Siegert pseudostate formulation of scattering theory: Nonzero angular momenta in the one-channel case

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The Siegert pseudostate (SPS) formulation of scattering theory, originally developed by Tolstikhin, Ostrovsky, and Nakamura [Phys. Rev. A, **58**, 2077 (1998)] for s-wave scattering in a spherically symmetric finite-range potential, is generalized to nonzero angular momenta. The orthogonality and completeness properties of SPSs are established and SPS expansions for the outgoing-wave Green's function, physical states, and scattering matrix are obtained. The present formulation completes the theory of SPSs in the one-channel case, making its application to three-dimensional problems possible. The results are illustrated by calculations for several model potentials.

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I. INTRODUCTION

Siegert states (SSs) are the solutions to the stationary Schrödinger equation, i.e., eigenfunctions of the Hamiltonian, which are regular everywhere and have only one type of waves, incoming or outgoing, in the asymptotic region. These boundary conditions can be satisfied simultaneously only for isolated generally complex values of the energy. The corresponding eigenvalue problem was first formulated in 1939 by Siegert [1] for s-wave scattering in a spherically symmetric finite-range potential.

The set of SSs is purely discrete. This is an important advantage over the more familiar set of physical states conventionally considered in scattering theory [2,3], which consists of discrete and continuous parts. At the same time, the two sets can be uniquely expressed in terms of each other. Thus it should be possible to reformulate scattering theory in terms of SSs. The goal of such an undertaking is an alternative approach to the theory of processes in the continuum which opens new analytical and computational perspectives in atomic physics.

Since the pioneering paper [1], the different issues in the theory of SSs have been addressed by many authors; the results are summarized in [3–6]. The main obstacle in the development of the theory is that, apart from a finite number of SSs representing bound states of the system, the SS eigenfunctions exponentially grow in the asymptotic region. As a consequence, SSs possess unusual orthogonality and completeness properties which hindered their incorporation into the formalism of scattering theory. The traditional approach based on the differential equations turned out to be not very fruitful in overcoming these difficulties; the available results [3–6] are fragmentary. Besides, they long remained useless for practical calculations because there was no an efficient method to numerically generate SSs.

The situation has changed after an algebraic approach and the concept of Siegert pseudostates (SPSs) were introduced in [7]. SPSs are a finite-basis representation of SSs for finite-range or cutoff potentials. The theory of SPSs gives an extension of the theory of SSs to finite values of N, where N is the dimension of the basis, in the same sense as quantum mechanics gives an extension of classical mechanics to nonzero values of $\hbar$. This means that all basic equations in the theory of SSs have their counterparts in terms of SPSs and can be obtained from the latter in the limit $N \to \infty$. SPSs suggest a very simple and transparent algebraic approach to the theory of SSs, which enables one not only to advance the theory, clarifying some of its mathematical aspects that are not readily apparent from the original differential equations, but also to implement the results.

So far, the theory of SPSs has been thoroughly developed only for s-wave scattering in one-channel [8] and two-channel [9] cases; recently, these formulations were supplemented by a discussion of the SPS perturbation theory [10]. In both cases, the task of generating the complete set of SPSs needed for the expansions in their terms to converge was reduced to a single-matrix diagonalization. The efficiency of this approach has been demonstrated by calculations for a number of model and realistic systems in the stationary [7–19] and time-dependent [20–24] frameworks. To make the approach applicable to more challenging three-dimensional problems it is necessary to extend it to higher partial waves.

In the present paper, the one-channel theory of [8] is generalized to nonzero angular momenta. Our presentation parallels that in [8]; however, the generalization is not straightforward. In Sec. II, we define the SPSs and establish their orthogonality, completeness, and some other properties. In Sec. III, all major objects of stationary scattering theory—namely, the outgoing-wave Green's function, physical states, and scattering matrix—are expressed in terms of SPSs. The corresponding results in terms of SSs follow in the limit $N \to \infty$. Some of the relations obtained have been known from previous studies, we simply rederive them in terms of SPSs, which is needed for consistency of the formulation as well as for its implementation, whereas others, to the best of our knowledge, have not appeared in the literature. We cite, where appropriate, only major original contributions to the subject; a concise review of the literature was given in [8], and much more extensive bibliography can be found in [3–6]. The results are illustrated by calculations of partial, differential, and total scattering cross sections and photoionization for several model potentials in Sec. IV. Section V concludes the paper.

II. SIEGERT PSEUDOSTATES AND THEIR PROPERTIES

In this section, we define the SPSs and establish their basic properties. The presentation may seem to be too technical, even though we try to skip details, but this is necessary for laying down a comprehensive foundation for the next section as well as future applications.

A. Siegert states: Basic differential equations

The radial Schrödinger equation describing the motion of a particle with angular momentum l in a spherically symmetric potential $V(r)$ reads [2,3] (a system of units in which $\hbar = m = 1$ and all the quantities involved in the analysis are dimensionless is used throughout the paper)

$$(H_l - E)\phi(r) = 0, \tag{1}$$

where

$$H_l = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + V(r). \tag{2}$$

We shall assume that the potential $V(r)$ has a finite range,

$$V(r)|_{r>a} = 0, \tag{3}$$

or decays sufficiently rapidly as r grows, so that cutting off its tail beyond $r=a$ does not produce any appreciable effect on the observables. The SSs are the solutions to Eq. (1) satisfying the regularity boundary condition at the origin,

$$\phi(0) = 0, \tag{4}$$

and the outgoing-wave boundary condition in the asymptotic region,

$$\left(\frac{d}{dr} - ik\right)\phi(r)\bigg|_{r\to\infty} = 0, \tag{5}$$

where the energy E and momentum k are related by

$$E = k^2/2. \tag{6}$$

This is an eigenvalue problem. The SS momentum and energy eigenvalues and eigenfunctions will be denoted by k_n, $E_n = k_n^2/2$, and $\phi_n(r)$. All the objects of scattering theory considered in this paper will be indicated by a subscript l, as in Eq. (2), in order to emphasize their dependence on the angular momentum; for brevity, we omit such a subscript in the notation for the SSs, but it should be remembered that they also depend on l.

We restrict our treatment to potentials that are not too singular at the origin,

$$r^2 V(r)|_{r\to 0} = 0. \tag{7}$$

In this case, the regularity boundary condition (4) can be specified as

$$\phi(r)|_{r\to 0} \propto r^{l+1}. \tag{8}$$

The outgoing-wave boundary condition (5) plays the central role in the present approach. It is well known that Eq. (5) uniquely selects one of the two linearly independent solutions to Eq. (1) at $r\to\infty$ only if $\mathrm{Im}\, k \geq 0$ [2]. Taking into account Eq. (3), it is possible to present the outgoing-wave boundary condition in a form applicable to any complex k. To this end, we note that Eq. (1) in the outer region $r \geq a$ has a pair of linearly independent solutions $e_l(\pm kr)$ with the asymptotic behavior $e_l(\pm kr)|_{r\to\infty} = e^{\pm ikr}$, where the function $e_l(z)$ is defined by Eqs. (A8) and (A9). Equation (5) implies that

$$\phi(r)|_{r\geq a} \propto e_l(kr). \tag{9}$$

From this and Eq. (A10) one obtains

$$\left(\frac{d}{dr} - ik + \frac{1}{r}\sum_{p=1}^{l}\frac{z_{lp}}{ikr + z_{lp}}\right)\phi(r)\bigg|_{r\geq a} = 0, \tag{10}$$

where z_{lp} are the zeros of the reverse Bessel polynomial $\theta_l(z)$; see the Appendix . Introducing the function and derivative value operators at $r=a$,

$$\mathcal{F} = \delta(r-a), \quad \mathcal{D} = \delta(r-a)\frac{d}{dr}, \tag{11}$$

one can rewrite Eq. (10) as

$$\mathcal{D}\phi(r) = \left(ik - \frac{1}{a}\sum_{p=1}^{l}\frac{z_{lp}}{ika + z_{lp}}\right)\mathcal{F}\phi(r). \tag{12}$$

This form of the outgoing-wave boundary condition will be used in the following.

B. Siegert pseudostates: Finite-basis representation

Let $\mathcal{H}$ denote the Hilbert space of functions square integrable on the interval $0 \leq r \leq a$ and satisfying the regularity boundary condition (8). The SSs belong to $\mathcal{H}$. Let $f_i(r)$, $i = 1, 2, \ldots$, be a real, orthonormal, and complete basis in $\mathcal{H}$, i.e.,

$$f_i(r)|_{r\to 0} \propto r^{l+1}, \tag{13a}$$

$$\int_0^a f_i(r) f_j(r) dr = \delta_{ij}, \tag{13b}$$

$$I_\infty(r,r') = \delta(r-r'), \quad 0 \leq r, \ r' \leq a, \tag{13c}$$

where

$$I_N(r,r') = \sum_{i=1}^{N} f_i(r) f_i(r'). \tag{14}$$

It will be assumed that for any well-behaved near $r=a$ function from $\mathcal{H}$ its expansion in terms of this basis converges at $r=a$; otherwise, the basis may be arbitrary. To transform the above differential equations to an algebraic form, we employ a finite basis set

$$f_i(r), \quad i=1,2,\ldots,N. \tag{15}$$

The N-dimensional space spanned by this basis will be denoted by $\mathcal{H}_N$. Function (14) is a projection of the unity operator onto this space.

The operator $\mathcal{D}$, Eq. (11), up to a constant factor, coincides with the Bloch operator [25], which is a well-known means to incorporate boundary conditions into the differential equation. Let us introduce Hermitized Hamiltonian

$$\widetilde{H}_l = H_l + \frac{1}{2}\mathcal{D}. \tag{16}$$

For any functions $u(r)$ and $v(r)$ from $\mathcal{H}$ we have

$$\int_0^a u(r)\widetilde{H}_l v(r)dr = \int_0^a v(r)\widetilde{H}_l u(r)dr; \tag{17}$$

i.e., $\widetilde{H}_l$ is a symmetric operator. Substituting Eq. (16) into Eq. (1), multiplying from the left by $f_i(r)$, and integrating over the interval $0 \le r \le a$, we obtain

$$\int_0^a f_i(r)\left(\widetilde{H}_l - \frac{1}{2}\mathcal{D} - E\right)\phi(r)dr = 0. \tag{18}$$

Since only the values of $\phi(r)$ for $r\in[0,a]$ appear in this equation, we can expand $\phi(r)$ in terms of the basis (15),

$$\phi(r) = \sum_{i=1}^{N} c_i f_i(r), \quad 0 \le r \le a. \tag{19}$$

Substituting this expansion into Eq. (18) and using Eqs. (6) and (12), we arrive at the algebraic eigenvalue problem

$$\left[\widetilde{\mathbf{H}}_l - \frac{1}{2}\left(\lambda - \frac{1}{a}\sum_{p=1}^{l}\frac{z_{lp}}{\lambda a + z_{lp}}\right)\mathbf{F} + \frac{\lambda^2}{2}\mathbf{I}\right]\mathbf{c} = \mathbf{0}. \tag{20}$$

Here, the eigenvalue λ is defined by

$$ik = \lambda, \tag{21}$$

the eigenvector $\mathbf{c}$ is a column vector of the dimension N composed of the coefficients c_i in Eq. (19) (the corresponding row vector will be denoted by $\mathbf{c}^T$, where T stands for transpose), $\widetilde{\mathbf{H}}_l$ and $\mathbf{F}$ are real symmetric matrices of the dimension $N\times N$ representing the operators $\widetilde{H}_l$ and $\mathcal{F}$ and having the elements

$$\widetilde{H}_{l,ij} = \int_0^a f_i(r)\widetilde{H}_l f_j(r)dr = \frac{1}{2}\int_0^a \frac{df_i(r)}{dr}\frac{df_j(r)}{dr}dr + \int_0^a f_i(r)\left[\frac{l(l+1)}{2r^2} + V(r)\right]f_j(r)dr, \tag{22a}$$

$$F_{ij} = \int_0^a f_i(r)\mathcal{F}f_j(r)dr = f_i(a)f_j(a), \tag{22b}$$

and $\mathbf{I}$ is an $N\times N$ unit matrix representing the unity operator (14). In this paper, $\mathbf{0}$ always denotes a generally rectangular zero matrix of appropriate dimension—e.g., a zero column vector in Eq. (20). It is convenient to introduce a vector $\mathbf{f}$ with the elements

$$f_i = f_i(a), \quad i=1,2,\ldots,N. \tag{23}$$

Then from Eq. (19) we have

$$\phi(a) = \mathbf{f}^T\mathbf{c} = \mathbf{c}^T\mathbf{f}, \tag{24}$$

and Eq. (22b) can be written as

$$\mathbf{F} = \mathbf{f}\mathbf{f}^T. \tag{25}$$

The fact that matrix $\mathbf{F}$ can be factorized in this way is very important for the following.

