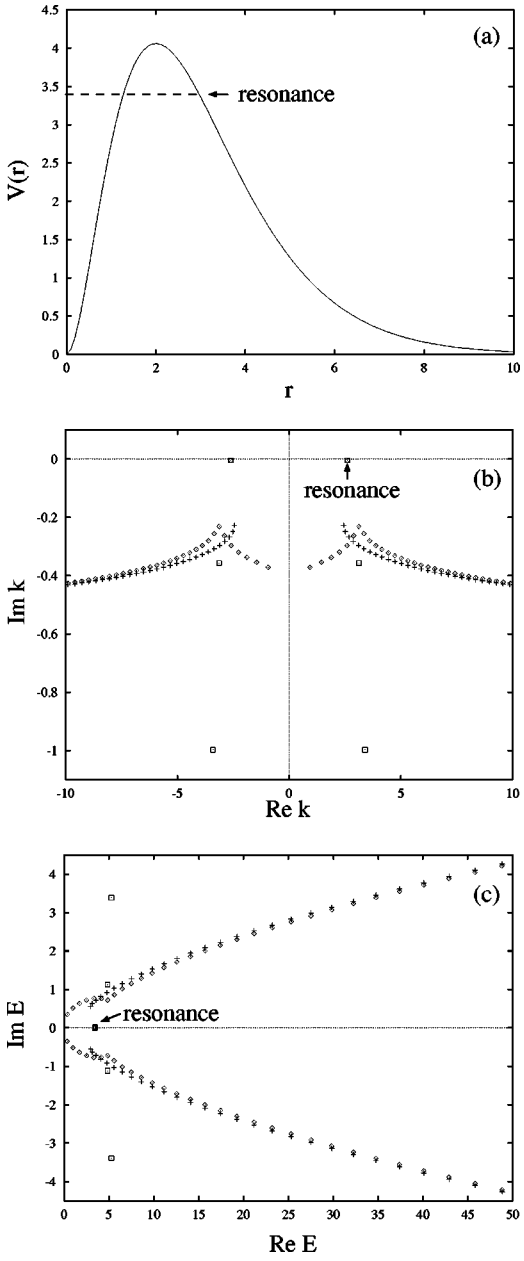

FIG. 4. Similar to Fig. 1, but for the potential (75) calculated with the cutoff radius $a=10$. (a) Solid line, the potential energy; dashed line, energy position of the resonance state. (b) Diamonds, low-lying SPS eigenvalues in the complex k plane; pluses, the results obtained from the SSCP asymptotic formula (71) shown for $n\geqslant 4$; squares, three lowest SS eigenvalues taken from Ref. [66] and their mirror images. (c) Same as in (b), but in the complex E plane. All the SPS eigenvalues shown are N-converged within the scale of the figure. The SPS representing the resonance state lies on the top of the lowest SS.

Table I demonstrates a remarkable accuracy of the present method for calculating true scattering resonances. The situation with the higher SSs, which do not reveal themselves as distinct resonances, is quite different. The second SS produces a cusplike structure in the distribution of the N-converged SPS eigenvalues shown in Figs. 4(b) and 4(c),

TABLE I. Convergence of the SPS calculations of a resonance state for the potential (75) with respect to the increase of the parameters a and N. The resonance position $E_{\rm res}$ and width Γ are defined by $k_n^2/2 = E_n = E_{\rm res} - i\Gamma/2$, where k_n is the corresponding SPS eigenvalue.

a	N	$E_{\rm res}$	$10\Gamma/2$
15	30	3.42639131031	0.127743607748
	40	3.42639141143	0.127744301272
	50	3.42639141144	0.127744301272
20	40	3.42639031473	0.127744665524
	50	3.42639031662	0.127744683508
	60	3.42639031662	0.127744683507
25	40	3.42639652531	0.127868298913
	50	3.42639031007	0.127744805012
	60	3.42639031007	0.127744804629
	70	3.42639031007	0.127744804628
30	50	3.42639023691	0.127746536919
	60	3.42639031015	0.127744805925
	70	3.42639031015	0.127744805930
	80	3.42639031014	0.127744805934
35	60	3.42639031121	0.127744818959
	70	3.42639031015	0.127744805930
	80	3.42639031015	0.127744805933
	90	3.42639031015	0.127744805932
Converged		3.42639031015(1)	0.12774480593(1)
Ref. [77]		3.42639031015	0.1277448059

but there is no individual SPS that would converge to it as a grows. The higher SSs produce even less of an effect on the SPS distribution. This agrees with the results of Refs. [44,45] and illustrates the hypersensitivity of the higher SSs to the asymptotic behavior of the potential.

