Siegert pseudostate perturbation theory: One- and two-threshold cases

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Perturbation theory for the Siegert pseudostates [Phys. Rev. A **58**, 2077 (1998) and Phys. Rev. A **67**, 032714 (2003)] is studied for the case of two energetically separated thresholds. The perturbation formulas for the one-threshold case are derived as a limiting case whereby we reconstruct More's theory for the decaying states [Phys. Rev. A **3**, 1217 (1971)] and amend an error. The perturbation formulas for the two-threshold case have additional terms due to the nonstandard orthogonality relationship of the Siegert pseudostates. We apply the theory to a two-channel model problem, and find that the rate of convergence of the perturbation expansion should be examined with the aide of the variance $D = \|E - \Sigma_n \lambda^n E^{(n)}\|$ instead of the real and imaginary parts of the perturbation energy individually.

I. INTRODUCTION

Resonances occur in a variety of fields of physical sciences. Despite their diversity, they are characterized by two parameters, the resonance energy position and width, apart from the coupling with the background continuum represented by the Fano profile [1]. A great deal of discussions have been given to the interpretation of resonance phenomena [1]. The most familiar parametrization of the resonances is condensed into the dispersion formula due to Breit and Wigner. Back in 1939, Siegert [2] developed a compact mathematical viewpoint for characterizing resonances as singular points of the dispersion relation. His idea requires the solution of the Schrödinger equation subject to the outgoing wave boundary condition,

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

where a is the radius beyond which the potential energy is negligible. The solution $\phi(r)$ is called the Siegert state (SS) and it behaves like e^{ikr} near $r=a$ and beyond. This boundary condition destroys the hermiticity of the Hamiltonian, thus entailing complex-valued eigenenergies, i.e.,

$$E = \frac{k^2}{2} = E_{\text{res}} - i \frac{\Gamma}{2}.$$

This is a most direct representation of both the resonance position and width. This mathematically appealing representation had been implemented with tedious iterations due to lack of suitable computational techniques until Tolstikhin *et al.* [3] made a breakthrough by introducing Siegert pseudostates (SPSs) for the one-threshold case. Their idea incorporates the boundary condition into the Schrödinger equation so that the dispersion relation is obtained by a single diagonalization of the Hamiltonian matrix. Previous applications of SPSs to resonances in three-body Coulomb problems indicate that it is not only a valid procedure but also a different perspective for the SPS representation of resonances and decay processes [4]. Another immediate application of the SPS theory is to the time-dependent problem [5,6] where the re-

flection off the exterior boundary incurs numerical instability. Tanabe and Watanabe [7] succeeded in describing the reflectionless time propagation based on the Siegert pseudostates. Indeed, applied to the half-cycle optical pulses, the Siegert boundary condition indeed was seen to eliminate the outgoing wave component perfectly.

Recently, Sitnikov and Tolstikhin [8,9] stretched the scope of the SPS theory by enabling the treatment of the two-threshold problem. Despite such progress, there remains in the theory of SPS a chapter still incompletely worked out. This is the Siegert perturbation theory. A pioneering work on this subject is due to More [10,11] who extended the Siegert state theory specifically to handle the decaying state. The main purpose of this paper is to complete the Siegert perturbation theory from the recently developed SPS viewpoint for both one- and two-threshold cases. Particularly, in the one-threshold case, we are able to reconstruct More's theory for decaying states [10] in terms of SPS but with an unexpected amendment to his theory. The SPS perturbation theory (SPSPT) is by no means straightforward owing to the nonstandard orthonormality of the eigenfunctions. This constraint also serves to fix the phase of the perturbed wave function, a feature which is absent from the standard perturbation theory. It is hoped that this paper serves to expose such noteworthy features of the SPSPT.

This paper is thus constructed as follows. In Sec. II, we review some basic ideas about the SPS as needed for an elementary presentation of the perturbation theory. Section III gives the details of the SPSPT for both one- and two-threshold cases. And Sec. III deals with a specific mathematical model as an example of the SPSPT. Atomic units are used throughout.

II. SIEGERT PSEUDOSTATES

Since the two-threshold SPS theory contains the one-threshold case in itself, we review the two-threshold case only, leaving the one-threshold case as the limit where the two thresholds become degenerate [8].

A. Mathematical settings

Suppose first that there are as many as q independent channels. The Schrödinger equation reads

$$\left[-\frac{1}{2}\frac{d^2}{dr^2} + V(r) - E \right]\phi(r) = 0, \qquad (1)$$

where

$$V(r) = \begin{pmatrix} V_1 & V_{12} & \cdots & V_{1q} \\ V_{12} & V_2 & \cdots & V_{2q} \\ \vdots & \vdots & \ddots & \vdots \\ V_{1q} & V_{2q} & \cdots & V_q \end{pmatrix},$$

$$\phi(r) = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_q \end{pmatrix},$$

and V_i pertains to the potential energy of channel i, and V_{ij} represents the interchannel coupling between channels i and j. We consider the situation where there are only two energetically distinct thresholds so that we separate V_i into two groups. A first group contains channels $1, \ldots, q_1$ and they converge to v_1 as $r \to a$ while the other group contains channels $q_1+1, \ldots, q$ and they converge to v_2, that is,