Equation (20) is a representation of the SS eigenvalue problem, Eqs. (1), (8), and (10), in the finite basis (15). The SPSs are the solutions to Eq. (20). The SPS eigenvalues and eigenvectors in the finite-basis representation will be denoted by λ_n and $\mathbf{c}_n$, where, for brevity, we again omit the subscript l. SPSs belong to $\mathcal{H}_N$. Since the basis (15) becomes complete in $\mathcal{H}$ when its dimension N grows, SPSs converge to SSs in the limit $N\to\infty$. However, for any finite N the SPSs and SSs are distinct; to emphasize this difference we have introduced a special notation λ for the SPS eigenvalue. All the results below will be derived in the finite-basis representation and expressed in terms of λ_n and $\mathbf{c}_n$. The final formulas will be given also in the coordinate representation. We shall use the same notation k_n and $\phi_n(r)$ for SPSs in the coordinate representation as for SSs; the transformation between the two representations is defined by Eqs. (19), (21), and (24). Setting in the final formulas $N\to\infty$, one obtains corresponding results in the basis-independent form in terms of SSs. In this form the present results can be compared with previous achievements in the theory of SSs.

C. General restrictions on the location of SPS eigenvalues

Some properties of the SPS eigenvalues λ_n can be deduced from Eq. (20) without solving the equation. First, using the properties of matrices $\widetilde{\mathbf{H}}_l$ and $\mathbf{F}$ and zeros z_{lp} (see the Appendix), it can be seen that if λ is an eigenvalue of Eq. (20), then λ^* also is an eigenvalue. This means that the eigenvalues λ_n are either pure real or occur in complex conjugate pairs λ_n and λ_n^*. Second, multiplying Eq. (20) from the left by $\mathbf{c}^{*T}$ and taking the imaginary part of the result, one obtains

$$\mathrm{Im}(\lambda)[2\mathrm{Re}(\lambda)\mathbf{c}^{*T}\mathbf{c} - \omega_l(-\lambda a)\mathbf{c}^{*T}\mathbf{F}\mathbf{c}] = 0, \tag{26}$$

where $\omega_l(z)$ is a universal (for the given l) function defined by Eq. (A11). This equation is evidently satisfied if $\mathrm{Im}\,\lambda = 0$; i.e., there may exist pure real eigenvalues. If $\mathrm{Im}\,\lambda \neq 0$, then Eq. (26) imposes some restrictions on the location of λ in the complex plane. Indeed, $\mathbf{c}^{*T}\mathbf{c}$ and $\mathbf{c}^{*T}\mathbf{F}\mathbf{c}$ are positive and non-negative real numbers, respectively. The function $\omega_l(z)$ is real for all complex z, and $\omega_l(z)<0$ [$\omega_l(z)=0$, $\omega_l(z)>0$] inside (on the boundary of, outside) a singly connected bounded domain $\Omega_l(z)$ which lies in the left half of the complex z plane, is symmetric with respect to the real axis, and touches the imaginary axis at the single point $z=0$ (see the Appendix). Then it can be seen from Eq. (26) that complex eigenvalues with $\mathrm{Im}\,\lambda \neq 0$ may appear only in the right half plane, $\mathrm{Re}\,\lambda > 0$, excluding the domain $\Omega_l(-\lambda a)$. For $l=0$ we have $\omega_0(z)=1$; hence, the domain $\Omega_0(z)$ is empty.

In the coordinate representation Eq. (26) reads

$$\mathrm{Re}(k)\left[2\,\mathrm{Im}(k)\int_0^a |\phi(r)|^2 dr + \omega_l(-ika)|\phi(a)|^2\right] = 0. \tag{27}$$

Translating the above results to the complex k plane, the SPS momentum eigenvalues k_n can be located either on the imaginary axis or occur in pairs k_n and $-k_n^*$ located in the lower half plane excluding the domain $\Omega_l(-ika)$. Thus SPSs can be conventionally divided into four groups, according to the position of k_n: bound ($\mathrm{Re}\,k_n=0$, $\mathrm{Im}\,k_n>0$), antibound ($\mathrm{Re}\,k_n=0$, $\mathrm{Im}\,k_n<0$), incoming ($\mathrm{Re}\,k_n>0$, $\mathrm{Im}\,k_n<0$), and outgoing ($\mathrm{Re}\,k_n<0$, $\mathrm{Im}\,k_n<0$). In the following, the set of subscripts n corresponding to the bound SPSs will be denoted by $\{b\}$. This classification remains unchanged from the case $l=0$ [8]. Equation (27) does not contain N, so it holds also for SSs, and hence the same classification applies to SSs. The corresponding well-known restrictions on the location of the SS eigenvalues are usually derived from the analytic properties of the Jost function [2,3]. The present derivation in terms of SPSs is solely based on the properties of function $\omega_l(z)$. It reveals a fact that, as far as we know, has not been noticed by previous authors: for $l \neq 0$, there exists a dead zone $\Omega_l(-ika)$ in the lower half plane where incoming and outgoing eigenvalues k_n cannot appear. The physical implications of this result will be discussed below (see Sec. IV B).

As can be seen from Eq. (9), the eigenfunctions $\phi_n(r)$ for the bound SSs decay in the asymptotic region, while for the other three groups they grow. Only bound SSs have a physical meaning—i.e., are observable—individually; all the other SSs serve to collectively represent the continuum. Yet there may appear SSs that, not being bound, approximately have the nature of individual states. Such SSs are associated with resonances, by which we mean sharp peaks in the scattering cross section. They can be distinguished from the others by some additional properties. We note that Eq. (27) does not forbid the eigenvalue k to lie on the real axis; i.e., there might exist a pair of incoming and outgoing SSs with $\mathrm{Im}\,k_n=0$ and $\mathrm{Re}\,k_n \neq 0$, which would correspond to a discrete state embedded in the continuum. The eigenfunctions for such states must satisfy $\phi_n(a)=0$. One may argue that in this case the derivative $\phi_n'(a)$ is also zero, as follows from Eq. (10), so such a solution to the second-order differential equation (1) must turn *identically* zero. That is true; strictly speaking, $\mathrm{Im}\,k_n$ can vanish only simultaneously with $\mathrm{Re}\,k_n$. However, $|\mathrm{Im}\,k_n|$ may have an arbitrarily small value. This may happen, e.g., if the sum of $V(r)$ and the centrifugal term in Eq. (2) has a barrier separating a potential well at $r<a$ from the asymptotic region, the situation commonly known as a shape resonance. Thus there may exist a pair of SSs for which $|\mathrm{Re}\,k_n| \gg |\mathrm{Im}\,k_n|$. The outgoing member of the pair satisfies

$$E_n = \mathcal{E} - i\Gamma/2, \quad \Gamma \ll \mathcal{E}. \tag{28}$$

It will reveal itself as a resonance at the energy $E=\mathcal{E}$ with width Γ. Another possibility is the existence of an SS with zero eigenvalue, $k_n=0$. As follows from Eq. (10), the eigenfunction for such a state must satisfy $\phi_n'(a)=-l\phi_n(a)/a$. By a small variation of the potential $V(r)$ this state can be turned into an antibound SS with a very small $|\mathrm{Im}\,k_n|$, often called a virtual state, which will reveal itself as a resonance at zero energy. In both cases, the eigenvalue k_n must lie close to the real axis, just below it. The degree of this closeness determines whether the SS reveals itself as a resonance. It can be controlled by varying some parameters defining the potential, which shows that resonance is an asymptotic notion.

D. Linearization

The SPS eigenvalue problem, Eq. (20), is nonlinear with respect to λ. This nonlinearity prevents the direct use of the standard methods of linear algebra. Indeed, it is not even clear at the moment how many solutions Eq. (20) has, i.e., how many SPS are there for a given value of N. A crucial observation is that Eq. (20) can be exactly linearized by increasing the dimension of the Hilbert space. To this end, let us introduce additional notation, in the coordinate and finite-basis representations,

$$\tilde{\phi}(r) = ik\phi(r), \quad \tilde{\mathbf{c}} = \lambda\mathbf{c}, \tag{29}$$

and

$$\xi_p = -\frac{z_{lp}\phi(a)}{ika + z_{lp}} = -\frac{z_{lp}\mathbf{f}^T\mathbf{c}}{\lambda a + z_{lp}}, \quad p = 1, \ldots, l. \tag{30}$$

The set of equations (20), (29), and (30) can be presented in the form

$$\left[\begin{pmatrix} \mathbf{0} & \mathbf{I} & \mathbf{0} & \ldots & \mathbf{0} \\ -2\tilde{\mathbf{H}}_l & \mathbf{F} & \mathbf{f}/a & \ldots & \mathbf{f}/a \\ -z_{l1}\mathbf{f}^T/a & \mathbf{0} & & & \\ \ldots\ldots\ldots\ldots & & & \boxed{-z_{lp}/a} & \\ -z_{ll}\mathbf{f}^T/a & \mathbf{0} & & & \end{pmatrix} - \lambda\right]\begin{pmatrix} \mathbf{c} \\ \tilde{\mathbf{c}} \\ \xi_1 \\ \ldots \\ \xi_l \end{pmatrix} = \mathbf{0}. \tag{31}$$

Here and in the following, boxed objects denote square diagonal matrices of dimension $l \times l$ with the elements inside the box standing on the diagonal; e.g., the box in Eq. (31) is an $l \times l$ diagonal matrix with the elements $-z_{lp}/a$, $p=1,\ldots,l$. There is a one-to-one correspondence between the solutions to Eqs. (20) and (31) established by Eqs. (29) and (30); for this reason, the solutions to Eq. (31) will be also called SPSs and denoted by λ_n, $\mathbf{c}_n$, $\tilde{\mathbf{c}}_n$, and ξ_{pn}. At the same time, Eq. (31) is a linear eigenvalue problem, which brings us to the solid grounds of simple linear algebra. Now it becomes clear that there are exactly $2N+l$ SPSs for a given N, this number being the dimension of the matrix in Eq. (31). Let us introduce an extended $(2N+l)$-dimensional Hilbert space $\mathcal{H}_{2N}^{(l)}$ defined by the direct product

$$\mathcal{H}_{2N}^{(l)} = \mathcal{H}_N \oplus \mathcal{H}_N \oplus \mathbb{C}^l, \tag{32}$$

where the first two factors stand for $\mathbf{c}$ and $\tilde{\mathbf{c}}$, and the l-dimensional complex vector space $\mathbb{C}^l$ corresponds to the set of ξ_p. The solutions to Eq. (31) belong to $\mathcal{H}_{2N}^{(l)}$. As we shall see, this is the natural space for the theory of SPSs. For example, the properties of SPSs look most simple in $\mathcal{H}_{2N}^{(l)}$. The linearization of the SPS eigenvalue problem on the step from Eq. (20) to Eq. (31), accompanied by the increase of the dimension of the Hilbert space from N to $2N+l$, generalizes the construction used in [8] to arbitrary values of l.

Equation (31) is a simple eigenvalue problem. It is suitable for the numerical solution, but for the discussion to follow it is convenient to transform it to another form. Multiplying Eq. (31) from the left by the weight matrix

$$\mathbb{W} = \begin{pmatrix} -\mathbf{F} & \mathbf{I} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{I} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & & & \\ \dots & \dots & & \boxed{-1/z_{lp}} & \\ \mathbf{0} & \mathbf{0} & & & \end{pmatrix}, \tag{33}$$

we obtain a generalized eigenvalue problem with symmetric matrices,

$$\left[\begin{pmatrix} -2\tilde{\mathbf{H}}_l & \mathbf{0} & \mathbf{f}/a & \dots & \mathbf{f}/a \\ \mathbf{0} & \mathbf{I} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{f}^T/a & \mathbf{0} & & & \\ \dots\dots & & & \boxed{1/a} & \\ \mathbf{f}^T/a & \mathbf{0} & & & \end{pmatrix} - \lambda\mathbb{W}\right]\begin{pmatrix} \mathbf{c} \\ \tilde{\mathbf{c}} \\ \xi_1 \\ \dots \\ \xi_l \end{pmatrix} = \mathbf{0}. \tag{34}$$

The orthogonality and completeness properties of SPSs immediately follow from this equation.