Next we discuss calculations of the scattering matrix. Table II presents the results for the phase shift $\delta(k)$ at $k=3$, i.e., at the energy $E=4.5$ just above the top of the potential barrier in Fig. 4(a), calculated using Eqs. (59) and (61). For each a, the presented results correspond to the minimum N for which Eq. (61) ensures convergence within all 12 quoted digits. One can see that the product formula

TABLE II. Convergence of the SPS calculations of the phase shift $\delta(k)$ (defined modulus π) produced by the potential (75) at $k=3$ using the sum (59) and the product (61) formulas. For each a, the presented results correspond to the minimum N for which Eq. (61) converges within all 12 quoted digits. Due to the numerical errors, convergence of Eq. (59) with respect to N at larger a becomes worse and for the last three entries in the second column it produces completely wrong numbers (not shown).

(a,N)	Eq. (59)	Eq. (61)
(10,40)	2.98030728982	2.98030728987
(20,55)	2.961	2.96617426069
(30,70)		2.96617194275
(40,85)		2.96617194254
(50,100)		2.96617194254
Converged		2.96617194254(1)

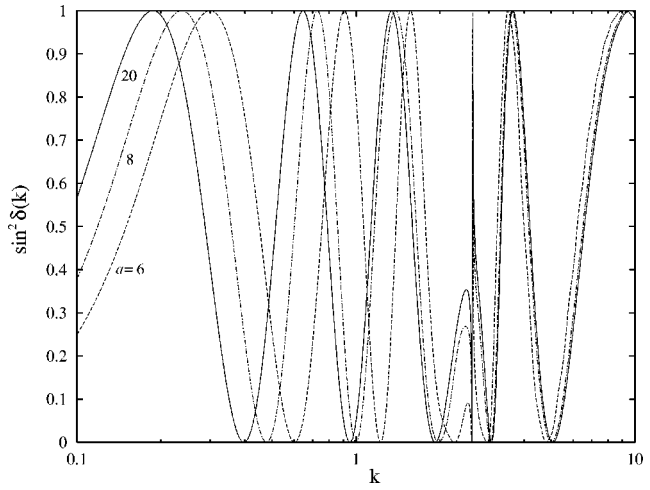

FIG. 5. Function characterizing the phase shift $\delta(k)$ produced by the potential (75). Different curves were calculated using Eq. (61) with $N=100$ for different values of a. All the curves are converged with respect to N. The solid curve ($a=20$) is also converged within the scale of the figure with respect to a.

(61) converges very fast with respect to both N and a. However, the results obtained from the sum formula (59), being in fair agreement with that from Eq. (61) for small a, demonstrate no convergence with the increase of N for larger a. This is due to the numerical errors, which for the present case play a much more violent role. Thus we arrive at the following practically important observation.

(v) Although the sum (59) and the product (61) formulas are algebraically equivalent, they are quite different in implementation and the latter, in addition to being explicitly unitary, is also numerically more stable.

Figure 5 shows the function $\sin^2\delta(k)$ calculated using Eq. (61) with $N=100$ for different values of a. For this N, the breakdown similar to that shown by broken lines in Fig. 3 happens just above $k=10$. The results for $a=20$ are fully converged within the scale of the figure. The resonance discussed above can be clearly seen at $k\approx 2.6$. This figure illustrates the following rather evident feature.

(vi) For infinite range potentials, the finiteness of the cutoff radius affects the low-energy behavior of the scattering matrix. The larger the cutoff radius a, the lower in energy the SPS expansions for $S(k)$ work well.

Thus the parameters a and N restrict the energy range that can be treated by the present method from below and above, respectively. The convergence of the phase shift demonstrated in Table II was achieved in the easy-to-do case of intermediate energies, which explains the incredibly high accuracy of the result. Table III shows how the method works in a wider energy range. Requesting a moderate six-digit accuracy within the interval of k from 0.1 to 10, i.e., E from 0.005 to 50, which is more than 10 times higher than the top of the potential barrier in Fig. 4(a), we achieved convergence with the minimum parameters $(a,N)=(30,170)$.

C. An exponential potential: Bound and antibound states

An exponential potential of the form

$$V(r) = V_0 \exp(-\alpha r) \tag{76}$$

TABLE III. Scattering cross section $\sigma(k)$ calculated for the potential (75) using the product formula (61) with the minimum parameters $(a,N)=(30,170)$, which ensure the requested convergence of all six quoted digits. $a[b]$ means $a\times 10^b$.

k	$\sigma(k)$	k	$\sigma(k)$
0.1	0.711493[3]	5.5	0.296230[−1]
0.5	0.202880[2]	6.0	0.901534[−1]
1.0	0.609153	6.5	0.138188
1.5	0.424456[1]	7.0	0.165388
2.0	0.631273[−1]	7.5	0.175290
2.5	0.710250	8.0	0.173537
3.0	0.425275[−1]	8.5	0.164887
3.5	0.928955	9.0	0.152685
4.0	0.583750	9.5	0.139081
4.5	0.129709	10.0	0.125363
5.0	0.157323[−2]		

allows an exact analytical solution in terms of Bessel functions; see, e.g., [65]. It is of interest in the present context for discussing calculations of bound and antibound states.