$$\lim_{r \to a} V(r) = \mathrm{diag}[\overbrace{v_1, \ldots, v_1}^{1, \ldots, q_1}, \overbrace{v_2, \ldots, v_2}^{q_1+1, \ldots, q}],$$

where v_1 and v_2 are the two constants representing the threshold energies. This allows us to use the *two-channel* SPS scheme even in the presence of *more than two channels*. The *two-channel* momenta are $k_1 = \sqrt{2(E-v_1)}$ and $k_2 = \sqrt{2(E-v_2)}$. The boundary conditions are thus

$$\phi_i(0) = 0$$

at $r=0$ and

$$\left.\left(\frac{d}{dr} - ik_j\right)\phi_i\right|_{r=a} = 0$$

at $r=a$ where $j=1$ for the first group, $i=1,\ldots,q_1$, and $j=2$ for the second group, $i=q_1+1,\ldots,q$. Now, consider to expand the wave function ϕ_i by a complete orthonormal basis set $\{\pi_l(r), (l=1,\ldots,N)\}$ over $r \in [0,a]$ such that

$$\phi_i(r) = \sum_{l=1}^{N} c_{i,l}\pi_l(r).$$

Substituting this into Eq. (1), and integrating over the interval $[0,a]$, we obtain the $M = q \times N$-dimensional eigenvalue problem,

$$\left[\tilde{H} - \frac{i}{2}B - EI_M\right]\vec{c} = 0, \qquad (2)$$

where

$$\tilde{H} = \begin{pmatrix} \tilde{H}^{(1)} & U^{(12)} & \cdots & U^{(1q)} \\ U^{(12)} & \tilde{H}^{(2)} & \cdots & U^{(2q)} \\ \vdots & \vdots & \ddots & \vdots \\ U^{(q1)} & U^{(q2)} & \cdots & \tilde{H}^{(q)} \end{pmatrix},$$

$$B = \begin{pmatrix} k_1 L & & & & & & \\ & \ddots & & & & 0 & \\ & & k_1 L & & & & \\ & & & k_2 L & & & \\ & 0 & & & \ddots & & \\ & & & & & k_2 L \end{pmatrix},$$

with column headers over B: $1 \cdots q_1 \quad q_1+1 \cdots q\text{th block}$

$$\vec{c} = \begin{pmatrix} c_{1,1} \\ \vdots \\ c_{1,N} \\ \vdots \\ c_{q,1} \\ \vdots \\ c_{q,N} \end{pmatrix},$$

and

$$\tilde{H}_{ij}^{(n)} = \frac{1}{2}\int_0^a \frac{d\pi_i}{dr}\frac{d\pi_j}{dr}dr + \int_0^a \pi_i V_n \pi_j dr,$$

$$U_{ij}^{(mn)} = \int_0^a \pi_i V_{mn}\pi_j dr,$$

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

In Eq. (2), I_M is an M-dimensional unit matrix. The eigensystem Eq. (2) involves a pair of eigenvalues, k_1 and k_2, which may be rewritten as a standard eigenvalue equation for a single variable u according to the following heuristic procedure. Let us note that energy E can be represented by both k_1 and k_2, namely

$$E = \frac{1}{2}k_1^2 + v_1 = \frac{1}{2}k_2^2 + v_2$$

so that

$$(k_1 + k_2)(k_1 - k_2) = 4\Delta^2, \qquad (3)$$

where

$$\Delta = \sqrt{\frac{v_2 - v_1}{2}}.$$

(Here, we assume $v_2 \geq v_1$ for simplicity.) Since the product of linearly independent combinations of k_1 and k_2 becomes constant, we require $k_1 \pm k_2$ to satisfy the following conditions:

$$k_1 + k_2 = 2i\Delta u,$$

$$k_1 - k_2 = -2i\Delta u^{-1}.$$

Thus

$$k_1 = i\Delta(u - u^{-1}),$$

$$k_2 = i\Delta(u + u^{-1}),$$

and

$$E = \bar{v} - \Delta^2 \frac{1 + u^4}{2u^2}$$

with

$$\bar{v} = \frac{v_1 + v_2}{2}.$$

This procedure of replacing a pair of variables k_1 and k_2 by a single variable u is called uniformization.

B. Tolstikhin-Siegert equation

The uniformization described above reduces Eq. (2) to

$$\mathcal{M}(u)\vec{c} = 0 \qquad (4)$$

with

$$\mathcal{M}(u) = I_M + uB^- + u^2 A + u^3 B^+ + u^4 I_M, \qquad (5)$$

where

$$A = \frac{2}{\Delta^2} \begin{pmatrix} \widetilde{H}^{(1)} - \bar{v}I_M & U^{(12)} & \cdots & U^{(1q)} \\ U^{(12)} & \widetilde{H}^{(2)} - \bar{v}I_M & \cdots & U^{(2q)} \\ \vdots & \vdots & \ddots & \vdots \\ U^{(1q)} & U^{(2q)} & \cdots & \widetilde{H}^{(q)} - \bar{v}I_M \end{pmatrix},$$

and

$$B^{\pm} = \frac{1}{\Delta} \begin{pmatrix} \pm L & & & & & \\ & \ddots & & & 0 & \\ & & \pm L & & & \\ & & & L & & \\ & 0 & & & \ddots & \\ & & & & & L \end{pmatrix} \begin{matrix} 1 \\ \cdots \\ q_1 \\ q_1+1 \\ \cdots \\ q\text{th block} \end{matrix} .$$