E. Orthogonality and normalization condition

Assuming that all SPS eigenvalues λ_n are distinct, the solutions to Eq. (34) are orthogonal with respect to the inner product

$$(\mathbf{c}_n^T \, \tilde{\mathbf{c}}_n^T \, \xi_{1n} \, \cdots \, \xi_{ln})\mathbb{W}\begin{pmatrix} \mathbf{c}_m \\ \tilde{\mathbf{c}}_m \\ \xi_{1m} \\ \dots \\ \xi_{lm} \end{pmatrix} = 2\lambda_n \delta_{nm}. \tag{35}$$

Substituting here Eq. (33), we obtain

$$\mathbf{c}_n^T\mathbf{c}_m - \frac{1}{\lambda_n + \lambda_m}\left[\mathbf{c}_n^T\mathbf{F}\mathbf{c}_m + \sum_{p=1}^{l}\frac{\xi_{pn}\xi_{pm}}{z_{lp}}\right] = \delta_{nm}. \tag{36}$$

In the coordinate representation this equation reads

$$\int_0^a \phi_n(r)\phi_m(r)dr + i\frac{\phi_n(a)\phi_m(a)}{k_n + k_m} \times \left[1 + \sum_{p=1}^{l}\frac{z_{lp}}{(ik_n a + z_{lp})(ik_m a + z_{lp})}\right] = \delta_{nm}. \tag{37}$$

It remains to explain our choice of the normalization factor on the right-hand side of Eq. (35). We can specify Eq. (9) as

$$\phi_n(r)|_{r\geq a} = \phi_n(a)\frac{e_l(kr)}{e_l(ka)}. \tag{38}$$

Using this and Eq. (A8), it can be verified that if both n and m correspond to bound SPSs, Eq. (37) can be rewritten as

$$\int_0^\infty \phi_n(r)\phi_m(r)dr = \delta_{nm}, \quad n,m \in \{b\}, \tag{39}$$

which coincides with the ordinary orthonormalization condition for bound states. Equations (36) and (37) express the orthonormalization condition for SPSs, generalizing the corresponding results of [8] to arbitrary l.

Equation (37) does not contain N, so it applies also to SSs. The normalization of SSs was a big problem in the development of the theory. The usual definition of the inner product is clearly not applicable because of the divergence of SS eigenfunctions at $r\to\infty$. This difficulty was resolved in [26] for the case $l=0$ by a regularization of the normalization integral. Another approach, based on the analytic continuation of the normalization condition for bound states (39) to the lower half of the complex k plane, was proposed independently in [27] for $l=0$ and in [28] for arbitrary l. In the most general form, which is applicable also to finite-range potentials without spherical symmetry, the orthonormalization condition for SSs was given in [29]. In the present notation, the result of [29] reads

$$\int_0^a \phi_n(r)\phi_m(r)dr + \frac{\phi_n'(a)\phi_m(a) - \phi_n(a)\phi_m'(a)}{k_n^2 - k_m^2} = \delta_{nm}. \tag{40}$$

Using Eq. (10), it can be easily seen that this coincides with Eq. (37). The orthonormalization condition for SSs in the form (37), as far as we know, has not appeared in the literature.

The inner product for SSs defined by the left-hand side of Eq. (37) or, equivalently, Eq. (40), differs from the usual inner product for physical states in three respects: the integration in the volume term extends over a finite interval $r \in [0,a]$, there is an additional surface term, and there is no complex conjugation. The algebraic derivation of this result in terms of SPSs complements the approaches used in [26–29], making the issue of normalization of SSs very simple. Indeed, Eq. (35) shows that SPSs are orthogonal in the usual sense of the word, but in the extended space $\mathcal{H}_{2N}^{(l)}$ and with a nonunit weight (33), while Eqs. (36) and (37) result from the projection of Eq. (35) onto the original Hilbert space $\mathcal{H}_N$. This projection and the structure of the weight matrix (33) explain the structure of Eqs. (37) and (40).

F. Completeness relations

The solutions to Eq. (34), being linearly independent, form a complete set in $\mathcal{H}_{2N}^{(l)}$. This fact is expressed by

$$\sum_{n=1}^{2N+l} \frac{1}{2\lambda_n} \begin{pmatrix} \mathbf{c}_n \\ \tilde{\mathbf{c}}_n \\ \xi_{1n} \\ \cdots \\ \xi_{ln} \end{pmatrix} (\mathbf{c}_n^T \; \tilde{\mathbf{c}}_n^T \; \xi_{1n} \; \cdots \; \xi_{ln}) = \mathbb{W}^{-1}, \tag{41}$$

where

$$\mathbb{W}^{-1} = \begin{pmatrix} \mathbf{0} & \mathbf{I} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{I} & \mathbf{F} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & & & \\ \cdots & \cdots & & \boxed{-z_{lp}} & \\ \mathbf{0} & \mathbf{0} & & & \end{pmatrix} \tag{42}$$

is the inverse of the weight matrix (33). Equation (41) amounts to the relations

$$\sum_{n=1}^{2N+l} \frac{\mathbf{c}_n\mathbf{c}_n^T}{\lambda_n} = \mathbf{0}, \tag{43a}$$

$$\sum_{n=1}^{2N+l} \mathbf{c}_n\mathbf{c}_n^T = 2\mathbf{I}, \tag{43b}$$

$$\sum_{n=1}^{2N+l} \lambda_n\mathbf{c}_n\mathbf{c}_n^T = 2\mathbf{F}, \tag{43c}$$

$$\sum_{n=1}^{2N+l} \frac{\xi_{pn}\mathbf{c}_n}{\lambda_n} = \mathbf{0}, \tag{43d}$$

$$\sum_{n=1}^{2N+l} \xi_{pn}\mathbf{c}_n = \mathbf{0}, \tag{43e}$$

$$\sum_{n=1}^{2N+l} \frac{\xi_{pn}\xi_{qn}}{\lambda_n} = -2z_{lp}\delta_{pq}. \tag{43f}$$

Using Eqs. (30), one can notice that Eq. (43d) is a consequence of Eqs. (43a) and (43e). Equation (43f) is a consequence of Eq. (43d) for $p \neq q$, but is an independent relation for $p=q$. In the coordinate representation, these relations read

$$\sum_{n=1}^{2N+l} \frac{1}{ik_n}\phi_n(r)\phi_n(r') = 0, \tag{44a}$$

$$\sum_{n=1}^{2N+l} \phi_n(r)\phi_n(r') = 2I_N(r,r'), \tag{44b}$$

$$\sum_{n=1}^{2N+l} ik_n\phi_n(r)\phi_n(r') = 2I_N(r,a)I_N(r',a), \tag{44c}$$

$$\sum_{n=1}^{2N+l} \frac{\phi_n(a)\phi_n(r)}{ik_n(ik_na + z_{lp})} = 0, \tag{44d}$$

$$\sum_{n=1}^{2N+l} \frac{\phi_n(a)\phi_n(r)}{ik_na + z_{lp}} = 0, \tag{44e}$$

$$\sum_{n=1}^{2N+l} \frac{[\phi_n(a)]^2}{ik_n(ik_na + z_{lp})(ik_na + z_{lq})} = -\frac{2\delta_{pq}}{z_{lp}}, \tag{44f}$$

where $0 \leq r, r' \leq a$. Equations (43) and (44) express the completeness properties of SPSs, generalizing the corresponding results of [8] to arbitrary l.

The completeness properties of SSs follow from Eqs. (44) in the limit $N \to \infty$. To obtain them, one has to extend the summations to infinity and substitute Eq. (13c) into the right-hand sides of Eqs. (44b) and (44c); for brevity, we do not reproduce the results here. The SS analogs of Eqs. (44a) and (44b) were first established for a δ-function potential and $l=0$ in [30] and then proved for a more general class of finite-range potentials and arbitrary l in [31]. In a somewhat less rigorous way these relations were obtained in [32]. In both cases, the derivation was based on the Mittag-Leffler expansion for the outgoing-wave Green's function [33]. Equation (44c) for $l=0$ was obtained within the SPS formulation in [8]. The properties of SSs following in the limit $N \to \infty$ from the other three relations, Eqs. (44d)–(44f), as far as we know, have never appeared in the literature.

As follows from Eqs. (44), the set of SS eigenfunctions $\phi_n(r)$ is linearly dependent and hence overcomplete in $\mathcal{H}$. This overcompleteness was another big problem in the development of the theory. The algebraic derivation of the completeness properties of SSs in terms of SPSs complements the approaches used in [30–32], clarifying the nature of the overcompleteness. Indeed, SPSs form a normal complete set [see Eq. (41)], but in the extended space $\mathcal{H}_{2N}^{(l)}$, while Eqs. (43) and (44) result from the projection of Eq. (41) onto the original Hilbert space $\mathcal{H}_N$. The overcompleteness of SSs is a consequence of this projection. This issue is further discussed from another viewpoint in the next subsection.

G. Expansion in terms of SPSs

Given a function $\psi(r) \in \mathcal{H}$, can it be expanded in terms of SS eigenfunctions $\phi_n(r)$? Is the expansion unique? How to find the coefficients? Many possible applications of SSs in atomic physics require answers to these questions. The overcompleteness of SSs makes the questions nontrivial. The SPS formulation enables one to find the answers.

Let $\psi(r)$ and $\tilde{\psi}(r)$ be two arbitrary functions from $\mathcal{H}_N$, i.e., they can be expanded on the interval $0 \leq r \leq a$ as

$$\psi(r) = \sum_{i=1}^{N} s_i f_i(r), \quad \tilde{\psi}(r) = \sum_{i=1}^{N} \tilde{s}_i f_i(r), \tag{45}$$

and η_p, $p=1,\ldots,l$, are arbitrary complex numbers. Let $\mathbf{s}$ and $\tilde{\mathbf{s}}$ be N-dimensional vectors composed of the coefficients in Eqs. (45). Then the vector $(\mathbf{s}^T, \tilde{\mathbf{s}}^T, \eta_1, \ldots, \eta_l)^T$ belongs to $\mathcal{H}_{2N}^{(l)}$; hence, it can be expanded in terms of the solutions to Eq. (34),

$$\begin{pmatrix} \mathbf{s} \\ \tilde{\mathbf{s}} \\ \eta_1 \\ \cdots \\ \eta_l \end{pmatrix} = \sum_{n=1}^{2N+l} a_n \begin{pmatrix} \mathbf{c}_n \\ \tilde{\mathbf{c}}_n \\ \xi_{1n} \\ \cdots \\ \xi_{ln} \end{pmatrix}. \tag{46}$$

Using Eq. (35), we find the coefficients

$$a_n = \frac{1}{2\lambda_n}\left[\mathbf{c}_n^T(\lambda_n \mathbf{s} + \tilde{\mathbf{s}}) - \mathbf{c}_n^T \mathbf{F}\mathbf{s} - \sum_{p=1}^{l} \frac{\xi_{pn}\eta_p}{z_{lp}} \right]. \tag{47}$$

In the coordinate representation the last two equations read

$$\begin{pmatrix} \psi(r) \\ \tilde{\psi}(r) \\ \eta_1 \\ \cdots \\ \eta_l \end{pmatrix} = \sum_{n=1}^{2N+l} a_n \begin{pmatrix} \phi_n(r) \\ \tilde{\phi}_n(r) \\ \xi_{1n} \\ \cdots \\ \xi_{ln} \end{pmatrix} \tag{48}$$

and

$$a_n = \frac{1}{2ik_n}\left[\int_0^a \phi_n(r)[ik_n\psi(r) + \tilde{\psi}(r)]dr - \phi_n(a)\psi(a) - \sum_{p=1}^{l} \frac{\xi_{pn}\eta_p}{z_{lp}} \right]. \tag{49}$$

In the limit $N\to\infty$, Eqs. (48) and (49) define the corresponding expansion in terms of SSs. These equations generalize the expansion discussed in [23] to arbitrary l.

Let us return to the above questions. Our derivation of Eqs. (48) and (49) shows that any function $\psi(r)$ from $\mathcal{H}$ can be expanded in terms of SS eigenfunctions $\phi_n(r)$, but the expansion is not unique. To make it unique, one has to consider a vector composed of $\psi(r)$, another function $\tilde{\psi}(r)$ from $\mathcal{H}$, and l complex numbers η_p, $p=1,\ldots,l$. Such a vector has a unique expansion in terms of SSs following from Eq. (48) in the limit $N\to\infty$, where the coefficients a_n are given by Eq. (49).