There are infinitely many SSs corresponding to antibound states for the potential (76). The positions of the lowest of them for $\alpha=2$ and V_0 varying from -15 to -8 are given in the second column of Table IV. The third column presents calculated results for the corresponding SPS eigenvalue. For $V_0=-15$, this eigenvalue lies rather close to the origin in the k plane and it rapidly converges when a and N increase. Convergence of all nine significant digits of the first entry in the third column of Table IV was achieved with the minimum parameters $(a,N)=(15,40)$. When the strength $|V_0|$ of the potential decreases, this eigenvalue moves downward along the negative imaginary semiaxis and the convergence with respect to the increase of a becomes worse. All the further results given in the third column of Table IV were obtained with the same a and N and we failed to improve on them by increasing these parameters.

TABLE IV. Calculations of the lowest bound (k_b) and antibound (k_a) SPS eigenvalues for the attractive exponential potential (76) for $\alpha=2$ and different values of V_0. The second column lists the analytical results for k_a. The third column lists the SPS results for k_a calculated with $(a,N)=(15,40)$ shown up to the first digit where the difference arises. When it goes deeper in the lower half plane, convergence of this SPS eigenvalue with respect to the increase of a becomes worse. The fourth column lists the SPS results for k_b, which coincide within all quoted digits with the analytical ones.

$-V_0$	ik_a (exact)	ik_a (SPS)	$-ik_b$
15	0.027345771893	0.02734577187	2.27081581770
14	0.144869197957	0.14486919801	2.12319588440
13	0.264888780251	0.264888782	1.97116889372
12	0.387573026885	0.38757305	1.81428218362
11	0.513105796277	0.513107	1.65199746581
10	0.641685750859	0.64172	1.48366586932
9	0.773523383889	0.7742	1.30849265602
8	0.908832940693	0.93	1.12548579773

However, we met no problems in achieving convergence for bound states. There is one bound state for the potential (76) in the interval of V_0 considered above. We could easily get its eigenvalue converged within 12 digits, as given in the last column of Table IV, in full agreement with the analytical results. Moreover, the lack of convergence of the antibound SPS to the corresponding SS does not cause any problems in calculations of the phase shift using the product formula (61): The convergence is similar to that demonstrated in the last column of Table II, although we do not report these results here. We have also checked the case of a repulsive potential (76) with the parameters $V_0=0.5$ and $\alpha=-2/3$ and could easily reproduce the analytical results reported in [65] within all eight quoted digits. These results add evidences to observation (iv) above.

D. Potential with a Coulomb singularity at the origin

In order to demonstrate the computational power of the method, following Ref. [80], we consider the potential

$$V(r)=-\frac{50}{r}\exp(-4r)+\frac{\lambda}{r}\exp(-r), \tag{77}$$

which has a Coulomb singularity at the origin. Čížek and Horáček [80] discussed the behavior of a pair of SS eigenvalues; let us call them k_1 and k_2, with the variation of the parameter λ. For $\lambda=7.5$, these eigenvalues correspond to a bound and an antibound state. In this case, Ref. [80] provides us with the estimate $-ik_1=0.2118$ and $ik_2=0.2251$. Our best results obtained with the minimum parameters $(a,N)=(20,100)$ are $-ik_1=0.211\,769\,667(1)$ and $ik_2=0.225\,082(1)$. Note that convergence for the antibound state (k_2) is worse than for the bound one (k_1). When λ increases, these eigenvalues approach each other, coalesce, and then leave the imaginary axis. For $\lambda=8$, their positions are estimated by $k_{1,2}=\pm 1.2059-i0.056$ [80]. Our calculation with $(a,N)=(30,140)$ yields $k_{1,2}=\pm 1.205\,942\,245\,0(1)-i0.056\,805\,038\,5(1)$. Thus, in all the cases our results agree with those of Ref. [80], but the present method provides a much higher accuracy.

E. Pure centrifugal potential

As the last example we consider a pure centrifugal potential

$$V(r)=\frac{l(l+1)}{2r^2}. \tag{78}$$

This has the purpose of testing the applicability of the method in the case of a nonzero angular momentum.

For $l\neq 0$, there is a phase difference in the conventional definition of the scattering matrix as compared to that given by Eq. (54c). However, if one still defines $S(k)$ by Eq. (54c), then for the case $l=1$ the phase shift $\delta(k)$ would be equal to $\pi/2$, independently of k. The results calculated by Eq. (61) for different values of a and N are shown in Fig. 6. At small k, the deviation from the correct value is due to the finiteness of a and at large k a breakdown similar to that shown in Fig. 3 happens due to the finiteness of N. However, the overall agreement now is much worse than in the previous cases.