By introducing a new vector

$$\begin{pmatrix} \vec{c} \\ u\vec{c} \\ u^2\vec{c} \\ u^3\vec{c} \end{pmatrix},$$

the nonlinear eigenvalue problem, Eq. (4), is reduced to a linear one such that

$$\begin{pmatrix} 0 & I_M & 0 & 0 \\ 0 & 0 & I_M & 0 \\ 0 & 0 & 0 & I_M \\ -I_M & -B^- & -A & -B^+ \end{pmatrix} \begin{pmatrix} \vec{c} \\ u\vec{c} \\ u^2\vec{c} \\ u^3\vec{c} \end{pmatrix} = u \begin{pmatrix} \vec{c} \\ u\vec{c} \\ u^2\vec{c} \\ u^3\vec{c} \end{pmatrix}. \qquad (6)$$

Furthermore, the above equation is symmetrizable as follows:

$$\begin{pmatrix} 0 & 0 & 0 & I_M \\ 0 & 0 & I_M & B^- \\ 0 & I_M & B^- & A \\ I_M & B^- & A & B^+ \end{pmatrix} \begin{pmatrix} \vec{c} \\ u\vec{c} \\ u^2\vec{c} \\ u^3\vec{c} \end{pmatrix} = u \begin{pmatrix} 0 & 0 & I_M & 0 \\ 0 & I_M & B^- & 0 \\ I_M & B^- & A & 0 \\ 0 & 0 & 0 & -I_M \end{pmatrix}$$

$$\times \begin{pmatrix} \vec{c} \\ u\vec{c} \\ u^2\vec{c} \\ u^3\vec{c} \end{pmatrix}. \qquad (7)$$

Let us refer to Eqs. (4), (6), and (7) as the Tolstikhin-Siegert equations (TSEs).

III. FIRST- AND SECOND-ORDER PERTURBATION THEORY

A. Derivation of perturbation formulas

Let us formulate the perturbation theory as appropriate for the SPS whose orthonormality relation is different from the standard one. Relegating the one-threshold case to the next subsection, we treat the general two-threshold case. We assume the perturbing potential energy $V'(r)$ vanishes beyond $r=a$, i.e.,

$$V'(r) = \begin{pmatrix} V'_{11} & V'_{12} & \cdots & V'_{1q} \\ V'_{12} & V'_{22} & \cdots & V'_{2q} \\ \vdots & \vdots & \ddots & \vdots \\ V'_{1q} & V'_{2q} & \cdots & V'_{qq} \end{pmatrix} = 0 \quad (r > a).$$

The TSE for the nth state including perturbing potential energy reads

$$\left(I_M + u_n B^- + u_n^2 A + 2\lambda \frac{u_n^2 U'}{\Delta^2} + u_n^3 B^+ + u_n^4 I_M \right) \vec{c}_n = 0, \qquad (8)$$

where

$$U' = \begin{pmatrix} U'^{(11)} & U'^{(12)} & \cdots & U'^{(1q)} \\ U'^{(12)} & U'^{(22)} & \cdots & U'^{(2q)} \\ \vdots & \vdots & \ddots & \vdots \\ U'^{(1q)} & U'^{(2q)} & \cdots & U'^{(qq)} \end{pmatrix},$$

$$U_{ij}'^{(mn)} = \int_0^a \pi_i V'_{mn} \pi_j dr.$$

Differentiating Eq. (8) with respect to λ and using the orthonormal relationship [see Eq. (44) in Ref. [8]]

$$\vec{c}_m^T \left[I_M + \frac{u_m u_n (B^- - u_m u_n B^+)}{(u_m + u_n)(1 - u_m^2 u_n^2)} \right] \vec{c}_n = \delta_{mn},$$

we obtain the Hellmann-Feynman theorem (HFT) in the present context, namely,

$$\vec{c}_n^T U' \vec{c}_n = \Delta^2 \frac{1 - u_n^4}{u_n^3} \frac{du_n}{d\lambda} = \frac{d}{d\lambda}\left(\bar{v} - \Delta^2 \frac{1 + u_n^4}{2u_n^2} \right) = \frac{dE_n}{d\lambda}. \quad (9)$$

Now, we consider the perturbation series of u_n and $\vec{c}_n$ such that

$$u_n = u_n^{(0)} + \lambda u_n^{(1)} + \lambda^2 u_n^{(2)} + \cdots, \quad (10)$$

$$\vec{c}_n = \vec{c}_n^{(0)} + \lambda \vec{c}_n^{(1)} + \lambda^2 \vec{c}_n^{(2)} + \cdots, \quad (11)$$

where $u_n^{(0)}$ and $\vec{c}_n^{(0)}$ are the nth solution to the unperturbed equation, Eq. (4),

$$\mathcal{M}(u_n^{(0)})\vec{c}_n^{(0)} = 0.$$

Substituting the perturbation series, Eqs. (10) and (11), into Eq. (9) and then comparing each power of λ, we obtain

$$\lambda^0 : \Delta^2 \frac{1 - u_n^{(0)4}}{u_n^{(0)3}} u_n^{(1)} = \vec{c}_n^{(0)T} U' \vec{c}_n^{(0)}, \quad (12)$$

$$\lambda^1 : \frac{\Delta^2}{2u_n^{(0)3}} \left[2u_n^{(2)}(1 - u_n^{(0)4}) - \frac{3u_n^{(1)2} + u_n^{(1)2} u_n^{(0)4}}{u_n^{(0)}} \right] = \vec{c}_n^{(0)T} U' \vec{c}_n^{(1)}. \quad (13)$$

