Siegert Pseudo-States as a Universal Tool: Resonances, S Matrix, Green Function

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The Siegert states have long been recognized as a potentially powerful tool in the formal scattering theory. Here we propose an efficient method to implement this power in practice. Our method yields bound states, complex-energy resonances, and scattering wave functions, i.e., a complete solution of the Schrödinger equation. We also obtain a representation of the Green function suitable for a variety of applications. The method is demonstrated by realistic examples of the eep and $dt\mu$ three-body Coulomb systems. [S0031-9007(97)03930-6]

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In 1939, in search of a formal derivation of the Breit-Wigner resonance formula, Siegert introduced [1] a class of solutions to the Schrödinger equation which now bear his name. The Siegert states satisfy outgoing wave boundary conditions, and, for the simplest generic scattering problem, they are defined by

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

$$\phi(r)|_{r=0} = 0, \quad \left(\frac{d}{dr} - ik\right)\phi(r)\Big|_{r\to\infty} = 0. \quad \text{(1b)}$$

These equations can be satisfied simultaneously only for a discrete set of generally complex momenta k_n; thus one should consider Eqs. (1a) and (1b) as an eigenvalue problem defining k_n and corresponding eigenfunctions $\phi_n(r)$. The eigenvalues k_n coincide with the poles of the S matrix in the complex k plane. Pure imaginary k_n with $\mathrm{Im}(k_n) > 0$ represent bound states of the system. Those lying close to the real k axis correspond to resonances. Others, though not observable directly, complement the set and, at least for finite range potentials, suffice to determine the S matrix in the entire k plane [2].

The significance of Siegert states within a general formalism of the scattering theory and their potential usefulness for computational implementations stem from the fact that they provide a possibility of unified description of bound states, resonances, and continuum spectrum in terms of a purely discrete set of states. For example, by virtue of the Mittag-Leffler expansion theorem (if applicable), one can construct the Green function simply in the form of a sum over the Siegert states, avoiding the annoying integral over the continuum [3]. Of course, there is a price to be paid for such a discretization. First, one must move away from the real energy axis to the complex energy plane. Second, for practical applications one must solve the problem of exponential divergence of $\phi_n(r)$ at $r \to \infty$, say, for instance, by making the radial variable r also complex as in the complex rotation method [4]. However, the most important point is that in order to achieve the completeness required for representing the continuum, one has to generate not just one or a few but *many* solutions of Eqs. (1a) and (1b). This causes an essential practical difficulty, because the nonlinearity of Eqs. (1a) and (1b) with respect to the eigenvalue k prohibits a direct application of the variational methods, which renders the problem tractable only by means of an iterative procedure. In fact, this difficulty was restricting the power of Siegert states to studying only individual resonances [5].

Here, we define Siegert *pseudo*-states by applying the asymptotic boundary condition (1b) at a finite distance $r_{\max}$. This eliminates the problem of exponential divergence of $\phi_n(r)$ and makes our method practical without going into the complex r. We propose an efficient method of constructing a large number of solutions to a thus modified eigenvalue problem (1a) and (1b), where the computational labor is reduced essentially to that of a single matrix diagonalization. The eigenvalues k_n, stable against variations of $r_{\max}$, represent bound states or true resonances. All others are dependent on $r_{\max}$ and serve to represent the continuum. We derive a representation of the Green function in the region $r < r_{\max}$ in terms of the Siegert pseudo-states which, with the aid of the Green formula, yield the scattering wave function and the S matrix, i.e., a complete solution of the scattering problem, though to the extent determined by the finiteness of $r_{\max}$.

The mathematical foundation of our method can be simply explained as follows. Consider a *quadratic* algebraic eigenvalue problem,

$$[\mathbf{A} + \lambda\mathbf{B} + \lambda^2\mathbf{I}]c = 0, \quad (2)$$

where $\mathbf{A}$ and $\mathbf{B}$ are square matrices, $\mathbf{I}$ is the unit matrix, and λ and c are the eigenvalue and the eigenvector to be found, respectively. If a given pair of λ and c satisfies Eq. (2), then the same λ and the vector of doubled dimension $(c^T, \lambda c^T)^T$, where T stands for transpose, satisfy the ordinary *linear* eigenvalue problem

$$\begin{pmatrix} \mathbf{0} & \mathbf{I} \\ -\mathbf{A} & -\mathbf{B} \end{pmatrix}\begin{pmatrix} c \\ \lambda c \end{pmatrix} = \lambda\begin{pmatrix} c \\ \lambda c \end{pmatrix}. \quad (3)$$

