Stable complex-rotation eigenvalues that correspond to no full resonances in scattering: Examples in positron scattering by the helium ion

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Hyperspherical close-coupling calculations for *S*- and *P*-wave positron scattering by He^+ ions produce no full resonances in the eigenphase sum $\delta(E)$ in the two regions of energy E where stable eigenvalues $E_r - i\Gamma/2$ with large Γ were found previously by the complex-rotation method (CRM); $\delta(E)$ increases only by one radian in the lower-E region, and even decreases almost monotonically in the higher-E region, implying time advance, rather than time delay, due to the collision. However, the peaks found in the trace of time-delay matrix, Tr $Q(E)$, are consistent with the CRM eigenvalues. This suggests that these eigenvalues indeed represent *S*-matrix poles in the complex-E plane, but that their effects on scattering are almost masked by the background δ due to the large Γ. This work uses a general relation Tr $Q(E)=2\hbar(d\delta/dE)$, proved here for *any functional form* of $\delta(E)$, and hence, both on and off resonance. This is a generalization of the well-known single-channel time-delay formula and of the multichannel formula proved previously for the Breit-Wigner resonance with a constant background *S* matrix.

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I. INTRODUCTION

The complex-coordinate rotation method (CRM) has proved to be powerful as a means to calculate simultaneously the positions and total widths of resonances in atomic physics [1,2]. With this method, the relative distance r_{ij} between each pair of particles i and j in the system is replaced by a complex variable $r_{ij}\exp(i\theta)$. Then, the Hamiltonian H is transformed into a non-Hermitian operator $H(\theta)$. The complex eigenvalues of a matrix of $H(\theta)$, constructed in terms of square-integrable (or L^2) basis functions $\{u_s\}$ with variable parameters, are found to be stable against the change in the rotation angle θ, in the size of the basis set, and in the nonlinear parameters in $\{u_s\}$, if these eigenvalues correspond to *S*-matrix poles $E_r - i\Gamma/2$ for $H(\theta=0)$ in the complex-energy plane. Each of them normally produces a resonance at the real energy E_r with a total width Γ, unless Γ is too large [1,2].

Ho [3] and Ho and Yan [4] used the CRM for the positron-involving three-body system $e^+e^-He^{2+}$, and found stable eigenvalues of $H(\theta)$ (for all partial waves $L\leqslant 6$) far from the real energy axis as well as close to it. In fact, the *S*-wave eigenvalues with large Γ had been suggested by the stabilization-method calculation of real eigenvalues of the matrix of $H(\theta=0)$, using L^2 basis functions [5]. In detailed *S*-wave *scattering* calculations with eigenphase-sum analysis by the present authors [6] and by Bransden *et al.* [7], however, no broad resonances occurred at the energies where the L^2-type calculations suggested *S*-matrix poles far from the real energy axis; Ref. [6] used the hyperspherical close-coupling (HSCC) method and Ref. [7] a least-squares method for the conventional close-coupling equations with pseudostates centered on the He^+ ion. No serious discrepancy exists between the CRM [3,4] and HSCC results [6,8] for the positions and total widths of the narrower resonances.

The present work sheds new light on the seemingly inconsistent results on the possible broad resonances found in the literature; they are shown to be consistent, in fact. We improve over and extend the previous HSCC calculations by coupling a larger number of hyperspherical channels, by covering the energy range up to the Ps($n=3$) threshold, and by going over to the *P* wave. We analyze the calculated results in terms of the time-delay matrix introduced by Smith [9].

II. THEORY

A. Hyperspherical close-coupling method

The HSCC method for three-body systems was described previously [6,10]. Here, only a brief reminder is given. The hyperradius ρ is defined by $\rho^2=r_1^2+r_2^2$ in terms of the electron ($\mathbf{r}_1$) and positron ($\mathbf{r}_2$) coordinates relative to the α particle. We choose ρ to be the reaction coordinate throughout the collision since the asymptotic channels of interest here, $e^+ + He^+$ and $Ps + He^{2+}$ (Ps denoting the positronium e^+e^-), are both represented by large values of ρ.

First, adiabatic separation is made between the motion in ρ and that in other coordinates. The adiabatic hyperspherical potentials thus obtained are a good initial approximation for elucidating the dominant dynamics of the system [6].