Next, let us evaluate the expansion coefficients over the unperturbed eigenstates. To this end, we rewrite Eq. (8) using Eq. (5), namely,

$$\mathcal{M}(u_n)\vec{c}_n = -\frac{2\lambda u_n^2}{\Delta^2} U' \vec{c}_n$$

so that

$$\vec{c}_n = -\frac{2\lambda u_n^2 \mathcal{M}^{-1}(u_n)}{\Delta^2} U' \vec{c}_n. \quad (14)$$

The spectral representation of $\mathcal{M}^{-1}$ is given by

$$\mathcal{M}^{-1}(u_n) = \sum_{l=1}^{4M} \frac{u_l^{(0)} \vec{c}_l^{(0)} \vec{c}_l^{(0)T}}{2(1 - u_l^{(0)4})(u_l^{(0)} - u_n)}.$$

[See Eq. (59) in Ref. [8].] Using the relations

$$\sum_{l=1}^{4M} \frac{u_l^{(0)p} \vec{c}_l^{(0)} \vec{c}_l^{(0)T}}{1 - u_l^{(0)4}} = 0 \quad (p = 1,2) \quad (15)$$

[see Eqs. (51) and (52) in Ref. [8]], we have

$$u_n^2 \mathcal{M}^{-1}(u_n) = \sum_{l=1}^{4M} \frac{u_l^{(0)3} \vec{c}_l^{(0)} \vec{c}_l^{(0)T}}{2(1 - u_l^{(0)4})(u_l^{(0)} - u_n)}. \quad (16)$$

Substituting this into Eq. (14) and comparing both hand sides power by power for λ, and then using Eqs. (12) and (13), we have

$$\lambda^0 : \vec{c}_n^{(0)} = \frac{1}{\Delta^2} \frac{u_n^{(0)3} \vec{c}_n^{(0)} \vec{c}_n^{(0)T}}{(1 - u_n^{(0)4}) u_n^{(1)}} U' \vec{c}_n^{(0)} = \vec{c}_n^{(0)}, \quad (17)$$

$$\lambda^1 : \vec{c}_n^{(1)} = \frac{1}{\Delta^2} \sum_{l \neq n}^{4M} \frac{u_l^{(0)3} W'_{ln}}{(1 - u_l^{(0)4})(u_n^{(0)} - u_l^{(0)})} \vec{c}_l^{(0)}$$

$$- \frac{u_n^{(0)4} + 3}{2u_n^{(0)}(1 - u_n^{(0)4})} u_n^{(1)} \vec{c}_n^{(0)}$$

$$= \frac{1}{\Delta^2} \sum_{l \neq n}^{4M} \frac{u_l^{(0)3} W'_{ln}}{(1 - u_l^{(0)4})(u_n^{(0)} - u_l^{(0)})} \vec{c}_l^{(0)}$$

$$+ \frac{W'_{nn}}{2}\left(\frac{1}{k_{1n}^{(0)2}} + \frac{1}{k_{2n}^{(0)2}} - \frac{1}{k_{1n}^{(0)} k_{2n}^{(0)}} \right)\vec{c}_n^{(0)}, \quad (18)$$

where

$$W'_{mn} = \vec{c}_m^{(0)T} U' \vec{c}_n^{(0)}$$

and, as before,

$$k_{1n}^{(0)} = i\Delta[u_n^{(0)} - (u_n^{(0)})^{-1}], \quad k_{2n}^{(0)} = i\Delta[u_n^{(0)} - (u_n^{(0)})^{-1}].$$

Let us note that for $\vec{c}_n^{(1)}$, there is a term on top of the summation, which is made absent in a standard perturbation theory because the normalization is unchanged in so far as this term is purely imaginary under the standard orthogonality relation. This freedom is not warranted in the present case.

Finally, we have the perturbation formulas for the two-threshold SPS,

$$E_n^{(1)} = \vec{c}_n^{(0)T} U' \vec{c}_n^{(0)}, \quad (19)$$

$$E_n^{(2)} = \vec{c}_n^{(0)T} U' \vec{c}_n^{(1)} = \frac{1}{\Delta^2} \sum_{l \neq n}^{4M} \frac{u_l^{(0)3} W'^2_{ln}}{(1 - u_l^{(0)4})(u_n^{(0)} - u_l^{(0)})}$$

$$+ \frac{W'^2_{nn}}{2}\left(\frac{1}{k_{1n}^{(0)2}} + \frac{1}{k_{2n}^{(0)2}} - \frac{1}{k_{1n}^{(0)} k_{2n}^{(0)}} \right). \quad (20)$$

In the same manner, it is possible to go on to the third- and higher-order formulas, and to examine how the complex eigenvalues converge to the exact ones. However, as seen from the unfortunate flaw in More's study, a careful and thorough assessment of each order of the expansion is absolutely necessary due to the manifestation of nonstandard terms. Therefore we forego this task as well as the derivation of partial widths by the perturbation theory at present.