This equation is equivalent to Eq. (2). Such *linearization* of the problem by means of doubling its dimension is similar to the well-known procedure of reducing a second order differential equation to a set of two first

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order equations. This technique is easily extendable to polynomial eigenvalue problems of an arbitrary order [6]. Equation (3) can be rewritten in the symmetric form,

$$\begin{pmatrix} -\mathbf{A} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \begin{pmatrix} c \\ \lambda c \end{pmatrix} = \lambda \begin{pmatrix} \mathbf{B} & \mathbf{I} \\ \mathbf{I} & \mathbf{0} \end{pmatrix} \begin{pmatrix} c \\ \lambda c \end{pmatrix}, \tag{4}$$

which is more convenient for deriving some general relations. In particular, for symmetric matrices $\mathbf{A}$ and $\mathbf{B}$, the eigenvectors of Eq. (4) are orthogonal with respect to the following inner product:

$$(\, c^{(n)T} \quad \lambda_n c^{(n)T} \,) \begin{pmatrix} \mathbf{B} & \mathbf{I} \\ \mathbf{I} & \mathbf{0} \end{pmatrix} \begin{pmatrix} c^{(m)} \\ \lambda_m c^{(m)} \end{pmatrix} = 2\lambda_n \delta_{nm} . \tag{5}$$

Here we have fixed the normalization constant convenient for further applications. The set of eigenvectors is complete in the space of doubled dimension, namely,

$$\sum_n \frac{1}{2\lambda_n} \begin{pmatrix} c^{(n)} \\ \lambda_n c^{(n)} \end{pmatrix} (\, c^{(n)T} \quad \lambda_n c^{(n)T} \,) = \begin{pmatrix} \mathbf{0} & \mathbf{I} \\ \mathbf{I} & -\mathbf{B} \end{pmatrix} . \tag{6}$$

An equation of the type (2) arises when one seeks solutions of Eqs. (1a) and (1b) as an expansion in terms of some basis. Here $\lambda = ik$, $\mathbf{A}$ stands for the Hamiltonian matrix, and the linear term in λ arises from the boundary conditions (1b) cast in the form of a Bloch operator [7]. We skip discussing the one-dimensional case based on Eqs. (1a) and (1b) and demonstrate our method by nontrivial realistic examples of resonances and scattering in three-body Coulomb systems. We use mass-scaled hyperspherical coordinates $\mathbf{R} = (R, \Omega)$, where Ω collectively denotes a set of angular variables. To utilize the smoothness of the Coulomb systems with respect to the hyperradius R, as discussed in [8], we consider the wave function multiplied by $R^{3/2}$. Then the Siegert pseudo-states are defined by

$$[H(\mathbf{R}) - E\rho(R)]\phi(\mathbf{R}) = 0 , \quad E = E_0 + \frac{1}{2}k^2, \tag{7a}$$

$$\phi(\mathbf{R})|_{R\to 0} \propto R^{3/2}, \qquad \left(\frac{\partial}{\partial R} - \frac{b}{R} - ik\right)\phi(\mathbf{R})\,\Big|_{R=R\max} = 0 , \tag{7b}$$

where (for more details and notation, see [8])

$$H(\mathbf{R}) = K(R) + H_{\rm ad}(\Omega; R) , \tag{8}$$

$$K(R) = -\frac{1}{2}\,\frac{\partial}{\partial R}\,\rho(R)\,\frac{\partial}{\partial R} + \frac{15}{8} , \qquad \rho(R) = R^2, \tag{9}$$

$$H_{\rm ad}(\Omega; R) = \frac{1}{2}\,\Lambda^2 + RC(\Omega) . \tag{10}$$

Two additional quantities, E_0 and b, are introduced in Eqs. (7a) and (7b) in comparison to Eqs. (1a) and (1b). We choose E_0 to be the lowest continuum threshold, e.g., $E_0 = -0.5m_p/(1 + m_p)$ a.u. for the eep system, and $b = 3/2 - 5/2 = -1$ for the present case of six-dimensional spherical wave.