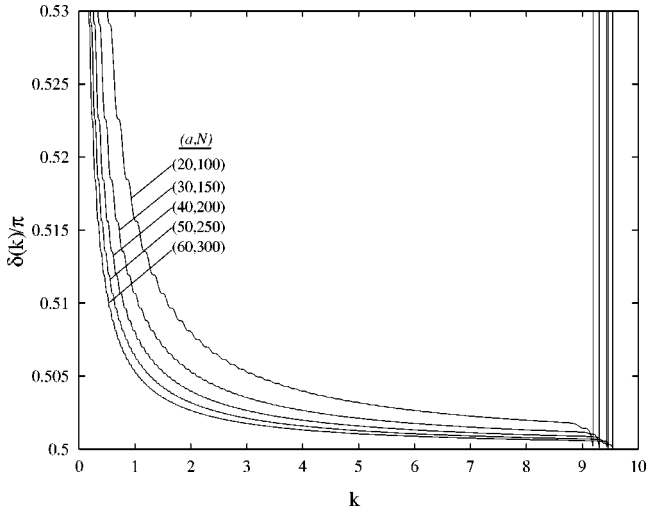

FIG. 6. Phase shift $\delta(k)$ produced by the pure centrifugal potential (78) for $l=1$ calculated with different values of the parameters a and N. The exact value for the present definition of $\delta(k)$ is $\pi/2$, independently of k.

With the increase of a the results do become better, but much slower. Thus, the nonzero angular momenta remain an open problem for the present method; a possibile approach to this problem is discussed in the next section.

VII. POSSIBLE GENERALIZATIONS AND OPEN PROBLEMS

In this section we point out possible generalizations of the SPS formulation and mention some open problems. Some of these generalizations seem to be rather straightforward and could be worked out without essential difficulties. At the same time, the most interesting for applications generalization to a multichannel case meets a problem whose solution is beyond us at the moment.

There are two directions where physically interesting generalizations could be sought. The first one consists in modification of the boundary condition (1c′) as

$$\left(\frac{d}{dr}-f(a,k)\right)\phi(r)\bigg|_{r=a}=0. \tag{1c″}$$

The function $f(a,k)$ here has the meaning of the logarithmic derivative of the outgoing wave soultion to Eq. (1a) at $r=a$. It is introduced to account for the effect due to the tail of the potential that extends beyond $r=a$. For all potentials decreasing faster than the Coulomb one, the following fundamental property holds:

$$f(a,k)|_{a\to\infty}=ik. \tag{79}$$

This relation shows that the SPS formulation exactly incorporates the leading term of $f(a,k)$ at $a\to\infty$ for all physically interesting potentials but the Coulomb one. For such potentials, the modification (1c″) is not essential since at most it can accelerate convergence with respect to the increase of a. However, for potentials with a Coulomb asymptote

$$V(r)|_{r\to\infty}=\alpha/r \tag{80}$$

the tail does produce a significant physical effect represented by the Coulomb logarithmic phase. In this case, one must take into account the next term in Eq. (79):

$$f(a,k)|_{a\to\infty}=ik-\frac{i\alpha}{ka}. \tag{81}$$

It is easy to see that Eqs. (1a), (1b), (1c″), (2), and (81) cast in an algebraic form similar to Eq. (9) result in a *cubic* eigenvalue problem with respect to k. This problem also can be linearized by means of tripling its dimension and treated along the lines of this paper, although all the derivations in this case must be repeated. For the potentials with a centrifugal tail (78) we have

$$f(a,k)|_{a\to\infty}=ik\left(1+\frac{l(l+1)}{2i(ka)^2}+\cdots\right). \tag{82}$$

Taking into account the second term on the right-hand side also leads to a qubic eigenvalue problem, which provides a possibility to remedy the problem of slow convergence met in Sec. VI E.

The other direction of generalization is to seek an extension of the SPS formulation to a multichannel case. Consider a matrix potential $V_{ij}(r)$ whose elements sufficiently rapidly approach constant values when r increases. The eigenvalues $E_1<E_2<\cdots<E_M$ of this matrix at $r\to\infty$ for the M-channel problem define the asymptotic threshold energies. We assume them all to be different; a possible degeneracy would only simplify the situation. It can be shown that in this case, instead of Eq. (16) SPSs are defined by an equation of the form

$$(\mathbf{A}+\sqrt{E-E_1}\mathbf{B}_1+\sqrt{E-E_2}\mathbf{B}_2+\cdots+\sqrt{E-E_M}\mathbf{B}_M+E\mathbf{I})c=0, \tag{83}$$