B. One-threshold case as a degenerate limit

It is important to clarify the relationship between one- and two-threshold cases. In the following, we prove that perturbation formulas for the one-threshold case are obtained when we implement a limit of $v_2 \rightarrow v_1$. In this limit, the following scaling clarified in Ref. [8]:

$$A \rightarrow \frac{1}{\Delta^2}\tilde{A}, \quad B^\pm \rightarrow \frac{1}{\Delta}\tilde{B}^\pm, \quad u \rightarrow \frac{-\kappa}{\Delta} \quad (21)$$

reduces the two-threshold TSE to a one-threshold one, namely,

$$(\tilde{A} + \kappa\tilde{B} + \kappa^2 I_M)\vec{c} = 0, \tag{22}$$

where

$$\tilde{A} = 2 \begin{pmatrix} \tilde{H}^{(1)} - \bar{v}I_M & U^{(12)} & \cdots & U^{(1q)} \\ U^{(12)} & \tilde{H}^{(2)} - \bar{v}I_M & \cdots & U^{(2q)} \\ \vdots & \vdots & \ddots & \vdots \\ U^{(1q)} & U^{(2q)} & \cdots & \tilde{H}^{(q)} - \bar{v}I_M \end{pmatrix},$$

and

$$\tilde{B} = \begin{pmatrix} 1 & \cdots & q\text{th block} \\ -L & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & -L \end{pmatrix}.$$

and $\kappa = ik_1 = ik_2$. This scaling corresponds to the solution $k_1 = k_2$ in Eq. (3) when $v_1 \to v_2$. Note that the solution $k_1 = -k_2$ in Eq. (3) is unphysical since the degenerate threshold here means the equivalence of asymptotic wave functions in this limit.

Thus the scaling leads us to the perturbation formulas for the one-threshold case, namely

$$\vec{c}_n^{(1)} = \sum_{l \neq n}^{2M} \frac{W'_{ln}}{k_l^{(0)}(k_n^{(0)} - k_l^{(0)})} \vec{c}_l^{(0)} + \frac{W'_{nn}}{2k_n^{(0)2}} \vec{c}_n^{(0)},$$

$$E_n^{(1)} = W'_{nn} = \vec{c}_n^{(0)T} V' \vec{c}_n^{(0)},$$

$$E_n^{(2)} = \sum_{l \neq n}^{2M} \frac{W'^2_{ln}}{k_l^{(0)}(k_n^{(0)} - k_l^{(0)})} + \frac{W'^2_{nn}}{2k_n^{(0)2}}.$$

Note that the summation runs over the branch of $k_1 = k_2$, that is only over a half of the full nondegenerate space. These correspond to the SPS representation of More's formulas [10]. Our expressions for the first-order eigenvector and for the second-order eigenenergy are different from his [11]. The origin of the discrepancy has been traced to an algebraic error in More's derivation of the first-order wave function. (One necessary term is unfortunately dropped during his derivation.) As a result of this, an extra term is restored in either formula. Here, one important difference from the standard perturbation theory is that no Hermitian conjugates appear in these formulas. This might suggest at first that there would remain phase ambiguity. However, any *ad hoc* additive phase would instead mar the orthogonality relation, that is, what is the relative phase in the standard theory is fixed in the SPS theory, thus leaving no ambiguity with the phase of eigenfunctions. It is thus worthwhile to see the consistency of the orthonormality relation and the Siegert boundary condition for the particular case of $\vec{c}_n^{(1)}$. This verification is worked out in the Appendix.

C. A model problem

Let us present an example of the perturbation theory for the two-threshold case. We revisit the two-channel model potential with two thresholds that is taken up in Ref. [8], i.e.,
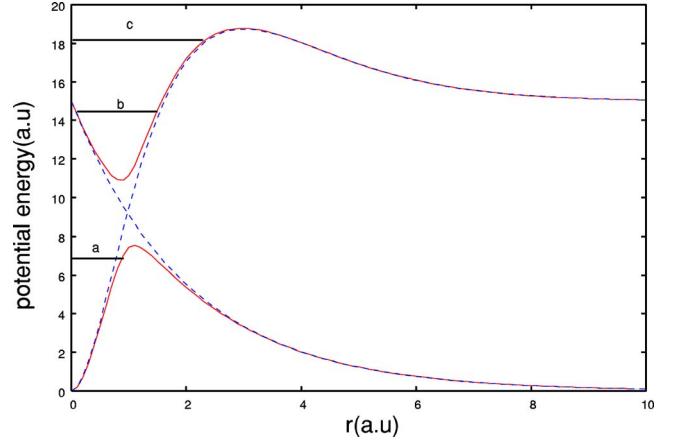

FIG. 1. (Color online) Broken lines: Diagonal elements of the potential matrix in Eq. (23). Solid lines: adiabatic potential energies. This system supports three resonances: shape type (a) in channel 1, Feshbach type (b), and shape type (c) in channel 2.

$$V(r) = \begin{pmatrix} 15e^{-0.5r} & 5re^{-r} \\ 5re^{-r} & 15(r^2 - r - 1)e^{-r} + 15 \end{pmatrix}. \tag{23}$$