We seek the solutions of Eqs. (7a) and (7b) in the form of the slow/smooth variable discretization (SVD) expansion [8]

$$\phi(\mathbf{R}) = \sum_{j=1}^{N} \sum_{\mu}^{M} s_{j\mu}\, \pi_j(R) \Phi_\mu(\Omega; R_j) . \tag{11}$$

Here $\pi_j(R)$ are the discrete variable representation (DVR) basis functions constructed from the Jacobi polynomials $P_n^{(0,3)}$, $\Phi_\mu(\Omega; R_j)$ are the hyperspherical adiabatic channel functions taken at the DVR quadrature points R_j, and $s_{j\mu}$ are the coefficients to be found. The channel functions have been calculated using the hyperspherical elliptic coordinates introduced in [9]. SVD provides a very powerful method for treating nonadiabatic couplings [8]. The whole computational scheme is highly efficient, and for a variety of three-body Coulomb systems it has been shown to yield an accuracy comparable with the best available variational results [8–10].

Substituting (11) into Eqs. (7a) and (7b) and introducing a new vector $c = \boldsymbol{\rho}^{1/2} s$, where $\boldsymbol{\rho}$ is the SVD matrix for $\rho(R)$, we obtain an algebraic equation of the type (2) with real symmetric matrices $\mathbf{A}$ and $\mathbf{B}$. By transforming it to the form (3), we construct a set of $2 \times N \times M$ Siegert pseudo-states $\phi_n(\mathbf{R})$. From Eq. (5) it follows that the functions $\phi_n(\mathbf{R})$ satisfy the following orthogonality condition:

$$\int_0^{R\max} dR\rho(R) \int d\Omega\, \phi_n(\mathbf{R})\phi_m(\mathbf{R}) - \frac{\rho(R_{\rm max})}{i(k_n + k_m)} \int d\Omega\, \phi_n(\mathbf{R})\phi_m(\mathbf{R})|_{R=R\max} = \delta_{nm} . \tag{12}$$

From (6), assuming the completeness of our SVD basis within the hypersphere $R < R_{\rm max}$ (which is the case for $N, M \to \infty$), we obtain the relations

$$\sum_n \frac{1}{ik_n}\, \phi_n(\mathbf{R})\phi_n(\mathbf{R}') = 0 , \tag{13}$$

$$\sum_n \phi_n(\mathbf{R})\phi_n(\mathbf{R}') = \frac{2}{\rho(R)}\, \delta(R - R')\delta(\Omega - \Omega') , \tag{14}$$

$$\sum_n ik_n \phi_n(\mathbf{R})\phi_n(\mathbf{R}') = \frac{2}{\rho(R_{\rm max})}\, \delta(R - R_{\rm max}) \times \delta(R' - R_{\rm max})\delta(\Omega - \Omega') . \tag{15}$$

Equations (13) and (14) are essential for deriving the following representation of the Green function:

$$G(\mathbf{R}, \mathbf{R}'; E) = \sum_n \frac{\phi_n(\mathbf{R})\phi_n(\mathbf{R}')}{k_n(k_n - k)} . \tag{16}$$

Finally, using the Green formula [11] and Eqs. (16) and (7b), we express a solution of the Schrödinger equation $\psi(\mathbf{R})$ in terms of its values on the hypersphere $R = R_{\rm max}$,

$$\psi(\mathbf{R}) = \frac{1}{2}\,\rho(R_{\rm max}) \int d\Omega' G(\mathbf{R}, \mathbf{R}'; E) \times \left(\frac{\partial}{\partial R'} - \frac{b}{R'} - ik\right)\psi(\mathbf{R}')\,\Big|_{R'=R\max} . \tag{17}$$

Before discussing numerical results, let us comment on Eqs. (13)–(16). Relations similar to (13) and (14) were known previously [12]. Equation (16) was given in [3]. However, our method of derivation is quite different. In order to prove Eq. (16), previous authors (see, e.g., [3]) had to assume some analytical properties of $G(\mathbf{R}, \mathbf{R}'; E)$ in the complex k plane, and then had to resort to the Mittag-Leffler expansion theorem. Instead, in our method, Eqs. (13)–(16) follow directly from Eq. (6) for a complete basis. Of course, there is a link between the two approaches: Our method explicitly treats a cutoff potential problem for which the required analytical properties are fulfilled.