H. Spectral matrix and its inverse

Let us introduce a matrix-valued function

$$\mathbf{M}(\lambda) = \tilde{\mathbf{H}}_l - \frac{1}{2}\left(\lambda - \frac{1}{a}\sum_{p=1}^{l} \frac{z_{lp}}{\lambda a + z_{lp}} \right)\mathbf{F} + \frac{\lambda^2}{2}\mathbf{I}, \tag{50}$$

which coincides with the matrix standing in the square brackets in Eq. (20). We call it the spectral matrix because its determinant turns zero whenever λ coincides with one of the SPS eigenvalues λ_n. Let us calculate $\det[\mathbf{M}(\lambda)]$. The determinant of a matrix is known to be independent of the basis. It is convenient to switch to a basis in which matrix $\mathbf{F}$ is diagonal; this can be done by an orthogonal transformation of the original basis (15). As follows from Eq. (25), $\mathbf{F}$ has rank 1 and hence only one nonzero eigenvalue. Using this, it can be shown that

$$\det[\mathbf{M}(\lambda)] = \frac{(-a)^l}{2^N \theta_l(-\lambda a)} \prod_{n=1}^{2N+l} (\lambda - \lambda_n). \tag{51}$$

The inverse matrix has the following spectral resolution in terms of SPSs:

$$\mathbf{M}^{-1}(\lambda) = \sum_{n=1}^{2N+l} \frac{\mathbf{c}_n \mathbf{c}_n^T}{\lambda_n(\lambda - \lambda_n)}. \tag{52}$$

The validity of this formula can be verified using Eqs. (20), (25), (30), and (43).

I. Surface amplitudes

The values of the SPS eigenfunctions at $r=a$—i.e., $\phi_n(a)$—which we call the surface amplitudes, play an important role in the present approach. Given the eigenvectors $\mathbf{c}_n$, they can be calculated from Eq. (24). It turns out that their squares can be calculated in another way, using only the eigenvalues λ_n.

From Eqs. (50) and (A17) we have

$$\mathbf{M}(\lambda) - \mathbf{M}(-\lambda) = -\frac{\lambda(i\lambda a)^{2l}}{\theta_l(\lambda a)\theta_l(-\lambda a)}\mathbf{F}. \tag{53}$$

Multiplying this equation from the right by $\mathbf{M}^{-1}(\lambda)$ we obtain

$$\mathbf{I} + \frac{\lambda(i\lambda a)^{2l}}{\theta_l(\lambda a)\theta_l(-\lambda a)}\mathbf{F}\mathbf{M}^{-1}(\lambda) = \mathbf{M}(-\lambda)\mathbf{M}^{-1}(\lambda). \tag{54}$$

An N-dimensional square matrix $\mathbf{P}$ is called a projector-type matrix if it can be presented in the form $\mathbf{P}=\mathbf{u}\mathbf{v}^T$, where $\mathbf{u}$ and $\mathbf{v}$ are N-dimensional vectors. It can be shown that for such a matrix $\det(\mathbf{I}+\mathbf{P}) = 1 + \mathrm{tr}(\mathbf{P})$ (see Appendix A in [8]). $\mathbf{F}$ is a projector-type matrix [see Eq. (25)] and hence so is $\mathbf{F}\mathbf{M}^{-1}(\lambda)$. Then we obtain from Eqs. (51) and (54)

$$\frac{\theta_l(\lambda a)}{\theta_l(-\lambda a)} + \frac{\lambda(i\lambda a)^{2l}}{\theta_l^2(-\lambda a)}\mathrm{tr}[\mathbf{F}\mathbf{M}^{-1}(\lambda)] = \prod_{n=1}^{2N+l} \frac{\lambda_n + \lambda}{\lambda_n - \lambda}. \tag{55}$$

Taking the residues of both sides of this equation at $\lambda \to \lambda_m$ using Eq. (52), we find

$$\mathbf{c}_m^T \mathbf{F} \mathbf{c}_m = -2\lambda_m \frac{\theta_l^2(-\lambda_m a)}{(i\lambda_m a)^{2l}} \prod_{n\neq m}^{2N+l} \frac{\lambda_n + \lambda_m}{\lambda_n - \lambda_m}. \tag{56}$$

In the coordinate representation the last two equations read

$$\frac{\theta_l(ika)}{\theta_l(-ika)} + \frac{ik(ka)^{2l}}{\theta_l^2(-ika)} \sum_{n=1}^{2N+l} \frac{[\phi_n(a)]^2}{k_n(k_n - k)} = \prod_{n=1}^{2N+l} \frac{k_n + k}{k_n - k} \tag{57}$$

and

$$[\phi_m(a)]^2 = -2ik_m \frac{\theta_l^2(-ik_m a)}{(k_m a)^{2l}} \prod_{n\neq m}^{2N+l} \frac{k_n + k_m}{k_n - k_m}. \qquad (58)$$

It may seem that the left-hand side of Eq. (57) is singular at $k=iz_{lp}/a$, where $\theta_l(-ika)$ standing in the denominators vanishes, which would contradict the equality, because the right-hand side is regular there. But this is not the case: using Eqs. (44d) and (A17), it can be shown that all singular terms (the first- and second-order poles) at $k=iz_{lp}/a$ on the left-hand side of Eq. (57) cancel.

Equations (55)–(58) generalize the corresponding results of [8] to arbitrary l. They reveal the existence of a nontrivial relation between the eigenvalues λ_n and eigenvectors $\mathbf{c}_n$ which results from the projector-type structure of matrix $\mathbf{F}$. As a consequence, the surface amplitudes $\phi_n(a)$ squared can be expressed in terms of the eigenvalues only, without knowing the eigenvectors. The corresponding properties of SSs follow from Eqs. (57) and (58) in the limit $N\to\infty$. As far as we know, they have never appeared in the literature, although the necessity of relations of this kind was pointed out in [34].

J. Sum rules

Another kind of relations, which we call the sum rules, reveal an interdependence between the eigenvalues λ_n. There are l such relations, and hence they exist only for $l>0$, representing a property absent in the case $l=0$ [8]. Let us rewrite Eq. (55) as

$$P(\lambda) - P(-\lambda) = \frac{\lambda(i\lambda a)^{2l}}{\theta_l(-\lambda a)} \prod_{n=1}^{2N+l} (\lambda_n - \lambda)\mathrm{tr}[\mathbf{F}\mathbf{M}^{-1}(\lambda)], \qquad (59)$$

where

$$P(\lambda) = \theta_l(-\lambda a) \prod_{n=1}^{2N+l} (\lambda_n + \lambda) \qquad (60)$$

is a polynomial of order $2(N+l)$. Consider Eq. (59) for $\lambda\to 0$. All the even powers of λ on the left-hand side exactly cancel. The first term in the expansion of the right-hand side is $\propto\lambda^{2l+1}$, which means that the coefficients of the odd powers in $P(\lambda)$ from 1 through $2l-1$ must vanish. This leads to the l relations mentioned above. In the most compact form, they can be expressed in terms of the elementary symmetric polynomials $\sigma_k(x_1,\ldots,x_n)$ defined as coefficients in the expansion [35]

$$\prod_{i=1}^{n} (x - x_i) = \sum_{k=0}^{n} (-1)^{n-k}\sigma_{n-k}(x_1,\ldots,x_n)x^k. \qquad (61)$$

One can easily find

$$\sigma_0(x_1,\ldots,x_n) = 1, \qquad (62a)$$

$$\sigma_1(x_1,\ldots,x_n) = \sum_{1\le i\le n} x_i, \qquad (62b)$$

$$\sigma_2(x_1,\ldots,x_n) = \sum_{1\le i<j\le n} x_i x_j, \qquad (62c)$$

etc. Let us define a set of x_i, $i=1,\ldots,2(N+l)$:

$$x_n = 1/\lambda_n, \quad n=1,\ldots,2N+l, \qquad (63a)$$

$$x_{2N+l+p} = a/z_{lp}, \quad p=1,\ldots,l. \qquad (63b)$$

Then the relations of interest read

$$\sigma_{2s+1}(x_1,\ldots,x_{2(N+l)}) = 0, \quad s=0,1,\ldots,l-1. \qquad (64)$$

We give here only the first of these relations in the coordinate representation. Setting in Eq. (64) $s=0$ and using Eq. (A7), we obtain

$$\sum_{n=1}^{2N+l} \frac{1}{k_n} = ia, \quad l\ge 1. \qquad (65)$$

The corresponding properties of SS eigenvalues k_n follow from Eqs. (64) and (65) in the limit $N\to\infty$. As far as we know, they do not have counterparts in the literature.

As can be seen from the derivation, Eqs. (64) are a consequence of Eq. (55). The peculiarity of these equations is that they relate the eigenvalues λ_n only. The relations obtained from the higher terms in the expansion of Eq. (59) in powers of λ involve both eigenvalues and eigenvectors. For example, equating the coefficient of λ^{2l+1} to zero, we obtain

$$\sum_{n=1}^{2N+l} \frac{[\phi_n(a)]^2}{k_n^2} = \frac{2\theta_l^2(0)}{(ia)^{2l}}\sigma_{2l+1}(x_1,\ldots,x_{2(N+l)}). \qquad (66)$$

One can proceed with the expansion and obtain higher relations of this type.

III. STATIONARY SCATTERING THEORY

In this section, on the basis of the above results we derive the expansions for all the major objects of stationary scattering theory in terms of SPSs. These expansions complete the present formulation, opening the way for its applications to many problems in atomic physics.

A. Outgoing-wave Green's function

The outgoing-wave Green's function is defined by

$$(H_l - E)G_l(r,r';k) = \delta(r-r'), \qquad (67a)$$

$$G_l(0,r';k) = 0, \qquad (67b)$$

$$\left.\left(\frac{d}{dr} - ik\right)G_l(r,r';k)\right|_{r\to\infty} = 0. \qquad (67c)$$

Taking into account the assumed properties of the potential, Eqs. (3) and (7), the regularity (67b) and outgoing-wave (67c) boundary conditions can be specified similarly to Eqs. (8) and (10) as

$$G_l(r,r';k)|_{r\to 0} \propto r^{l+1}, \quad r'>0, \qquad (68)$$

and

$$\left(\frac{d}{dr} - ik + \frac{1}{r}\sum_{p=1}^{l}\frac{z_{lp}}{ikr + z_{lp}}\right)G_l(r,r';k) = 0,$$
$$r \ge a, \quad 0 \le r' < a. \tag{69}$$

The solution to these equations in the inner region can be sought as an expansion in terms of the basis (15),

$$G_l(r,r';k) = \sum_{i,j=1}^{N} G_{ij}(\lambda) f_i(r) f_j(r'), \quad 0 \le r,\ r' \le a. \tag{70}$$

Substituting this into Eq. (67a) and acting as in the derivation of Eq. (20), we arrive at the algebraic equation

$$\left[\tilde{\mathbf{H}}_l - \frac{1}{2}\left(\lambda - \frac{1}{a}\sum_{p=1}^{l}\frac{z_{lp}}{\lambda a + z_{lp}}\right)\mathbf{F} + \frac{\lambda^2}{2}\mathbf{I}\right]\mathbf{G}(\lambda) = \mathbf{I}, \tag{71}$$

where $\mathbf{G}(\lambda)$ is a matrix composed of the coefficients in Eq. (70). Using Eq. (52), we obtain

$$\mathbf{G}(\lambda) = \sum_{n=1}^{2N+l}\frac{\mathbf{c}_n\mathbf{c}_n^T}{\lambda_n(\lambda - \lambda_n)}. \tag{72}$$

In the coordinate representation this equation reads

$$G_l(r,r';k) = \sum_{n=1}^{2N+l}\frac{\phi_n(r)\phi_n(r')}{k_n(k_n - k)}, \quad 0 \le r,\ r' \le a. \tag{73}$$

The expansion of the outgoing-wave Green's function in terms of SSs follows from Eq. (73) in the limit $N \to \infty$. This fundamental result was obtained in [33]. These and the majority of other authors in the field followed the same logical route based on the argument of analyticity first employed in [36]: namely, under certain conditions satisfied by the potential, $G(r,r';k)$ is a meromorphic function of k, and then the SS analog of Eq. (73) results from the Mittag-Leffler expansion theorem [37]. In the SPS formulation, Eq. (73) follows from the completeness properties of SPSs expressed by Eqs. (43) and (44), which are rather simple algebraic relations. Remarkably, expansion (73) has the same form for all l, provided that by k_n and $\phi_n(r)$ one means appropriate SPSs, only the number of terms changes in accordance with the number of SPSs.