The adiabatic hyperspherical channels are then coupled by the nonadiabatic operator. In the present HSCC calculation, all channels up to those dissociating asymptotically into $He^{2+} + Ps(n=3)$ are coupled. They include all channels disintegrating into $e^+ + He^+(n\leqslant 8)$. Thus, substantial improvement has been achieved over the previous calculation [6,11]. The asymptotic form of the scattering wave function is used to

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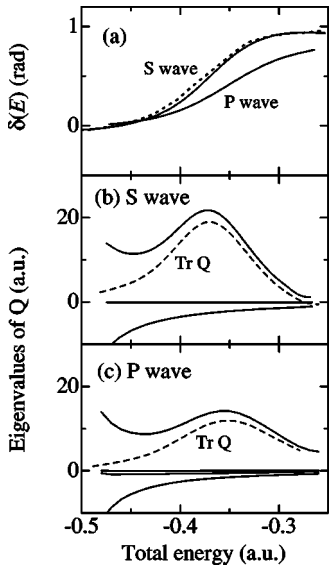

FIG. 1. *S*- and *P*-wave positron scattering by He^+ at energies E of the total system below the energy level of Ps($n=1$). (a) Eigenphase sum $\delta(E)$. Full curves: present results. Dotted curve: *S*-wave result by Bransden *et al.* [7]. (b) Eigenvalues of the *S*-wave time-delay matrix $Q(E)$ (full curves) and Tr $Q(E)=2\hbar(d\delta/dE)$ (broken curve). (c) Eigenvalues of the *P*-wave $Q(E)$ (full curves) and Tr $Q(E)$ (broken curve).

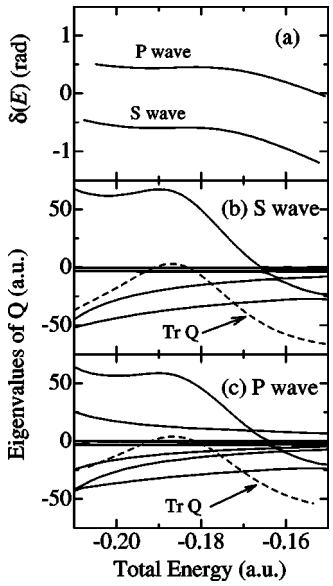

FIG. 2. *S*- and *P*-wave positron scattering by He^+ at energies E of the total system above the energy level of Ps($n=1$). (a) Eigenphase sum $\delta(E)$. (b) Eigenvalues of the *S*-wave time-delay matrix $Q(E)$ (full curves) and Tr $Q(E)=2\hbar(d\delta/dE)$ (broken curve). (c) Eigenvalues of the *P*-wave $Q(E)$ (full curves) and Tr $Q(E)$ (broken curve).

obtain the S matrix, the eigenphases δ_α, and state-to-state partial-wave cross sections $\sigma_L(i\to f)$.

B. Resonances and the time-delay matrix

A hump in a cross section as a function of the total energy E is not necessarily associated with a resonance. In the presence of an isolated narrow resonance, the sum of all eigenphases δ_α, or the eigenphase sum $\delta(E)$, follows the Breit-Wigner one-level formula in a good approximation [12], and increases nearly by π radians in an energy region having a width of the order of Γ.

Resonances may also be analyzed by observing the time-delay or lifetime matrix $Q(E)=i\hbar S(dS^\dagger/dE)$ [9]. The trace of $Q(E)$, which has a significance of average time delay due to the collision, is proved in the Appendix to satisfy a relation

$$\text{Tr } Q(E) = 2\hbar\frac{d\delta}{dE}, \tag{1}$$

whatever energy dependence $Q(E)$ or $\delta(E)$ may have. If $\delta(E)$ follows approximately the Breit-Wigner formula with a background phase changing linearly with E as $(C/2)E+C'$, then Tr $Q(E)$ behaves as

$$\text{Tr } Q(E) \simeq \frac{\hbar\Gamma}{(E-E_r)^2+(\Gamma/2)^2}+\hbar C, \tag{2}$$

according to Eq. (A12).