We now consider bound states and resonances. In both cases the problem reduces to finding such eigenvalues of Eqs. (7a) and (7b) that are stable against an increase of $R_{\max}$. Here, we report our results for the eep and $dt\mu$ systems for zero total angular momentum. Instead of the complex momenta k_n, we look into the distribution of the Siegert eigenenergies $E_n = E_0 + k_n^2/2$ in the complex E plane. Our computational strategy is as follows. For a given $R_{\max}$, by increasing N and M we achieve convergence for some representative group of eigenvalues. For higher roots, which lie far on the right of the continuum threshold E_0 and correspond to more rapidly oscillating wave functions, the convergence is slower. Thus we obtain the basis-independent roots. Then we increase $R_{\max}$, repeat the procedure, and select those roots which are stable. Figure 1 illustrates a distribution of the basis-independent roots for eep. Its qualitative features are the same for other studied systems. Real roots appear only on the left of E_0; they represent bound $[\mathrm{Im}(k_n) > 0]$ or antibound $[\mathrm{Im}(k_n) < 0]$ states. We found that the bound and antibound roots appear in pairs which rapidly coalesce in the E plane with the increase of $R_{\max}$. In addition, there is one unpaired real root closest to E_0. For eep and $dt\mu$ it corresponds to an antibound state and keeps approaching E_0 from the left in the interval of $R_{\max}$ considered here. All other roots are complex and appear in conjugate pairs. Most of them lie along the parabolalike branches with apexes located on the real axis at the thresholds of different channels. These roots essentially depend on $R_{\max}$ and represent discretized continua for the corresponding channels. With the increase of $R_{\max}$, new continuum branches separate out and become clearly visible. Far on the right in Fig. 1 these branches obey the law $\mathrm{Re}E_n \sim (\mathrm{Im}E_n)^2$, valid for arbitrary cutoff potentials [2]. Resonances which are stable against the increase of $R_{\max}$ appear as precursors to the continuum branches. All these features can be seen in Fig. 1.

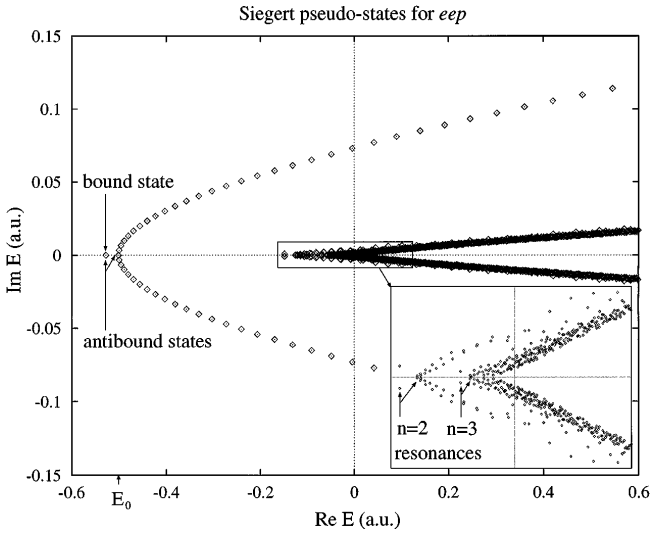

FIG. 1. Basis-independent Siegert eigenenergies for eep calculated for $R_{\max} = 70$.

From the above discussion it can be seen that the parameter E_0 plays an important role in our formulation, setting the origin of the branch cut along the real axis in Fig. 1. Here we chose E_0 to be the lowest continuum threshold. The threshold energies for the higher channels, though they appear effectively in Fig. 1, are not included in the formulation explicitly. At this stage, it is not clear how our method accounts for the multisheet structure of the complex energy surface discussed in [13], and further studies in this direction are required.

Tables I and II present our results. Masses of the particles were taken to be the same as in [8]. The converged results are obtained with $(N, M, R_{\max}) = (60, 30, 50)$ and $(80, 40, 150)$ for eep and $dt\mu$, respectively. Good accuracy of the bound state energies verifies our numerical procedure. To confirm eligibility of the present method for calculating resonances, we considered the mandatory test example of the lowest $^1S^e$ resonance in eep. For the infinite proton mass, our results are in excellent agreement with other precision calculations. We also report results for the finite proton mass. For $dt\mu$, we investigated the three lowest resonances below the $t\mu(n = 2)$ threshold. Our results for the resonance energies are close to the best available variational calculations [19], and are somewhat better than the results of the complex rotation method [20,21]. However, our values for the resonance widths differ by an order of magnitude from that of [20] and [21] which, in turn, also quite disagree with each other. To clarify the situation, we thoroughly analyzed the convergence and found that for such narrow resonances the width is very sensitive to all the parameters N, M, and $R_{\max}$, and to achieve convergence for $dt\mu$ was more difficult than for eep. We also performed calculations for $dd\mu$, which is computationally

TABLE I. $L = 0$ bound states of eep (in a.u.) and $dt\mu$ (in μa.u.). E—present results, E_{var}—variational calculations.