B. Physical states

The set of stationary states conventionally considered in scattering theory [2,3] includes bound states $\varphi_{nl}(r)$, $n = 1,2,\ldots$, and scattering states $\varphi_l(r,k)$, $0 \le k < \infty$. The bound states satisfy the Schrödinger equation (1), the regularity boundary condition (4), and the asymptotic boundary condition

$$\varphi_{nl}(r)\big|_{r\to\infty} = 0. \tag{74}$$

Upon appropriate enumeration of SPSs, bound states coincide with the corresponding bound SPSs,

$$\varphi_{nl}(r) = \phi_n(r), \quad 0 \le r < \infty, \quad n \in \{b\}. \tag{75}$$

The scattering states satisfy Eqs. (1) and (4) and the asymptotic boundary condition

$$\varphi_l(r,k)\big|_{r\to\infty} = e^{-ikr} - (-1)^l S_l(k) e^{ikr}, \tag{76}$$

where $S_l(k)$ is the scattering matrix. Taking into account Eq. (3), in the outer region we have [see Eqs. (A9)]

$$\varphi_l(r,k)\big|_{r\ge a} = e_l(-kr) - (-1)^l S_l(k) e_l(kr). \tag{77}$$

This function is related to $G_l(r,r';k)$ by

$$G_l(r,r';k) = \frac{i}{k}\varphi_l(r_<,k)e_l(kr_>), \quad r_> \ge a, \tag{78}$$

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

$$\varphi_l(r,k) = \frac{-ikG_l(r,a;k)}{e_l(ka)}, \quad 0 \le r \le a. \tag{79}$$

Substituting here Eq. (73), we obtain

$$\varphi_l(r,k) = -ike^{-ika}\frac{(-ika)^l}{\theta_l(-ika)}\sum_{n=1}^{2N+l}\frac{\phi_n(r)\phi_n(a)}{k_n(k_n - k)}, \quad 0 \le r \le a. \tag{80}$$

The expansion of the scattering state wave function in terms of SSs follows from Eq. (80) in the limit $N \to \infty$. It was first obtained for $l=0$ in [38] by directly applying the Mittag-Leffler expansion theorem to $\varphi_l(r,k)$ as a function of k. Later, the same result for $l=0$ was rederived in [39] by substituting the Mittag-Leffler expansion for $G_l(r,r';k)$ [33] into Eq. (79). The second approach is applicable to any l, as was pointed out in [31], and we have used it in the above derivation.

It is instructive to take a look at Eq. (80) from the viewpoint of the expansion discussed in Sec. II G. Setting in Eq. (48) $\psi(r) = \varphi_l(r,k)$, what are the corresponding $\tilde{\psi}(r)$ and η_p that lead to Eq. (80)? Using Eqs. (44), it can be shown that

$$\tilde{\psi}(r) = ik\varphi_l(r,k), \quad \eta_p = -\frac{z_{lp}\varphi_l(a,k)}{ika + z_{lp}}. \tag{81}$$

These equations are similar to Eqs. (29) and (30) for an individual SPS. They are essential for the extension of the time-dependent approach proposed in [23] to arbitrary l.

C. Scattering matrix

The final goal of scattering theory is the scattering matrix, and this applies to the present formulation as well. In the one-channel case under consideration, the scattering matrix $S_l(k)$ is simply a complex number defined by Eq. (76). From Eqs. (77) and (79), requiring continuity of $\varphi_l(r,k)$ at $r=a$, we find

$$S_l(k) = (-1)^l\left[\frac{e_l(-ka)}{e_l(ka)} + \frac{ikG_l(a,a;k)}{e_l^2(ka)}\right]. \tag{82}$$

Substituting here Eq. (73) and using Eq. (A8), we obtain an expansion for $S_l(k)$,

$$S_l(k) = e^{-2ika}\left[\frac{\theta_l(ika)}{\theta_l(-ika)} + \frac{ik(ka)^{2l}}{\theta_l^2(-ika)}\sum_{n=1}^{2N+l}\frac{[\phi_n(a)]^2}{k_n(k_n-k)}\right]. \tag{83}$$

Following [8], we shall call this expansion the sum formula. To implement it, one needs to know the SPS eigenvalues k_n and surface amplitudes $\phi_n(a)$. Equation (83) shows that $S_l(k)$ has simple poles at $k=k_n$ with the residues

$$(k-k_n)S(k)|_{k=k_n} = \frac{-ie^{-2ik_na}(k_na)^{2l}[\phi_n(a)]^2}{\theta_l^2(-ik_na)}. \tag{84}$$

We note that the right-hand side of Eq. (83) is regular at $k=iz_{lp}/a$, where $\theta_l(-ika)$ vanishes, as has been explained just after Eq. (58). Using Eq. (57), we obtain from Eq. (83) another expansion for $S_l(k)$,

$$S_l(k) = e^{-2ika}\prod_{n=1}^{2N+l}\frac{k_n+k}{k_n-k}. \tag{85}$$

This will be called the product formula. For its implementation, it is sufficient to know only the SPS eigenvalues k_n. Even though Eqs. (83) and (85) look very different, they are algebraically equivalent, as has been shown above. These equations generalize the sum and product formulas obtained in [8] to arbitrary l.

The corresponding expansions for the scattering matrix in terms of SSs follow from Eqs. (83) and (85) in the limit $N\to\infty$. The traditional approach to the derivation of the sum formula based on the argument of analyticity and Mittag-Leffler expansion theorem failed: all the expansions of the type (83) discussed in the literature contain some undefined quantities (see, e.g., [3]). The closed-form expression following from Eq. (83) in the limit $N\to\infty$ was first obtained within the SPS formulation for $l=0$ in [8]. The product formula was first given without due proof in [40]. Later, it was rigorously derived using Hadamard's form of the Weierstrass expansion theorem [37] for potentials decaying faster than any exponential function and $l=0$ in [41]. Within the SPS formulation, the product formula (85) follows from relation (57) which has simple algebraic origin. The fact that the scattering matrix can be expressed in terms of its poles—i.e., SS eigenvalues k_n—only, without knowing the residues, can be understood from Eq. (58) which shows that the residues [see Eq. (84)] can be expressed in terms of the poles.

Equation (85) explicitly ensures unitarity of the scattering matrix. Hence $S_l(k)$ can be conventionally presented in the form

$$S_l(k) = \exp[2i\delta_l(k)], \tag{86}$$

where $\delta_l(k)$ is the phase shift. The partial $\sigma_l(k)$, differential $d\sigma(\theta,k)/d\Omega$, and total $\sigma_{\text{tot}}(k)$ scattering cross sections are given in terms of $\delta_l(k)$ by standard formulas [3,42].

The present approach, being in a sense variational, does not reproduce the correct behavior of $S_l(k)$ in the Born region; the validity of Eqs. (83) and (85) at high energies is limited by the finite dimension N of the basis (15). But it should be noted that for any finite N Eqs. (83) and (85) are in accordance with the Wigner threshold low. Indeed, at low energies $\delta_l(k)$ behaves as [3,42]

$$\delta_l(k) = A_l(ka)^{2l+1}, \quad k\to 0. \tag{87}$$

The same behavior follows from Eq. (83). We obtain using Eq. (A19)

$$A_l = \frac{1}{\theta_l^2(0)}\left[\frac{-1}{2l+1} + \frac{1}{2a}\sum_{n=1}^{2N+l}\frac{[\phi_n(a)]^2}{k_n^2}\right]. \tag{88}$$

Using Eqs. (58) or (66), this coefficient can be expressed in terms of the eigenvalues k_n only. We consider only the scattering length $\alpha=-A_0a$, which is of main interest for applications. Its expansion can be obtained by substituting Eq. (66) into Eq. (88) or directly from Eq. (85),

$$\alpha = -\left.\frac{\delta_0(k)}{k}\right|_{k\to 0} = a + \sum_{n=1}^{2N}\frac{i}{k_n}. \tag{89}$$

In the limit $N\to\infty$, this formula gives an expansion for α in terms of SSs. This result pertains to the case $l=0$ treated in [8], but was not given there explicitly.

IV. ILLUSTRATIVE EXAMPLES

In this section we illustrate the above results by calculations for several model potentials. While the purpose of more extensive calculations for the case $l=0$ reported in [8] was to provide sufficient and convincing evidences that the SPS formulation works at all, the experience gained since then [7–24]has left no doubts in its consistency and efficiency. So in the calculations below we restrict ourselves to fewer examples.

A. Computational aspects

To implement the present approach, we use the numerical procedure described in [8]. It is based on a discrete variable representation (DVR) [43–45] constructed from Jacobi polynomials compatible with the boundary conditions (8) and (10). For the numerical treatment, instead of r it is convenient to introduce a new variable x,

$$r = a(1+x)/2. \tag{90}$$

This equation transforms the interval $0\le r\le a$ into $-1\le x\le 1$. Let

$$\varphi_n(x) = (1+x)^l\tilde{P}_{n-1}^{(0,2l)}(x), \quad n=1,2,\ldots,N, \tag{91}$$

and

$$\pi_i(x) = \sum_{n=1}^{N} T_{ni}\varphi_n(x), \quad i=1,2,\ldots,N, \tag{92}$$

where

$$T_{ni} = \frac{\sqrt{\omega_i}\varphi_n(x_i)}{(1+x_i)^l}. \tag{93}$$

Here $\tilde{P}_n^{(0,2l)}(x)$ are the normalized Jacobi polynomials, x_i and ω_i are the abscissas and weights of the corresponding Gaussian quadrature, and T_{ni} is an orthogonal matrix defining the transformation from the polynomials (91) to the DVR basis $\pi_i(x)$. Then the basis (15) is defined by

$$f_i(r) = \sqrt{\frac{2}{a}\frac{1+x}{1+x_i}}\pi_i(x). \tag{94}$$

These functions satisfy Eqs. (13) if the integrals are calculated using the Gaussian quadrature. In the same way the matrix elements of the Hamiltonian (22a) can be calculated (see Appendix C in [8]). This is a global basis, since functions (94) extend all over the interval $0 \leq r \leq a$. Our experience shows that it gives very high rate of convergence, provided that the potential $V(r)$ is an infinitely differentiable function on the interval $0 \leq r \leq a$. If this is not the case, finite elements [18,22] or any other local basis may turn out to be more preferable.

The matrix in the SPS eigenvalue problem (31) is complex, because the zeros z_{lp} are generally complex. For the numerical solution, it is better to switch to a real matrix: this saves computation time and ensures that all eigenvalues are either exactly real or appear in complex conjugate pairs. To this end, we note that all complex zeros z_{lp} occur in complex conjugate pairs (see the Appendix). Let z_{lp} and z_{lq} be such a pair, i.e., $z_{lq}=z^*_{lp}$. Let us introduce instead of ξ_p and ξ_q a pair of new variables,

$$\xi'_p = \frac{\xi_p + \xi_q}{2}, \quad \xi'_q = \frac{\xi_p - \xi_q}{2i}. \tag{95}$$

Switching in Eq. (31) to such variables for each pair of complex conjugate zeros z_{lp}, one obtains an algebraic eigenvalue problem with a real matrix. This problem can be solved by any standard linear algebra routine.

We calculate zeros z_{lp}, $p=1,\ldots,l$, as roots of the polynomial $\theta_l(z)$ [see Eq. (A2)] using Laguerre's method implemented in the IMSL library. This algorithm works for $l \leq 28$, but does not converge for larger l. The procedure of recovering z_{lp} from the coefficients in Eq. (A2) becomes unstable in this case. This difficulty should not be fatal, since the table of z_{lp} up to a sufficiently large l is to be generated only once for all times. However, this remains an open problem. Therefore, in the present calculations we are limited to $l \leq 28$.

One should distinguish truly finite-range potentials, when Eq. (3) is exactly satisfied for some a, and cutoff potentials. In the former case, the dimension N of the basis is the only parameter of the computational scheme. The larger N, the higher the maximum energy up to which Eqs. (73), (80), (83), and (85) yield converged results. This convergence is rather rapid and similar to that demonstrated for $l=0$ in [8], so we shall not discuss it here; all the results presented below are converged with respect to N. In the latter case, there is an additional parameter, the cutoff radius a. The convergence with respect to a is an important issue and will be illustrated below.

Finally, although the sum (83) and product (85) formulas were shown to be algebraically equivalent, they are quite different in implementation. The sum formula involves SPS surface amplitudes $\phi_n(a)$, which exponentially grow with a. Hence, for a sufficiently large a, the numerical value of the sum in Eq. (83) may be severely affected by round-off errors. The product formula involves only SPS eigenvalues k_n and is much more robust against such kind of errors. This situation is similar to that discussed in [8,9]. We have confirmed that both formulas yield identical results when round-off errors can be ignored. In the calculations below we use Eq. (85).