Here, the threshold energies of the first and second channels are 0 and 15, respectively. The potential $V(r)$ supports three resonances. The adiabatic potential energy curve of the first channel supports one shape type resonance (a) while the other channel supports one Feshbach type (b) and one shape type (c) resonance. These resonances are depicted in Fig. 1. We carried out the diagonalization of the TSE, Eq. (6), using the discrete variable representation (DVR) functions as a basis set. The calculated resonance energies and widths with different numbers of the basis functions are given in Table I. Let us call these results *direct numerical solutions*. To implement perturbation calculations, we separate $V(r)$ into

$$V(r) = V_0(r) + V'(r),$$

where

$$V_0(r) = \begin{pmatrix} 15e^{-0.5r} & 4re^{-r} \\ 4re^{-r} & 15(r^2 - r - 1)e^{-r} + 15 \end{pmatrix},$$

$$V'(r) = \begin{pmatrix} 0 & re^{-r} \\ re^{-r} & 0 \end{pmatrix}.$$

We regard V_0 as the unperturbed potential energy and V' as the perturbation potential energy. We calculate perturbation energies using the unperturbed solutions of TSE for the same box size $a = 50$ as in Ref. [8]. Table I shows the results of first- and second-order perturbation calculations, and Figs. 2–4 epict how the numerical solutions converge in the complex plane. In the present model problem, the first-order resonance energy agrees with the direct numerical solutions to about two to four digits while the width agrees to about two to three digits. And the second-oder resonance energy agrees to about three to five digits while the width agrees to about one to three digits. An important fact which we must remark is that the resonance energy and width do not appear to converge in pace. For instance, the width of resonance "c"

TABLE I. Columns Re, Im, D, and N represent the real and imaginary parts of resonance energies, error variance in the complex plane, and the dimension of the DVR basis set, respectively.

	Resonance a			Resonance b			Resonance c		
N	Re	Im	D	Re	Im	D	Re	Im	D
					$E^{(0)}$				
100	7.13731291	−0.04777819	0.17022398	14.36514823	−0.00441589	0.08759123	18.25940438	−0.04709964	0.02402711
300	7.13739307	−0.04774929	0.17034758	14.36548638	−0.00426431	0.08762023	18.26200618	−0.04826379	0.02526594
500	7.13739307	−0.04774929	0.17034758	14.36548638	−0.00426431	0.08762023	18.26200618	−0.04826379	0.02526594
700	7.13739307	−0.04774929	0.17034758	14.36548638	−0.00426431	0.08762023	18.26200619	−0.04826379	0.02526594
					$E^{(0)}+E^{(1)}$				
100	6.98368137	−0.06730063	0.01543038	14.44177638	−0.00607880	0.01094681	18.27770236	−0.05762106	0.00327772
300	6.98382603	−0.06744164	0.01560641	14.44219720	−0.00577079	0.01089678	18.28142974	−0.05926301	0.00330703
500	6.98382602	−0.06744165	0.01560641	14.44219720	−0.00577079	0.01089678	18.28142974	−0.05926301	0.00330703
700	6.98382603	−0.06744162	0.01560643	14.44219720	−0.00577079	0.01089678	18.28142974	−0.05926301	0.00330702
					$E^{(0)}+E^{(1)}+E^{(2)}$				
100	6.96760487	−0.06783608	0.00067084	14.45258871	−0.00611007	0.00013451	18.28074487	−0.05788235	0.00031413
300	6.96755505	−0.06807440	0.00074684	14.45297412	−0.00575530	0.00011988	18.28452186	−0.05952953	0.00031773
500	6.96755905	−0.06807406	0.00074312	14.45297384	−0.00575631	0.00012019	18.28452397	−0.05952538	0.00031324
700	6.96756395	−0.06807313	0.00073832	14.45297366	−0.00575513	0.00012033	18.28452412	−0.05952393	0.00031208
					E (Direct numerical solution)				
100	6.96825547	−0.06767254		14.45272315	−0.00610584		18.28097965	−0.05767365	
300	6.96822245	−0.06773922		14.45309397	−0.00575250		18.28473661	−0.05929537	
500	6.96822245	−0.06773921		14.45309397	−0.00575250		18.28473661	−0.05929537	
700	6.96822244	−0.06773923		14.45309397	−0.00575250		18.28473661	−0.05929536	

evaluated by the second-order perturbation theory appears less accurate than the first-order one while the resonance energy appears to have improved. The seeming deterioration of the width is a little overwhelming, all the more so for the improvement of the resonance energy. Nonetheless, the distance between the second-order result and the direct numerical one becomes rather small (see Fig. 4) in the complex plane, that is, in the Siegert state perturbation theory the convergence is to be measured with respect to the variance

$$D = \left\| E - \sum_n \lambda^n E^{(n)} \right\| \tag{24}$$

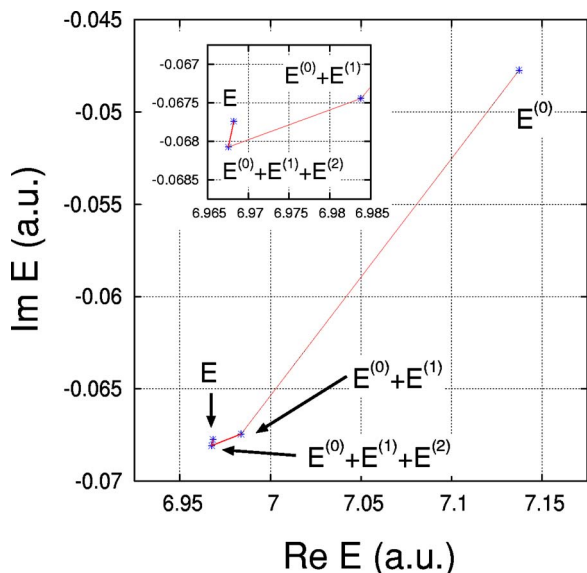rather than with respect to the real and imaginary parts of the sum, individually.