where $\mathbf{A}$ again represents the Hermitized Hamiltonian and $\mathbf{B}_i$ is proportional to the Bloch operator for the outgoing wave solutions in the channel i. This equation is an eigenvalue problem defining the energy E. Because of the square roots, it is essentially nonlinear with respect to E. If there exists such a uniformization mapping $E(u)$ that reduces Eq. (83) to a polynomial eigenvalue problem in terms of the new variable u, via subsequent linearization of this problem the SPS formulation could be extended to the multichannel case. In the one-channel case, the uniformization mapping is given by Eq. (2). In the two-channel case, such mapping is also known and is defined by the equations (see Sec. 17.1 in [12])

$$\sqrt{E-E_1}=\Delta\frac{1+u^2}{1-u^2},\quad \sqrt{E-E_2}=\Delta\frac{2u}{1-u^2}, \tag{84}$$

where

$$\Delta=\sqrt{E_2-E_1}. \tag{85}$$

It is easy to see that upon substitution of Eqs. (84) into Eq. (83), the latter reduces to a *quartic* eigenvalue problem with respect to u. It would be very interesting and instructive to investigate this problem along the lines of this paper and to establish the structure of the scattering matrix in terms of the

SPS eigenvalues u_n, similar to that given by Eq. (61). We leave this program for future studies. Note that there are some results to this point available in the literature [82,83], although they have never been scrutinized numerically.

For more than two channels, the uniformization mapping $E(u)$ is not known to us. Moreover, even if it exists, there is a circumstance that may require the introduction of an essentially different element in the formulation. Namely, the Riemann surface spanned by the uniformization variable u in this case is known to have a nonzero genus, i.e., it cannot be topologically mapped onto an ordinary complex plane [84,12]. For example, for the three-channel problem this surface is topologically equivalent to a torus. In one- and two-channel cases the uniformization mapping, whose purpose is to make the scattering matrix a single-valued function, simultaneously reduces Eq. (83) to a polynomial form. Whether such polynomial form of the problem is possible to achieve for more than two channels remains an open question.

Although the multichannel case is forbidden at the moment, the present formulation should work for multidimensional but exactly separable problems. An interesting example of such a situation is given by the two-center Coulomb problem. In this case, instead of the radial equation (1a) one should deal with a quasiradial equation in spheroidal coordinates, which has quite a different mathematical nature. A Sturmian basis for this problem has been discussed recently [85]. We also mention an interesting possibility to apply the machinary of the polynomial eigenvalue problems [41] to calculations of Regge states [86].

Finally, the following comment concerning our previous paper [5] is in order here. In [5] we calculated positions and widths for several resonances in eep, $dt\mu$, and $dd\mu$ three-body Coulomb systems lying below the $n=2$ threshold. The discussion above may raise a question regarding the consistency of the calculations reported in [5]. The answer is given as follows: The present formulation is completely eligible to be used even in multichannel problems in the situations where there is only one open channel. This is the case for the $n=2$ resonances in the symmetric three-body Coulomb systems such as eep and $dd\mu$. In the case of $dt\mu$, by virtue of the weakness of the coupling with the $t+d\mu(n=1)$ decay channel, the results reported in [5] are numerically correct, as is confirmed by the good agreement with the results of Ref. [87], of which we became aware recently.

VIII. SUMMARY AND DISCUSSION

To summarize this work, its principal achievment consists in finding a way to implement the power of Siegert states as a universal tool for treating the whole spectrum of collision phenomena. This became possible via doubling the dimension of the original Hilbert space and introducing Siegert pseudostates that actually make our method practical. A rederivation of the basic results of the theory of Siegert states in terms of SPSs has led us to a new formulation of the scattering theory for the simplest generic scattering problem considered here. The main results of this formulation are presented by the SPS expansions for the outgoing wave Green's function (52), continuous-energy wave function (57), and the scattering matrix (59) and (61). These representations are easy to implement and their computational efficiency was demonstrated by a number of numerical examples.