III. RESULTS

A. Quest for possible broad resonances

The *S*- and *P*-wave eigenphase sums are shown in Fig. 1(a) at energies between the levels of $He^+(n=2)$ and Ps($n=1$) and in Fig. 2(a) between those of $He^+(n=3)$ and $He^+(n=4)$, where Ho [3] located complex eigenvalues with large Γ. The eigenvalues and the traces of the time-delay matrices are presented in Figs. 1(b), 1(c), 2(b), and 2(c). The present result for the *S*-wave eigenphase sum in Fig. 1(a) compares well with the result by Bransden *et al.* [7]. For both *S* and *P* waves, the eigenphase sum increases only by less than 1 radian in this energy region, much less than a value of π radians for a full resonance. In other words, clearly, no full broad resonances occur below the energy level of Ps($n=1$).

A striking aspect of Figs. 1(b) and 1(c) is the clear peak in Tr $Q(E)$ found for both *S* and *P* waves. Although Eq. (2) applies accurately to narrow resonances only, in principle, an attempt was made to fit the HSCC values of Tr $Q(E)$ to this equation in a limited energy range ΔE around the peak center. With a choice $\Delta E=0.1$ a.u., the fit was fairly accurate and it yielded parameters $(E_r,\Gamma)=(-0.371,0.136)$ in a.u. (with $C=-10.6$) for the *S* wave and $(-0.352,0.188)$ (with $C=-9.2$) for the *P* wave. These parameters, which depend slightly on the choice of ΔE, are seen to be consistent with Ho's results $(-0.3705,0.1294)$ for the *S* wave and $(-0.3544,0.178)$ for the *P* wave [3], though, naturally, the agreement is not perfect and the fitting becomes inaccurate outside of ΔE $(<\Gamma)$. We note also that only one eigenvalue of the time-delay matrix has a clear peak and that the other eigenvalues are slowly varying with E, just like the case of true resonances [9,13].

These observations may be interpreted as follows. The CRM eigenvalues indeed represent *S*-matrix poles in the complex energy plane. The *S*-matrix poles lying far from the real energy axis weakly affect scattering for real energies E,

but the background eigenphases decrease so much in the relevant, broad energy region (see the large negative values of C) that no full resonances are seen in the eigenphase sums.

An even more striking case is the eigenphase sums $\delta(E)$ in Fig. 2(a). They are seen to decrease nearly monotonically with energy in this region, implying a negative time delay on the average, or implying that the average collision time is shorter than the case of no collision interaction, unlike any resonance process. Nevertheless, the values of Tr $Q(E)$ in Figs. 2(b) and 2(c) show clear peaks just as in Figs. 1(b) and 1(c). Their fit to Eq. (2) in a limited energy range $\Delta E = 0.03$ a.u. around their peak center yields $(E_r, \Gamma) = (-0.188, 0.045)$ for the S wave with C as large as -87.2, and $(-0.188, 0.051)$ for the P wave with $C = -75.9$ for $\Delta E = 0.035$ a.u., in fair accord with Ho's results $(-0.1856, 0.0393)$ for the S wave and $(-0.1848, 0.0432)$ for the P wave [3]. For both S and P waves, the background eigenphase sum, decreasing drastically between the thresholds of $He^+(n=3)$ and $He^+(n=4)$, seems to wash out any appreciable effects of the S-matrix pole on $\delta(E)$ in Fig. 2(a). By monitoring Tr $Q(E)$, however, the existence of the S-matrix poles far from the real energy axis may be inferred according to argument similar to the one about Fig. 1. In the energy region of Fig. 2, too, only one eigenvalue of the time-delay matrix has a peak-like structure with a large negative background, and the other eigenvalues vary slowly with energy, again showing a behavior similar to true resonances.

B. Narrow resonances

Many narrow resonances are calculated accurately in this work. Their positions and total widths, obtained by fitting to Eq. (2), are summarized in Tables I and II, together with the stable CRM eigenvalues found in Refs. [3] and [4]. Some HSCC resonances were reported previously [6,8]. In particular, the one with $E_r = -0.075\,39$ and reported in Ref. [6] as extremely narrow ($\Gamma \sim 10^{-13}$ a.u.) was corrected in Ref. [8] as $\Gamma = 5.3 \times 10^{-4}$ a.u. This broader Γ was confirmed later in Ref. [4]. This resonance is supported by the well of the adiabatic hyperspherical potential formed, essentially, by the avoided crossings between an asymptotically attractive potential dissociating into $Ps(n=2) + He^{2+}$ and asymptotically repulsive potentials leading to channels $He^+(n=4,5) + e^+$; see Fig. 2 in Ref. [6]. The decay mechanism of this resonance is mainly the coupling with a channel leading asymptotically to $He^+(n=4) + e^+$, and partly the coupling with a channel leading to $He^+(n=3) + e^+$, instead of the inefficient tunneling through the barrier in the adiabatic potential.