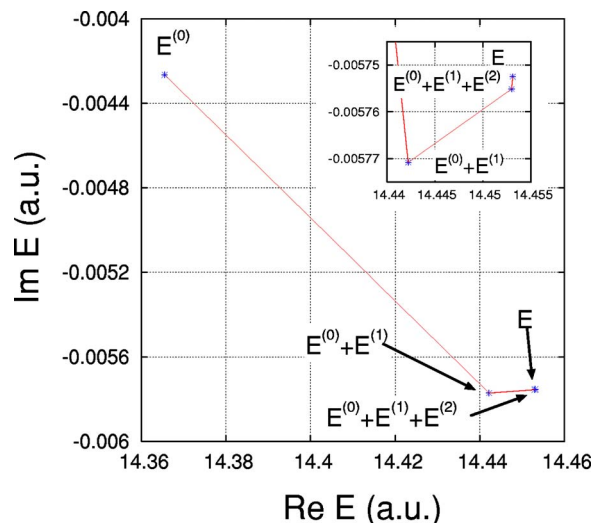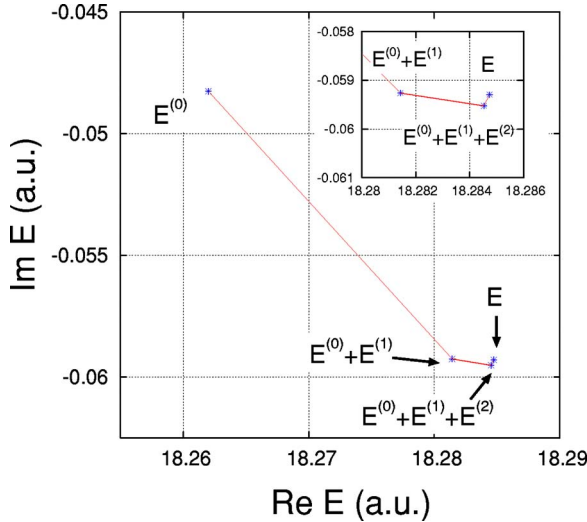
FIG. 2. (Color online) Complex energies for resonance a.

FIG. 3. (Color online) Complex energies for resonance b.

FIG. 4. (Color online) Complex energies for resonance c.

IV. CONCLUSIONS

In this paper we formulated one- and two-threshold SPSPT. The unusual orthonormality relationship of the SPSs results in somewhat nontrivial additional terms in SPSPT, and also it determines the phase of the perturbation wave function. In the degenerate threshold case, the one-threshold SPSPT formulas are obtained by appropriate scaling, and we also obtained an up-to-date correction to More's theory. The numerical calculations show how the perturbation results converge. The convergence is achieved in the sense of the variance, Eq. (24), but not the resonance energy and width independently.

It is of interest to speculate on possible uses of SPSPT. One immediate application would be to the manipulation of Siegert poles. The shadow poles located near the physical sheet may be transformed to physical resonances by an appropriate perturbation. We leave issues such as this for a future task.

APPENDIX: CONSISTENCY WITH ORTHONORMALITY RELATIONSHIP AND SIEGERT BOUNDARY CONDITION IN FIRST ORDER

Here, we prove that the first-order wave function satisfies the orthonormality relationship and the Siegert boundary condition consistently. First of all, we expand

$$\vec{c}_n^T\left(I_N + \frac{1}{\kappa_n + \kappa_m}B\right)\vec{c}_m = \delta_{mn}, \tag{A1}$$

into perturbation series, and compare both sides power by power for λ. The first-order equation shows

$$\vec{c}_n^{(0)T}\left(I_N - \frac{i}{k_n^{(0)} + k_m^{(0)}}B\right)\vec{c}_m^{(1)} + c_n^{(0)T}\frac{i(k_n^{(1)} + k_m^{(1)})}{(k_n^{(0)} + k_m^{(0)})^2}B\vec{c}_m^{(0)}$$

$$+ \vec{c}_n^{(1)T}\left(I_N - \frac{i}{k_n^{(0)} + k_m^{(0)}}B\right)c_m^{(0)} = 0. \tag{A2}$$