Before closing the paper, it is worthwhile to compare the SPS formulation with other computational approaches in scattering theory. The universality of the present method should be viewed from the perspective of the diversity of the existing methods for a separate treatment of bound states, resonances, and continuum spectrum. Perhaps our method has no advantages over variational calculations of bound states, but it does provide the best accuracy in calculating complex-energy resonances, as was demonstrated above. Besides the high accuracy, there are also certain conceptual advantages; thus, in contrast to the complex rotation method, the present method does not require analytical continuation of the potential energy $V(r)$ into the complex r plane and in contrast to the stabilization method and scattering calculations, it yields the resonance position and width directly, without any fitting procedure. Among the methods for treating continuum, the SPS formulation should be compared with the R-matrix method. The two approaches have many features in common. In each of them, the heavy part of the calculations should be done only once and consists in diagonalization of a ''big'' matrix and constructing a set of energy-independent information that then can be used for high-resolution scattering calculations in a wide energy range, whose size grows with the dimension of the matrix. The difference lies in the basis states and can be characterized briefly by saying that the SPS basis incorporates more physics and better portrays the individuality of the system, while the R-matrix basis is more on the side of a mere computational tool. Thus the existence of scattering resonances within the SPS formulation can be seen already from the SPS eigenvalues, without doing the scattering calculations. This may present an important technical merit in the case of very narrow resonances, which are difficult to locate by scanning the energy range. Another technical merit is that due to the complexity of the SPS eigenvalues, the well-known problem of singularities of the R-matrix method [88] does not arise. The SPS formulation also has advantages as a method of discretization of the continuum. SPSs could be used as a basis for expanding the target states in time-dependent close-coupling calculations, which would lead to a consistent way of treating the ionization and enable one to distinguish between excitation of a resonance state and the underlying continuum scattering. Another advantage stems from the fact that the SPS expansion for the outgoing wave Green's function (52) has a very simple dependence on the energy, which opens a way to study the time-evolution problems [89]. Finally, we wish to emphasize the product formula (61) which has no analog in other methods of scattering calculations. The price for all this is doubling the dimension of the matrix to be diagonalized.

In conclusion, there are still many problems and some of them may turn out to be difficult to solve, but we believe that the approach initiated in [5] and more fully developed in the present paper is worth pursuing, and that the SPS formulation will find applications in the theory of atomic and molecular collisions.

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APPENDIX A: SOME PROPERTIES OF THE PROJECTOR-TYPE MATRICES

Let $\mathbf{P}=uv^T$, where $\mathbf{P}$ is an $N\times N$ matrix and u and v are some N-dimensional column vectors. We call such $\mathbf{P}$ a projector-type matrix. First, we note that

$$\mathbf{P}^2=\mathrm{tr}(\mathbf{P})\mathbf{P}, \tag{A1}$$

which is obvious. Second, we prove the identity

$$\det(\mathbf{I}+\mathbf{P})=1+\mathrm{tr}(\mathbf{P}). \tag{A2}$$

Indeed, let us introduce a new orthonormal basis such that the first two basis vectors e_1 and e_2 lie in the plane of the vectors u and v and all others e_i, $i=3,\ \ldots\ ,N$ are perpendicular to that plane. Let e_1 be directed along u, with e_2 thus being perpendicular to u. In the new basis the matrix $\mathbf{P}$ has only two nonzero elements $e_1^T\mathbf{P}e_1=\mathrm{tr}(\mathbf{P})$ and $e_1^T\mathbf{P}e_2$, while the unit matrix $\mathbf{I}$, of course, remains unchanged. Now it can be easily seen that in the new basis Eq. (A2) holds. Hence it holds in any basis since both determinant of a matrix and its trace are invariant under a change of basis.

APPENDIX B: DERIVATION OF EQ. (71)

Here we give some details needed for the derivation of Eq. (71). Assuming the expansion (71a), we have

$$s(a)=k_n a-\frac{a}{\pi n}\int_0^a V(r)dr+O\left(\frac{\ln n}{n^2}\right), \tag{B1}$$

$$\ln\frac{k_n+p(a)}{k_n-p(a)}=2\ln n+\ln\frac{2\pi^2}{a^2V(a)}-\frac{2i}{\pi}\frac{\ln n}{n}+\frac{2\alpha_0}{\pi n}+\frac{1}{\pi^2}\left(\frac{\ln n}{n}\right)^2+O\left(\frac{\ln n}{n^2}\right), \tag{B2}$$

and from Eq. (68)

$$\theta(a)=\frac{a^3V'(a)e^{2i\alpha_0}}{8\pi^3 n}+O\left(\frac{\ln n}{n^2}\right). \tag{B3}$$

Substituting these expansions into Eq. (70), we confirm the assumed form of Eq. (71a) and obtain the coefficients (71b)–(71e).

APPENDIX C: NUMERICAL PROCEDURE

Here we describe the numerical procedure used for calculating SPSs in this paper as well as for treating the radial part of the three-body Coulomb problems in [5]. For practical reasons, it is more convenient to consider a somewhat modified form of Eqs. (1a), (1b), and (1c′). To avoid introducing new notation for only slightly modified quantities, such quantities will be denoted by the same symbols as their counterparts in the main text, although they are not always identical. A link with the notation above will be established by specification of the matrices $\mathbf{A}$ and $\mathbf{B}$ in Eq. (16).

The SPSs were calculated by solving the equations

$$\left[H-\frac{1}{2}k^2\rho(r)\right]\phi(r)=0, \tag{C1a}$$

$$\phi(r)|_{r\to 0}\propto r^l, \tag{C1b}$$

$$\left(\frac{d}{dr}-\frac{b}{r}-ik\right)\phi(r)\bigg|_{r=a}=0. \tag{C1c}$$

Here l is the angular momentum, $b=-1$ for the present case of three-dimensional spherical wave, and the Hamiltonian H is defined by

$$H=K+U(r), \tag{C2}$$

$$K=-\frac{1}{2}\frac{d}{dr}\rho(r)\frac{d}{dr},\quad \rho(r)=r^2, \tag{C3}$$

$$U(r)=\frac{1}{2}l(l+1)+\rho(r)V(r), \tag{C4}$$

where $V(r)$ is the potential energy and it is assumed that $\rho(a)V(a)=0$.