System	v	$-E$	$-E_{\mathrm{var}}$	Ref.
eep, $m_p = \infty$	0	0.5277497	0.5277510	[14]
eep, $m_p = 1836.1527$	0	0.5274454	0.5274459	[14]
$dt\mu$	0	0.5385939	0.5385949	[15]
$dt\mu$	1	0.4880628	0.4880653	[15]

TABLE II. Lowest $L = 0$ resonances in eep (in a.u.) and $dt\mu$ (in μa.u.). Resonance positions and widths are related to Siegert eigenenergies by $E_n = E_{\rm res} - i\Gamma/2$. The numbers in parentheses give the uncertainty in the last digit quoted. Results of Refs. [16–18] are for $m_p = \infty$.

Method	v	$-E_{\rm res}$	$\Gamma \times 10^a$	Ref.
$eep(^1S^e)$, $a = 4$				
Kohn variational	0	0.148774	0.1735	[16]
Feshbach formalism	0	0.148777(2)	0.17334(7)	[17]
Complex rotation	0	0.148777(2)	0.1731(4)	[18]
Present, $m_p = \infty$	0	0.148776(1)	0.1734(1)	
Present, $m_p = 1836.1527$	0	0.148695(1)	0.1731(1)	
$dt\mu$, $a = 9$				
Variational	0	0.1591945		[19]
⋯	1	0.1453017		⋯
⋯	2	0.1345261		⋯
Complex rotation	0	0.1591910	0.64×10^4	[20]
⋯	1	0.1452625	0.14×10^5	⋯
⋯	2	0.1344000	0.20×10^6	⋯
Complex rotation	0	0.1591938	0.36×10^3	[21]
⋯	1	0.1452985	0.50×10^4	⋯
⋯	2	0.1344978	0.12×10^5	⋯
Present	0	0.1591938	0.354	
⋯	1	0.1453015	0.839	
⋯	2	0.1345291	1.15	

much simpler owing to its symmetry. For the lowest $^1S^e$ resonance in $dd\mu$ we obtained $E_{\rm res} = -0.1570989$ μa.u. and $\Gamma = 0.687 \times 10^{-9}$ μa.u. The same order of magnitude of Γ, as compared to the $dt\mu$ case, supports our confidence in the present results for $dt\mu$. We found *no* such stable root for $dt\mu$ as the resonance discussed in [22].

Finally, to demonstrate the power of our method as a universal tool for calculating not only bound states and resonances but also the S matrix, in Table III we report results for the $^1S^e$ elastic phase shift in the $e + ep$ system. These results were obtained using Eqs. (16) and (17). More details of these calculations will be given elsewhere.

In conclusion, we have proposed an efficient method for scattering calculations capable of describing the whole spectrum of the scattering phenomena. Formula (16) for the Green function implemented via Siegert pseudo-states may find wide applications for a variety of collision processes, including chemical reactions [25].

TABLE III. Elastic $^1S^e$ phase shift for $e + ep$. δ and δ_∞ are the present results for $m_p = 1836.1527$ and $m_p = \infty$, respectively. In both cases, k was determined by $E = E_0 + k^2/2$ with an appropriate E_0. Results of Refs. [23,24] are for $m_p = \infty$.

k (a.u.)	δ	δ_∞	Ref. [23]	Ref. [24]
0.1	2.5532	2.5535	2.553(1)	2.5561
0.2	2.0663	2.0668	2.0673(9)	2.0666
0.3	1.6961	1.6966	1.6964(5)	1.6963
0.4	1.4149	1.4154	1.4146(4)	1.4152
0.5	1.2004	1.2009	1.202(1)	1.2010
0.6	1.0404	1.0409	1.041(1)	1.0408
0.7	0.9303	0.9307	0.930(1)	0.9303
0.8	0.8873	0.8874	0.886(1)	0.887

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