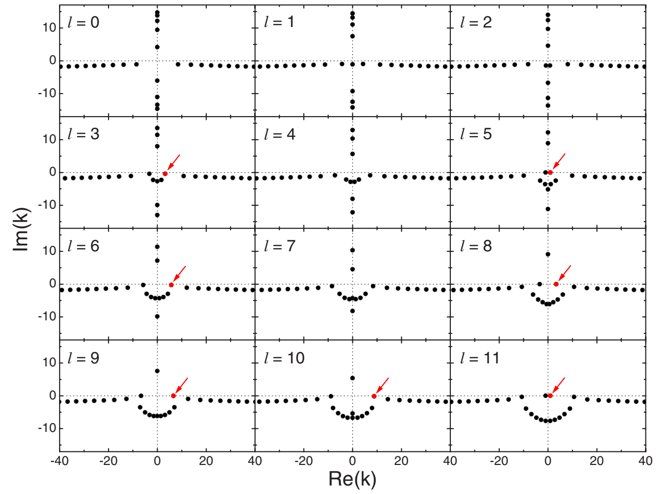

FIG. 1. (Color online) SPS momentum eigenvalues k_n for the rectangular potential (96). The arrows indicate states responsible for the appearance of resonance peaks seen in Fig. 3.

B. Rectangular potential: General features

We start with a rectangular potential well

$$V(r) = \begin{cases} V_0, & r \leq a, \\ 0, & r > a, \end{cases} \tag{96}$$

with the same values of the parameters $V_0=-112.5$ and $a=1$ as were used in [8]. This is the simplest example of a finite-range potential. Numerical studies of SSs were pioneered in [46] by the analysis of poles of the scattering matrix for this model as functions of V_0 for $l=0$. Recently, this analysis has been extended to complex V_0 and higher l [47].

The distributions of SPS eigenvalues k_n in the complex k plane for several lowest l are shown in Fig. 1. For $l=0$, potential (96) supports five bound states. As l grows, the centrifugal term in Eq. (2) also grows, the number of bound states decreases, and eventually there remains none for $l=11$. The behavior of the bound state poles as l varies explains the origin of resonances. Let us discuss this behavior, temporarily treating l as a continuous variable. The critical values of l for which there exists a bound state with zero energy, and hence the number of bound states jumps by 1, can be found from

$$zJ_{l+3/2}(z) - (2l+1)J_{l+1/2}(z) = 0, \tag{97}$$

where $z=\varkappa a$ and $\varkappa=\sqrt{-2V_0}$. For the present case $z=15$ and Eq. (97) has five roots, $l_c \approx 0.54$, 2.64, 4.97, 7.65, and 10.97, which agrees with the results in Fig. 1. In fact, it can be shown that at these critical values of l pairs of poles coalesce at $k=0$. As l approaches one of the l_c from below, a pair of

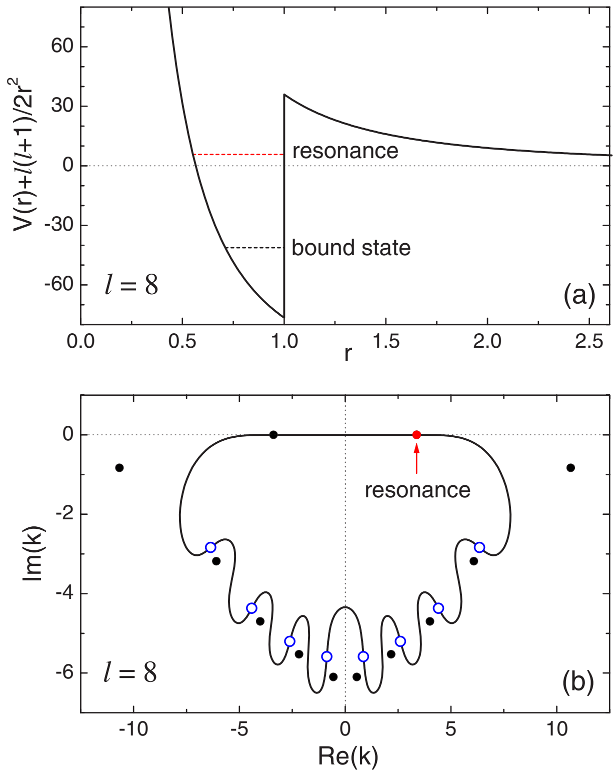

FIG. 2. (Color online) (a) Sum of the rectangular (96) and centrifugal potentials for $l=8$. There is one bound state and one pronounced resonance in this case (see Fig. 3). (b) Solid circles, SPS eigenvalues k_n, same as in the $l=8$ panel in Fig. 1. Open circles, poles iz_{lp}/a, $p=1,\ldots,l$, of the function $\omega_l(-ika)$ in Eq. (27). Solid curve outlines the dead zone $\Omega_l(-ika)$ [see Eq. (A16)].

bound and antibound poles approach the point $k=0$ from opposite sides in the vertical direction. They coalesce at $k=0$ for $l=l_c$ and then turn into a pair of incoming and outgoing poles receding from each other in the horizontal direction as l grows further. Now, we recall that there is a dead zone $\Omega_l(-ika)$ in the lower half plane, inside which incoming and outgoing eigenvalues cannot appear (see Sec. II C). It touches the real axis at $k=0$; therefore, the receding poles are confined for a while to a narrow corridor between the real axis and $\Omega_l(-ika)$, as is illustrated in Fig. 2(b) for $l=8$. In this interval of l, the outgoing member of the pair satisfies Eq. (28) and may reveal itself as a resonance in the corresponding partial cross section. The poles leave the corridor as they reach a distance $\sim l/a$ from the imaginary axis. This distance is determined by the size of the domain $\Omega_l(-ika)$ (see Appendix) and can be simply estimated on semiclassical grounds by equating the energy of the resonance pole $k^2/2$ to the height of the centrifugal barrier $l(l+1)/2a^2$ [see Fig. 2(a)]. As l grows even further, the poles depart from the real axis and rapidly lose the character of resonance. Figure 1 shows snapshots of this behavior taken at integer values of l.

The partial and total scattering cross sections are shown in Fig. 3. The numerical results obtained from Eq. (85) coincide with the analytical ones available for this model. Convergence of $\sigma_{\text{tot}}(k)$ in the interval of k considered is achieved with $l\leq 15$. The behavior of $\sigma_{\text{tot}}(k)$ in this interval is dominated by a number of more or less pronounce resonance

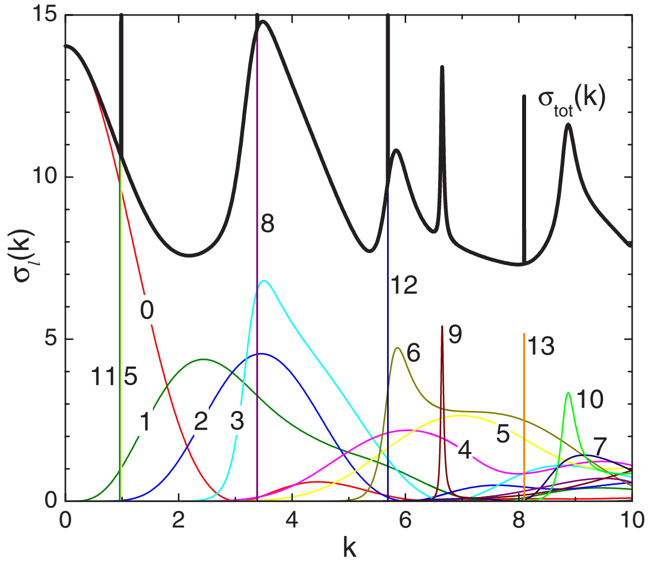

FIG. 3. (Color online) The thick curve, total cross section $\sigma_{\text{tot}}(k)$ for the rectangular potential (96). Thin curves labeled by l, partial cross sections $\sigma_l(k)$. The individual SPSs giving rise to the resonance peaks for $l\leq 11$ are indicated in Fig. 1 by arrows. The two peaks at $k\approx 0.958$ ($l=11$) and $k\approx 0.986$ ($l=5$) almost overlap.

peaks, each coming from an individual partial-wave contribution. The SPS formulation enables one to trace each of these peaks to an individual SPS (see Fig. 1).

We have also calculated the scattering length. The result $\alpha=1.057\,066\,227$ obtained from Eq. (89) with only $N=17$ is in full agreement with the analytical result for the present model, $\alpha=a-\varkappa^{-1}\tan\varkappa a$.

C. Eckart potential: Convergence with respect to the cutoff radius

To illustrate convergence with respect to the cutoff radius a, we consider an Eckart potential well

$$V(r)=-\frac{21}{\cosh^2 r}. \tag{98}$$

For $l=0$, this potential supports three bound states with energies -12.5, -4.5, and -0.5 [42,48]. The distributions of SPS eigenvalues k_n calculated with $a=10$ for the three values of l at which the number of bound states decreases by 1 are shown in Fig. 4. These distributions look similar to the previous case. In particular, the mechanism of transformation of bound-state poles into resonances as l grows remains the same. A new feature of this model is that, except for a finite

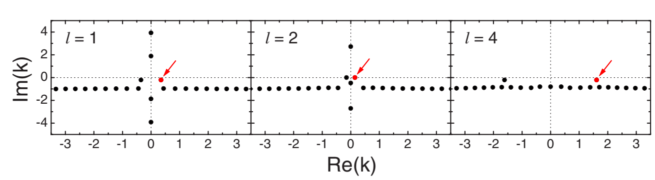

FIG. 4. (Color online) SPS momentum eigenvalues k_n for the Eckart potential (98) calculated with the cutoff radius $a=10$. The arrows indicate resonances seen in Fig. 5.

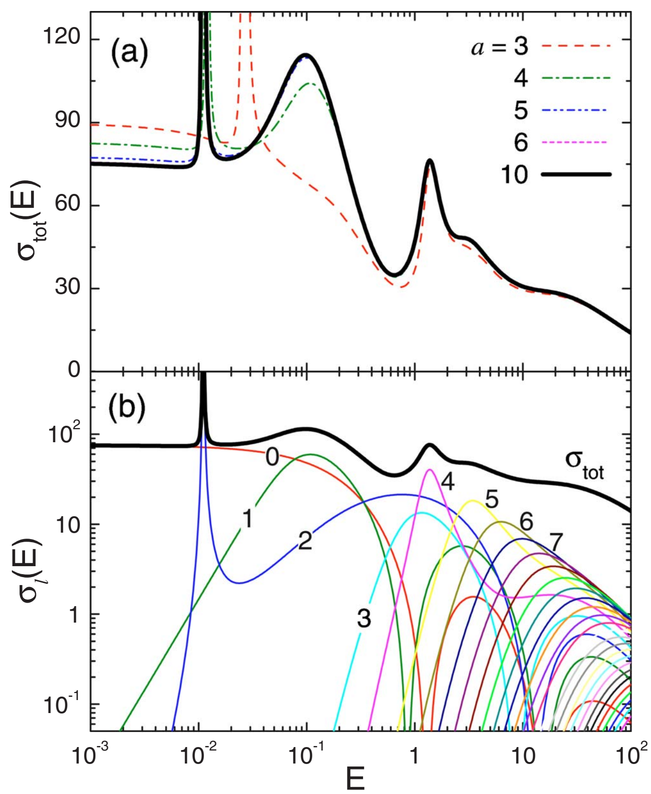

FIG. 5. (Color online) (a) Convergence of the total cross section for the Eckart potential (98) with respect to the cutoff radius a. (b) The converged results for the total (the thick curve) and partial wave (thin curves labeled by l) cross sections.