For the numerical treatment, instead of r we introduce a new variable x,

$$r=\frac{a}{2}(1+x). \tag{C5}$$

Then the interval $r\in[0,a]$ maps onto $x\in[-1,1]$. As a basis in $L^2[-1,1]$ one can employ the set of functions

$$\varphi_n(x)=\sqrt{\frac{w(x)}{h_{n-1}}}P_{n-1}^{(\alpha,\beta)}(x),\quad n=1,\ \ldots\ ,N, \tag{C6}$$

where $P_n^{(\alpha,\beta)}(x)$ are the Jacobi polynomials orthogonal on the interval $x\in[-1,1]$ with the weight

$$w(x)=(1-x)^\alpha(1+x)^\beta \tag{C7}$$

and h_n are corresponding normalization constants [90]. In order to satisfy the boundary conditions (C1b) and (C1c) we choose $\alpha=0$ and $\beta=2l$. The basis (C6) is orthonormal and becomes complete in $L^2[-1,1]$ when $N\to\infty$. However, in practical calculations one can operate with only a finite number N of the basis functions. Such truncation of the basis is known as a finite basis representation (FBR). Given the value of N, for a number of practical reasons it is convenient to switch from the FBR to a discrete variable representation (DVR) [91]. The polynomials $P_n^{(\alpha,\beta)}(x)$ define an associate N-point Gauss-Jacobi quadrature

$$\int_{-1}^{1}F(x)w(x)dx\approx\sum_{i=1}^{N}\omega_i F(x_i), \tag{C8}$$

where $F(x)$ is an arbitrary function such that the integral on the left-hand side of Eq. (C8) exists and x_i and w_i are quadrature abscissas and weights, respectively. Note that formula (C8) gives an exact result for $F(x)$ polynomial of degree $2N-1$ or less. The quadrature (C8) and the related Christoffel-Darboux identity provide a foundation for the FBR-DVR transformation [92]:

$$\varphi_n(x)=\sum_{i=1}^{N} T_{ni}\pi_i(x), \quad \pi_i(x)=\sum_{n=1}^{N} T_{ni}\varphi_n(x), \quad \text{(C9)}$$

where

$$T_{ni}=(T^{-1})_{in}=\kappa_i\varphi_n(x_i) \quad \text{(C10)}$$

and

$$\kappa_i=\sqrt{\frac{\omega_i}{w(x_i)}}. \quad \text{(C11)}$$

The DVR basis functions

$$\pi_i(x), \quad n=1, \ \ldots \ ,N, \quad \text{(C12)}$$

also form an orthonormal set on the interval $[-1,1]$ and have the property

$$\pi_i(x_j)=\kappa_i^{-1}\delta_{ij}, \quad \text{(C13)}$$

which reveals them as a *pointwise* basis conjugate to the *polynomialwise* basis (C6).

We expand the solutions of Eq. (C1) in terms of the DVR basis

$$\phi(x)=\sum_{j=1}^{N} c_j\pi_j(x), \quad -1\leqslant x\leqslant 1. \quad \text{(C14)}$$

Substituting this into Eq. (C1a), premultiplying by $\pi_i(x)$, integrating over $x\in[-1,1]$, and using the boundary conditions (C1b) and (C1c), we arrive at the algebraic eigenvalue problem

$$\left[\tilde{\mathbf{H}}-(b+ika)\mathbf{L}-\frac{1}{2}k^2\boldsymbol{\rho}\right]c=0, \quad \text{(C15)}$$

where c is the vector of coefficients in Eq. (C14) and the boldface characters denote matrices defined with respect to the DVR basis:

$$\tilde{H}_{ij}=\tilde{K}_{ij}+U(r_i)\delta_{ij}, \quad \text{(C16)}$$

$$\tilde{K}_{ij}=\frac{1}{2}\int_{-1}^{1}\frac{d\pi_i(x)}{dx}(1+x)^2\frac{d\pi_j(x)}{dx}dx, \quad \text{(C17)}$$

$$L_{ij}=\pi_i(1)\pi_j(1), \quad \text{(C18)}$$

$$\rho_{ij}=\frac{a^2}{4}\int_{-1}^{1}\pi_i(x)(1+x)^2\pi_j(x)dx. \quad \text{(C19)}$$