And each term of the above equation reduces to

$$\text{(1st term)} = \sum_{l\neq m}^{2N}\frac{W_{lm}'\vec{c}_n^{(0)T}\vec{c}_l^{(0)}}{k_l^{(0)}(k_n^{(0)} + k_m^{(0)})} + \frac{2W_{nm}'}{(k_n^{(0)} + k_m^{(0)})(k_m^{(0)} - k_n^{(0)})}$$

$$+ \frac{W_{mm}'}{2k_m^{(0)2}}\delta_{nm},$$

$$\text{(2nd term)} = \frac{W_{nn}'/k_n^{(0)} + W_{mm}'/k_m^{(0)}}{k_n^{(0)} + k_m^{(0)}}(\vec{c}_n^{(0)T}\vec{c}_m^{(0)} - \delta_{mn})$$

and

$$\text{(3rd term)} = \sum_{l\neq n}^{2N}\frac{W_{ln}'\vec{c}_l^{(0)T}\vec{c}_m^{(0)}}{k_l^{(0)}(k_n^{(0)} + k_m^{(0)})} - \frac{2W_{nm}'}{(k_n^{(0)} + k_m^{(0)})(k_m^{(0)} - k_n^{(0)})}$$

$$+ \frac{W_{nn}'}{2k_n^{(0)2}}\delta_{nm}.$$

Hence the left-hand side of Eq. (A2) reduces to

[left-hand side (A2)]

$$= \sum_{l=1}^{2N}\frac{W_{lm}'\vec{c}_n^{(0)T}\vec{c}_l^{(0)}}{k_l^{(0)}(k_n^{(0)} + k_m^{(0)})} + \sum_{l=1}^{2N}\frac{W_{ln}'\vec{c}_l^{(0)T}\vec{c}_m^{(0)}}{k_l^{(0)}(k_n^{(0)} + k_m^{(0)})}$$

$$+ \frac{W_{mm}'}{k_m^{(0)}}\left(\frac{1}{2k_m^{(0)}} - \frac{1}{k_n^{(0)} + k_m^{(0)}}\right)\delta_{mn}$$

$$+ \frac{W_{mm}'}{k_m^{(0)}}\left(\frac{1}{2k_m^{(0)}} - \frac{1}{k_n^{(0)} + k_m^{(0)}}\right)\delta_{mn}$$

$$= \frac{1}{k_n^{(0)} + k_m^{(0)}}\left(\sum_{l=1}^{2N}\frac{W_{lm}'\vec{c}_n^{(0)T}\vec{c}_l^{(0)}}{k_l^{(0)}} + \sum_{l=1}^{2N}\frac{W_{ln}'\vec{c}_l^{(0)T}\vec{c}_m^{(0)}}{k_l^{(0)}}\right).$$

By using a SPS sum rule,

$$\sum_{l=1}^{2N}\frac{1}{k_l^{(0)}}\vec{c}_l^{(0)}\vec{c}_l^{(0)T} = 0,$$

we obtain

$$\sum_{l=1}^{2N}\frac{1}{k_l^{(0)}}W_{lm}'\vec{c}_n^{(0)T}\vec{c}_l^{(0)} = \vec{c}_n^{(0)T}\left(\sum_{l=1}^{2N}\frac{1}{k_l^{(0)}}c_l^{(0)}\vec{c}_l^{(0)T}\right)U'\vec{c}_m^{(0)} = 0$$

and

$$\sum_{l=1}^{2N}\frac{1}{k_l^{(0)}}W_{ln}'\vec{c}_l^{(0)T}\vec{c}_m^{(0)} = \sum_{l=1}^{2N}\frac{1}{k_l^{(0)}}W_{nl}'\vec{c}_l^{(0)T}\vec{c}_m^{(0)}$$

$$= \vec{c}_n^{(0)T}U'\left(\sum_{l=1}^{2N}\frac{1}{k_l^{(0)}}\vec{c}_l^{(0)}\vec{c}_l^{(0)T}\right)\vec{c}_m^{(0)} = 0.$$

Therefore the first-order wave function is consistent with the orthonormality relationship.

Next, let us consider the Siegert boundary condition. We expand the Siegert boundary condition and compare both sides power by power for λ. The first-order equation shows

$$\left(\frac{d}{dr} - ik_n^{(0)}\right)\phi_n^{(0)} - ik_n^{(1)}\phi_n^{(0)}\bigg|_{r=a} = 0.$$

Then by using the coordinate representation of the SPS sum rule, namely

$$\sum_{l=1}^{2N} \frac{1}{k_l^{(0)}}\phi_l^{(0)}(r)\phi_l^{(0)}(r') = 0,$$

we get

$$\left(\frac{d}{dr} - ik_n^{(0)}\right)\phi_n^{(0)}\bigg|_{r=a} = \sum_{l\neq n}^{2N} \frac{W_{ln}'}{k_l^{(0)}(k_n^{(0)} - k_l^{(0)})}\left(\frac{d\phi_l^{(0)}}{dr}\right)_{r=a}$$

$$- k_n^{(0)}\sum_{l\neq n}^{2N} \frac{W_{ln}'}{k_l^{(0)}(k_n^{(0)} - k_l^{(0)})}\phi_l^{(0)}(a)$$

$$= -i\sum_{l\neq n}^{2N} \frac{1}{k_l^{(0)}}W_{ln}'\phi_l^{(0)}(a)$$

$$= -i\sum_{l=1}^{2N} \frac{1}{k_l^{(0)}}W_{ln}'\phi_l^{(0)}(a) + i\frac{W_{nn}'}{k_n^{(0)}}\phi_n^{(0)}(a)$$

$$= -i\int_0^a \left(\sum_{l=1}^{2N} \frac{1}{k_l^{(0)}}\phi_l^{(0)}(a)\phi_l^{(0)}\right)U'\phi_n^{(0)}dr$$

$$+ ik_n^{(1)}\phi_n^{(0)}(a) = ik_n^{(1)}\phi_n^{(0)}(a).$$

Hence the first-order wave function is consistent with the Siegert boundary condition.

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