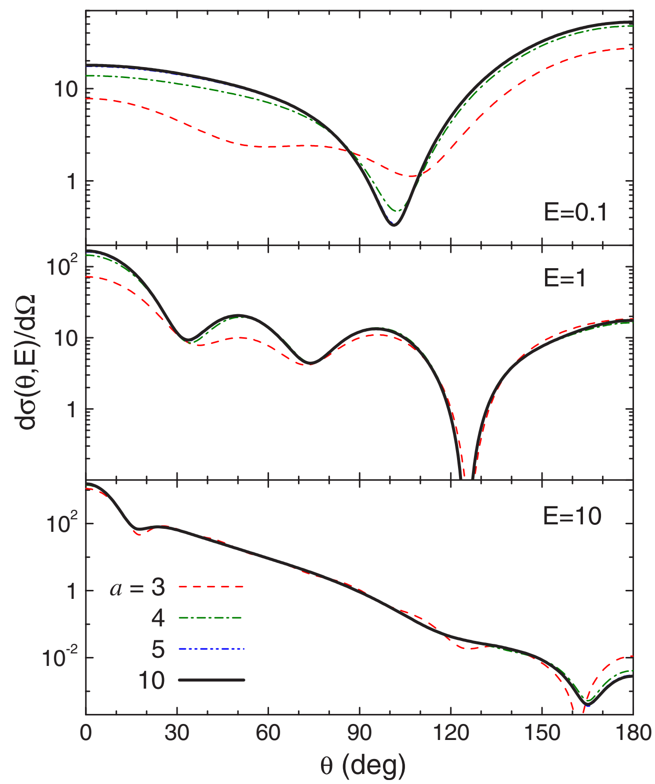

FIG. 6. (Color online) Convergence of differential cross sections for the Eckart potential (98) at three energies (see Fig. 5).

number of states observable individually—i.e., bound states and resonances—all the other SPSs now essentially depend on a. Nevertheless, the scattering results obtained from Eqs. (83), (85), and (89) rapidly converge as a grows.

Convergence of bound states and resonances is similar to the case $l=0$ [8], so we shall not discuss it here. Convergence of the scattering length calculated from Eq. (89) is shown in Table I. Note that larger a naturally require larger N, but with the present basis the rate of growth of N is close to the minimum. Figure 5(a) illustrates convergence of the total cross section. At lower energies this convergence is slower, because lower partial waves, which dominantly contribute there [see Fig. 5(b)] are more affected by the cutoff. At higher energies, the dominant contribution comes from higher partial waves and the convergence becomes faster. The upper boundary of the energy interval shown in Fig. 5 is limited by the maximum number of partial waves, $l \leq 28$, that can be included in the present calculations. Similarly to the previous case, one can clearly see three resonance peaks in the total cross section coming from partial waves with $l=1$, 2, and 4 (one can also notice a shoulder of the fourth peak from $l=5$); the corresponding resonance states are indicated in Fig. 4 by arrows. Figure 6 illustrates convergence of the differential cross section. At $E=0.1$, there are non-negligible contributions from only three lowest l [see Fig. 5(b)]; in this case, the results obtained with $a=3$ are far from convergence. At $E=10$, the dominant contributions come from higher partial waves and even the results for $a=3$ are uniformly in θ not too different from the converged ones.

TABLE I. Convergence of the scattering length α for the Eckart potential (98) with respect to the cutoff radius a. For each a, N gives the minimal dimension of our basis for which all digits quoted are converged.

a	N	α
6	29	2.458 575
8	33	2.450 348
10	37	2.450 011
12	40	2.450 000
Exact [48]		2.45

The approach based on Eq. (3) could be called a "hard cutoff." It works well for potentials decaying exponentially or faster, ensuring rapid monotonic convergence with respect to a. For potentials decaying as powers of $1/r$ the convergence is also achievable, but it may be nonmonotonic. Artificial reflections from the stepwise discontinuity at $r=a$ may cause oscillations in the partial cross sections. In this case, the use of a "soft cutoff," when the original potential $V(r)$ is multiplied by a smooth switching off function rapidly approaching 1 (0) at $r<a$ ($r>a$), accelerates the convergence.

D. Yukawa potential: Photoionization

As the last example, we consider photoionization of a particle bound by the Yukawa potential

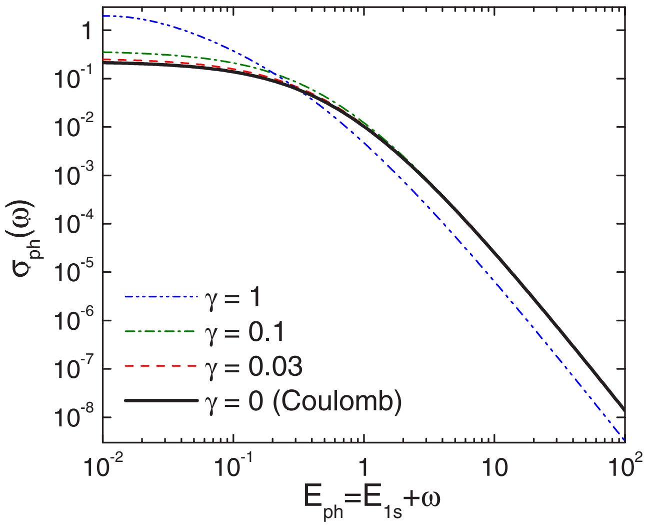

FIG. 7. (Color online) Dashed curves: the photoionization cross section from the $1s$ state in the Yukawa potential (99) calculated using Eq. (100). Solid curve: similar results for the Coulomb potential obtained from Eq. (102).

$$V(r) = -\frac{e^{-\gamma r}}{r}. \tag{99}$$

This will illustrate the performance of the approach for potentials with the Coulomb singularity at $r=0$.

The photoionization cross section from a ground $1s$ state to a continuum p state by a photon with the energy ω is given by [49]

$$\sigma_{\rm ph}(\omega) = \frac{2\pi\omega}{3ck_{\rm ph}}\left|\int_0^\infty \varphi_{1s}(r) r \varphi_p(r,k_{\rm ph}) dr\right|^2, \tag{100}$$

where

$$k_{\rm ph} = \sqrt{2E_{\rm ph}}, \quad E_{\rm ph} = E_{1s} + \omega. \tag{101}$$

The bound and scattering states were calculated using Eqs. (75), (77), and (80). The results for several values of γ are shown in Fig. 7. For $\gamma=1$, 0.1, and 0.03, the ground-state energy is $E_{1s}=-0.010\,286$, $-0.407\,058$, and $-0.470\,662$ and convergence of the results in Fig. 7 is achieved with the minimal parameters $(a,N)=(4,20)$, $(35,70)$, and $(90,130)$, respectively, with a affecting the convergence near the threshold and N at large energies. As $\gamma\to 0$, the matrix element in Eq. (100) becomes insensitive to a difference between the Yukawa and Coulomb potentials, and the calculated results converge to the photoionization cross section from the Coulomb potential given by [49]

$$\sigma_{\rm ph}(\omega) = \frac{32\pi^2}{3c\omega^4}\frac{\exp(-4x\,\mathrm{arccot}\,x)}{1-\exp(-2\pi x)}, \tag{102}$$

where $x=1/k_{\rm ph}$. This type of convergence illustrates the soft cutoff approach mentioned above. One of the most interesting applications of SPSs is to use them as a basis for the expansion in the problem of an atom interacting with a strong laser field. The results in Fig. 7 show that the effects of the Coulomb tail of the atomic potential can be recovered by using the Yukawa potential (99) and achieving convergence as $\gamma\to 0$.

V. CONCLUSIONS

This work generalizes the SPS formulation of scattering theory, originally developed in [8] for s-wave scattering in a spherically symmetric finite-range potential, to arbitrary angular momenta l. Its main results consist in defining the SPSs as the solutions to a linear eigenvalue problem in the extended Hilbert space [Eqs. (31) and (34)], establishing their basic orthogonality [Eqs. (36) and (37)] and completeness [Eqs. (43) and (44)] properties, and the derivation of SPS expansions for the outgoing-wave Green's function [Eq. (73)], physical states [Eqs. (75), (77), and (80)], and scattering matrix [Eqs. (83) and (85)]. This completes the theory of SPSs in the one-channel case, making its application to three-dimensional problems possible. The results are illustrated by calculations for several model potentials.

Technical merits of SPSs as a computational tool in comparison with other computational approaches in scattering theory, especially with the R-matrix method, were discussed in the concluding section in [8]; all the arguments remain the same, so we do not repeat them here. The only difference is that the size of the matrix to be diagonalized in the general case is $2N+l$. Fortunately, this is not much larger than $2N$, as in the case $l=0$ [8], at least in situations when the partial-wave expansion is expected to converge within reasonably moderate values of l. The main conceptual advantage of the SPS formulation is that the whole spectrum of scattering phenomena can be described by means of a pure discrete set of states. This advantage becomes even more important in the nonstationary framework. An extension of the present formulation to the nonstationary case along the lines of the approach initiated in [23] is the next goal in the development of the theory.

APPENDIX: BESSEL POLYNOMIALS AND RELATED FUNCTIONS

The Bessel polynomials are defined by [50]

$$y_l(z) = \sum_{m=0}^{l}\frac{(l+m)!}{m!\,(l-m)!}\frac{z^m}{2^m}, \tag{A1}$$

and the reverse Bessel polynomials are defined by [51]

$$\theta_l(z) \equiv z^l y_l(1/z) = \sum_{m=0}^{l}\frac{(2l-m)!}{m!\,(l-m)!}\frac{z^m}{2^{l-m}}. \tag{A2}$$

For our purposes, it is more convenient to work with $\theta_l(z)$. The relevance of these polynomials to the present subject is seen from the fact that spherical Hankel functions [52] can be expressed in their terms,

$$h_l^{(1,2)}(z) = \mp i e^{\pm iz} z^{-l-1}\theta_l(\mp iz). \tag{A3}$$

Here, we summarize some properties of $\theta_l(z)$ used in the above discussion.

The polynomials $\theta_l(z)$ satisfy the recurrence relations

$$\theta_0(z) = 1, \quad \theta_1(z) = z + 1, \tag{A4a}$$

$$\theta_l(z) = (2l-1)\theta_{l-1}(z) + z^2\theta_{l-2}(z), \quad l \geq 2, \tag{A4b}$$

and

$$\frac{d\theta_l(z)}{dz} = \theta_l(z) - z\theta_{l-1}(z), \quad l \geq 1. \tag{A5}$$

Let z_{lp}, $p=1,\ldots,l$, denote the zeros of $\theta_l(z)$. Then

$$\theta_l(z) = \prod_{p=1}^{l}(z - z_{lp}). \tag{A6}$$

The zeros z_{lp} are well studied [53]. We mention only several of their properties: for even l, there are no real zeros and all the zeros occur in complex conjugate pairs; for odd l, there is only one unpaired real zero; all the zeros are simple and lie in the half plane $\mathrm{Re}\, z \leq -1$, approximately on an arc joining $z=-il$ and $z=il$. Using Eqs. (A2) and (A6) it can be shown that

$$\sum_{p=1}^{l}\frac{1}{z_{lp}} = -1. \tag{A7}$$

The position of z_{lp} in the complex plane for several lowest l is shown in Fig. 8.

It is convenient to introduce a function

$$e_l(z) = e^{iz}\frac{\theta_l(-iz)}{(-iz)^l}, \tag{A8}$$

which, up to a constant phase factor, coincides with $zh_l^{(1)}(z)$. It satisfies

$$\left[\frac{d^2}{dz^2} - \frac{l(l+1)}{z^2} + 1\right]e_l(z) = 0, \tag{A9a}$$

$$e_l(z)\big|_{|z|\to\infty} = e^{iz}. \tag{A9b}$$

Using Eq. (A6), we obtain

$$\frac{1}{e_l(z)}\frac{de_l(z)}{dz} = i - \frac{1}{z}\sum_{p=1}^{l}\frac{z_{lp}}{iz + z_{lp}}. \tag{A10}$$

This equation enables one to formulate the outgoing-wave boundary condition for SSs (see Sec. II A).