All these matrices are real and symmetric. The tilde over $\tilde{\mathbf{H}}$ and $\tilde{\mathbf{K}}$ indicates that they represent Hermitized versions of the operators H and K, respectively. Matrix elements of $U(r)$ in Eq. (C16), where r_i is related to x_i by Eq. (C5), were calculated *approximately*, using the quadrature (C8). However, the result is exact for the centrifugal part of $U(r)$ [the first term in Eq. (C4)] and for the Coulomb singularity of $V(r)$, if any. The exactness of the potential matrix in Eq. (C16) for purely Coulomb $V(r)$ reveals a computational advantage of Eq. (C1a) over Eq. (1a). We refrain from using the quadrature for calculating the matrix $\boldsymbol{\rho}$ since this may lead to an unnecessary slowing down of the convergence with respect to the increase of N. Without derivation we give formulas used for calculating the matrices $\tilde{\mathbf{K}}$ and $\boldsymbol{\rho}$ ($\alpha=0$ is assumed here as above). For $\tilde{\mathbf{K}}$ we have

$$\tilde{K}_{ij}=\sum_{n,m=1}^{N} T_{ni}\tilde{K}^{(\varphi)}_{nm}T_{mj}, \quad \text{(C20)}$$

where

$$\tilde{K}^{(\varphi)}_{nm}=\varphi_n(1)\varphi_m(1)\left[2\sum_{k=1}^{n-1}\varphi_k^2(1)+\varphi_n^2(1)-\frac{1}{2}\right], \quad \text{(C21a)}$$

for $n<m$,

$$\tilde{K}^{(\varphi)}_{nn}=2\varphi_n^2(1)\sum_{k=1}^{n-1}\varphi_k^2(1)+\frac{1}{2}\left(\varphi_n^2(1)-\frac{1}{2}\right)^2, \quad \text{(C21b)}$$

and $\tilde{K}^{(\varphi)}_{nm}=\tilde{K}^{(\varphi)}_{mn}$. The matrix $\boldsymbol{\rho}$ is given by

$$\rho_{ij}=\frac{a^2}{4}[(1+x_i)^2\delta_{ij}+\Delta(N)T_{Ni}T_{Nj}], \quad \text{(C22)}$$

where the first term coincides with what would be obtained using the quadrature (C8), and

$$\Delta(N)=\frac{4N^2(N+\beta)^2}{(2N+\beta)^2[(2N+\beta)^2-1]}. \quad \text{(C23)}$$

The polynomials $P_n^{(\alpha,\beta)}(x)$, quadrature abscissas x_i, and weights ω_i were calculated using the algorithms of Ref. [93].

After the differential eigenvalue problem (C1) is cast into an algebraic form (C15), there are two ways to transform it further to the required form of Eq. (16). One can premultiply Eq. (C15) by $2\boldsymbol{\rho}^{-1}$ and obtain for the vector c an equation of the type (16) where $\lambda=ik$ and

$$\mathbf{A}=2\boldsymbol{\rho}^{-1}(\tilde{\mathbf{H}}-b\mathbf{L}), \quad \text{(C24a)}$$

$$\mathbf{B}=-2a\boldsymbol{\rho}^{-1}\mathbf{L}. \quad \text{(C24b)}$$

However, these matrices are not symmetric, in contradiction to what has been assumed in writing Eqs. (25) and (31). Another approach is to introduce a new vector of coefficients

$$s=\boldsymbol{\rho}^{1/2}c. \quad \text{(C25)}$$

Then premultiplying Eq. (C15) by $2\boldsymbol{\rho}^{-1/2}$ for the vector s we again obtain Eq. (16), now with symmetric matrices

$$\mathbf{A}=2\boldsymbol{\rho}^{-1/2}(\tilde{\mathbf{H}}-b\mathbf{L})\boldsymbol{\rho}^{-1/2}, \tag{C26a}$$

$$\mathbf{B}=-2a\boldsymbol{\rho}^{-1/2}\mathbf{L}\boldsymbol{\rho}^{-1/2}. \tag{C26b}$$

In our calculations we solved Eq. (20) using a general eigenvalue problem solver. In this case, it is simpler to use Eqs. (C24). If in doing this linear algebra part of the calculations one is going to utilize some advantages of the symmetric form Eq. (23), then Eqs. (C26) must be used.

Finally, we note the relation

$$\begin{pmatrix} \mathbf{B} & \mathbf{I} \\ \mathbf{I} & \mathbf{0} \end{pmatrix}=\begin{pmatrix} -\mathbf{D}-i\mathbf{D}^{-1} & i\mathbf{D} \\ i\mathbf{D} & \mathbf{D} \end{pmatrix}^2, \tag{C27}$$

where

$$\mathbf{D}=(2i\mathbf{I}-\mathbf{B})^{-2}. \tag{C28}$$

This permits one to reduce the generalized algebraic eigenvalue problem Eq. (23) to an ordinary one with a symmetric but explicitly complex matrix.

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