Consider the function

$$\omega_l(z) = 1 + \sum_{p=1}^{l}\frac{z_{lp}}{(z - z_{lp})(z^* - z_{lp})}, \quad l \geq 1. \tag{A11}$$

Its properties are needed for the discussion of the distribution of SS eigenvalues in the complex plane (see Sec. II C). We are not aware of any studies of this function in the literature, so it is worthwhile to give some details here. Using the properties of z_{lp}, it can be shown that $\omega_l(z)$ takes real values for all complex z. The most important for the present purposes results are

$$\omega_l(0) = 0, \tag{A12a}$$

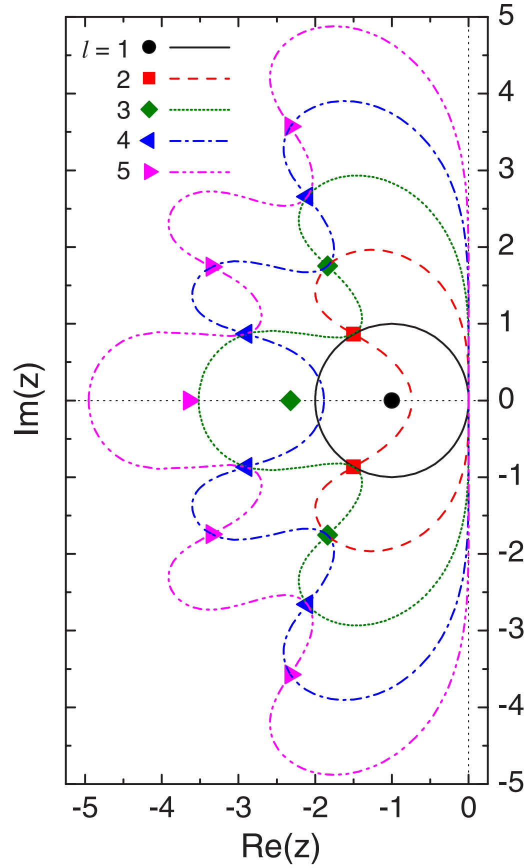

FIG. 8. (Color online) Symbols show the zeros z_{lp}, $p=1,\ldots,l$, of inverse Bessel polynomials $\theta_l(z)$. Curves outline domains $\Omega_l(z)$ defined by Eq. (A16).

$$\omega_l(z) > 0, \quad |z| > 0, \quad -\pi/2 \leq \arg z \leq \pi/2. \tag{A12b}$$

Equation (A12a) follows from Eq. (A7). Let us prove inequality (A12b). It is sufficient to consider the first quadrant $0 \leq \arg z \leq \pi/2$ because $\omega_l(z) = \omega_l(z^*)$. The proof is based on the equation which follows from Eqs. (A5) and (A6),

$$\mathrm{Im}\, z \times \omega_l(z) = \mathrm{Im}\, F_l(z), \tag{A13}$$

where

$$F_l(z) = \frac{z^2\theta_{l-1}(z)}{\theta_l(z)}. \tag{A14}$$

We proceed in three steps. First, consider the ray $|z|>0$, $\arg z = \pi/2$. Using Eqs. (A4), function (A14) satisfies the recurrence

$$F_1(z) = \frac{z^2}{1+z}, \tag{A15a}$$

$$F_l(z) = \frac{z^2}{2l - 1 + F_{l-1}(z)}, \quad l \geq 2. \tag{A15b}$$

Substituting here $z=iy$, where $y>0$ is real, it can be shown that $\mathrm{Im}\, F_l(iy) > 0$ for all l. Then the validity of (A12b) follows from Eq. (A13). Second, consider the sector $|z|>0$, 0

$<\arg z<\pi/2$. Function (A14) is analytic in the first quadrant; therefore, $\text{Im}\, F_l(z)$ is a harmonic function there, and hence $\text{Im}\, F_l(z)$ attains its minimum value in the first quadrant on the boundary of the quadrant (the maximum principle for harmonic functions). Using the above result and the fact that $F_l(z)=z$ for $|z|\to\infty$, it can be seen that this happens on the real axis, where $\text{Im}\, F_l(z)=0$. Consequently, $\text{Im}\, F_l(z)>0$, in the sector under consideration and the validity of (A12b) again follows from Eq. (A13). Finally, the function $\omega_l(z)$ cannot have zeros on the ray $|z|>0$, $\arg z=0$, because this would contradict its positiveness inside the first quadrant. From $\omega_l(+\infty)=1$ we obtain that inequality (A12b) holds on this ray too. This completes the proof.

Let $\Omega_l(z)$, $l\geq 1$, denote a domain in the complex z plane where

$$\omega_l(z)\leq 0,\quad z\in\Omega_l(z). \tag{A16}$$

This domain defines the dead zone where SS eigenvalues cannot appear (see Sec. II C). The following properties of $\Omega_l(z)$, which we give without proof, can be deduced from the above considerations: $\Omega_l(z)$ is bounded, singly connected, symmetric with respect to the real axis, lies in the left half plane, $\text{Re}\, z<0$, and touches the imaginary axis at the single point $z=0$. On the boundary of $\Omega_l(z)$ we have $\omega_l(z)=0$. For $l=1$, it is a circle of radius 1 with the center at $z=z_{11}=-1$; for $l>1$, it is a closed artichoke like curve with l petals. It also can be shown that all complex zeros z_{lp} for the given l lie on the boundary of $\Omega_l(z)$, the straight line connecting a complex zero z_{lp} and $z=0$ is tangential to the boundary of $\Omega_l(z)$ at $z=z_{lp}$, and each complex zero z_{lp} belongs simultaneously to the boundaries of $\Omega_l(z)$ and $\Omega_{l\pm1}(z)$. All these properties are illustrated in Fig. 8.

Finally, we mention two more relations satisfied by reverse Bessel polynomials. The first one reads

$$1-\sum_{p=1}^{l}\frac{z_{lp}}{z^2-z_{lp}^2}=\frac{(-1)^l z^{2l}}{\theta_l(z)\,\theta_l(-z)}. \tag{A17}$$

This equation is needed for the derivation of Eq. (58). It can be obtained using Eqs. (A5), (A6), and

$$\theta_{l-1}(z)\,\theta_l(-z)-\theta_{l-1}(-z)\,\theta_l(z)=2(-1)^l z^{2l-1}, \tag{A18}$$

which in turn follows from Eqs. (A4). The second relation expresses a property that holds for $z\to 0$,

$$\frac{e^{-2z}\theta_l(z)}{\theta_l(-z)}=1-\frac{(-1)^l z^{2l+1}}{(l+1/2)\,\theta_l^2(0)}+O(z^{2l+3}). \tag{A19}$$

It is used in the derivation of Eq. (88). The fact that there are no terms in this expansion with powers between 0 and $2l+1$ underlies the principle of so-called Bessel filters well known in electronics and signal processing (see, e.g., [54]).

[1] A. J. F. Siegert, Phys. Rev. **56**, 750 (1939).
[2] V. de Alfaro and T. Regge, *Potential Scattering* (North-Holland, Amsterdam, 1965).
[3] R. G. Newton, *Scattering Theory of Waves and Particles* (Springer-Verlag, New York, 1982).
[4] A. I. Baz', Ya. B. Zel'dovich, and A. M. Perelomov, *Scattering, Reactions, and Decays in Nonrelativistic Quantum Mechanics* (Nauka, Moscow, 1971).
[5] H. M. Nussenzveig, *Causality and Dispersion Relations* (Academic Press, New York, 1972).
[6] V. I. Kukulin, V. M. Krasnopol'sky, and J. Horáček, *Theory of Resonances: Principles and Applications* (Academia, Praha, 1989).
[7] O. I. Tolstikhin, V. N. Ostrovsky, and H. Nakamura, Phys. Rev. Lett. **79**, 2026 (1997).
[8] O. I. Tolstikhin, V. N. Ostrovsky, and H. Nakamura, Phys. Rev. A **58**, 2077 (1998).
[9] G. V. Sitnikov and O. I. Tolstikhin, Phys. Rev. A **67**, 032714 (2003).
[10] K. Toyota, T. Morishita, and S. Watanabe, Phys. Rev. A **72**, 062718 (2005).
[11] O. I. Tolstikhin, I. Yu. Tolstikhina, and C. Namba, Phys. Rev. A **60**, 4673 (1999).
[12] O. I. Tolstikhin, V. N. Ostrovsky, and H. Nakamura, Phys. Rev. A **63**, 042707 (2001).
[13] E. L. Hamilton and C. H. Greene, Phys. Rev. Lett. **89**, 263003 (2002).
[14] K. Toyota and S. Watanabe, Phys. Rev. A **68**, 062504 (2003).
[15] V. Kokoouline and C. H. Greene, Phys. Rev. Lett. **90**, 133201 (2003); Phys. Rev. A **68**, 012703 (2003); **69**, 032711 (2004).
[16] Å. Larson, S. Tonzani, R. Santra, and C. H Greene, J. Phys.: Conf. Ser. **4**, 148 (2005).
[17] G. V. Sitnikov and O. I. Tolstikhin, Phys. Rev. A **71**, 022708 (2005).
[18] V. N. Ostrovsky and N. Elander, Phys. Rev. A **71**, 052707 (2005); Chem. Phys. Lett. **411**, 155 (2005).
[19] A. I. Smolyakov, S. I. Krasheninnikov, and O. I. Tolstikhin, Phys. Plasmas **12**, 052112 (2005).
[20] S. Yoshida, S. Watanabe, C. O. Reinhold, and J. Burgdörfer, Phys. Rev. A **60**, 1113 (1999).
[21] S. Tanabe, S. Watanabe, N. Sato, M. Matsuzawa, S. Yoshida, C. O. Reinhold, and J. Burgdörfer, Phys. Rev. A **63**, 052721 (2001).
[22] R. Santra, J. M. Shainline, and C. H. Greene, Phys. Rev. A **71**, 032703 (2005).
[23] O. I. Tolstikhin, Phys. Rev. A **73**, 062705 (2006).
[24] O. I. Tolstikhin, Phys. Rev. A **74**, 042719 (2006).
[25] C. Bloch, Nucl. Phys. **4**, 503 (1957).
[26] Ya. B. Zel'dovich, Zh. Eksp. Teor. Fiz. **39**, 776 (1960) [Sov. Phys. JETP **12**, 542 (1961)].
[27] V. S. Rudakov, Vestn. Leningr. Univ., Ser. 4: Fiz., Khim. **16**, 143 (1966).
[28] W. J. Romo, Nucl. Phys. A **116**, 617 (1968).
[29] É. É. Shnol, Teor. Mat. Fiz. **8**, 140 (1971) [Theor. Math. Phys. **8**, 729 (1971)].
[30] W. J. Romo, Nucl. Phys. A **237**, 275 (1975).

[31] W. J. Romo, J. Math. Phys. **21**, 311 (1980).
[32] J. Bang, F. A. Gareev, M. H. Gizzatkulov, and S. A. Goncharov, Nucl. Phys. A **309**, 381 (1978).
[33] R. M. More and E. Gerjuoy, Phys. Rev. A **7**, 1288 (1973).
[34] R. E. Peierls, Proc. R. Soc. London, Ser. A **253**, 16 (1959).
[35] V. V. Prasolov, *Polynomials* (Springer, Berlin, 2004).
[36] J. Humblet, Mem. Soc. R. Sci. Liege Collect. in-8 **12**, No. 4 (1952).
[37] A. I. Markushevich, *Theory of Functions of a Complex Variable* (Chelsea, New York, 1985).
[38] V. I. Serdobol'skiĭ, Zh. Eksp. Teor. Fiz. **36**, 1903 (1959) [Sov. Phys. JETP **9**, 1354 (1959)].
[39] G. García-Calderón, Nucl. Phys. A **261**, 130 (1976).
[40] N. Hu, Phys. Rev. **74**, 131 (1948).
[41] T. Regge, Nuovo Cimento **8**, 671 (1958).
[42] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics (Nonrelativistic Theory)* (Pergamon Press, Oxford, 1977).
[43] D. O. Harris, G. G. Engerholm, and W. D. Gwinn, J. Chem. Phys. **43**, 1515 (1965).
[44] A. S. Dickinson and P. R. Certain, J. Chem. Phys. **49**, 4209 (1968).
[45] J. C. Light, I. P. Hamilton, and J. V. Lill, J. Chem. Phys. **82**, 1400 (1985).
[46] H. M. Nussenzveig, Nucl. Phys. **11**, 499 (1959).
[47] C. Grama, N. Grama, and I. Zamfirescu, Phys. Rev. A **61**, 032716 (2000).
[48] S. Flügge, *Practical Quantum Mechanics* (Springer, Berlin, 1999).
[49] A. F. Starace, *Theory of Atomic Photoionization, Handbuch der Physik*, Vol. 31, edited by W. Mehlhorn (Springer-Verlag, Berlin, 1982); M. Ya. Amusia, *Atomic Photoeffect* (Plenum Press, New York, 1990).
[50] H. L. Krall and O. Fink, Trans. Am. Math. Soc. **65**, 100 (1948).
[51] E. Grosswald, *Bessel Polynomials Lecture Notes in Mathematics* , Vol. 698 (Springer-Verlag, New York, 1978).
[52] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1972).
[53] M. G. de Bruin, E. B. Saff, and R. S. Varga, Nederl. Akad. Wetensch. Indag. Math. **43**, 1 (1981); **43**, 14 (1981).
[54] S. Winder, *Analog and Digital Filter Design* (Newnes, Boston, 2002).