Including this case, E_r and Γ values for all the narrow resonances lying below the $Ps(n=2)$ threshold calculated by both the HSCC method and CRM agree well with each other. The Feshbach resonances lying below the $Ps(n=3)$ threshold are reported for the first time in this paper, as far as we are aware.

Resonances in the system $e^+e^-He^{2+}$ are particularly of interest because there are distinct kinds of asymptotic channels, namely, the ones dissociating into two charged particles repelling each other, and the ones dissociating into a charged particle and a hydrogenlike atom, either in the ground state (attracting each other by the polarization potential) or in an excited state (either attracting or repelling each other by a dipole potential). Avoided crossings between potentials with different asymptotic energies occur quite frequently, and result in rich physics, such as the resonance mentioned above as previously thought to be quite narrow. The attractive dipole potential supports an infinite number of Feshbach resonances if the dipole is strong enough, and their resonance parameters satisfy simple formulas in a good approximation [14,15]. We find such Feshbach series below the $Ps(n=2)$ and $Ps(n=3)$ thresholds in Tables I and II. The infinite series actually become finite because of the sublevel splitting due to the relativistic and quantum electrodynamic effects.

TABLE I. S-wave resonances in the system e^+He^+. HSCC: present 42-channel hyperspherical close-coupling calculation. CRM: complex-rotation method. E_r: resonance energy. Γ: total width. $x[y] = x \times 10^y$.

Energy level (a.u.)		HSCC		CRM	
		E_r (a.u.)	Γ (a.u.)	E_r (a.u.)	Γ (a.u.)
Ps(3)	−0.027 78				
$He^+(8)$	−0.031 25				
		−0.032 64	1.2[−3]		
		−0.035 12	1.5[−3]		
		−0.037 42	3.1[−4]		
$He^+(7)$	−0.040 82				
		−0.047 55	8.9[−4]		
$He^+(6)$	−0.055 56				
Ps(2)	−0.0625				
		−0.064 31	4.1[−4]	−0.064 33[a]	3.9[−4][a]
		−0.067 42	7.3[−4]	−0.067 43[a]	7.9[−4][a]
		−0.075 39	5.3[−4]	−0.075 40[a]	5.4[−4][a]
$He^+(5)$	−0.0800				
		−0.1039	5.0[−3]		
$He^+(4)$	−0.1250				
				−0.1856[b]	0.0393[b]
$He^+(3)$	−0.2222				
Ps(1)	−0.2500				
		−0.250 014	7.4[−6]		
				−0.3705[b]	0.1294[b]
$He^+(2)$	−0.5000				

[a]Reference [4].
[b]Reference [3].

IV. CONCLUSION

We have discussed examples of stable complex-rotation eigenvalues, lying far from the real energy axis, that produce no full resonances but that can be assessed by monitoring the time-delay matrix. Attention should also be drawn to the fact that the Breit-Wigner one-level formula with constant resonance parameters can often be an unsatisfactory approximation for broad resonances, in which case the energy dependence of the resonance parameters should be taken into account [16,17].

TABLE II. *P*-wave resonances in the system e^+He^+. HSCC: present 73-channel hyperspherical close-coupling calculation. CRM: complex-rotation method. E_r: resonance energy. Γ: total width. $x[y]=x\times 10^y$.

Energy level		HSCC		CRM	
	(a.u.)	E_r (a.u.)	Γ (a.u.)	E_r (a.u.)	Γ (a.u.)
Ps(3)	−0.027 78				
$He^+(8)$	−0.031 25				
		−0.034 20	1.4[−4]		
		−0.035 01	1.5[−4]		
		−0.037 30	2.8[−4]		
$He^+(7)$	−0.040 82				
		−0.0474	9.7[−3]		
$He^+(6)$	−0.05556				
Ps(2)	−0.0625				
		−0.063 13	1.3[−4]		
		−0.063 95	4.1[−4]	−0.063 97[a]	3.8[−4][a]
		−0.064 30	4.0[−4]	−0.064 29[a]	4.1[−4][a]
		−0.067 15	6.3[−4]	−0.067 11[a]	6.7[−4][a]
		−0.074 84	4.4[−4]	−0.074 86[a]	4.5[−4][a]
$He^+(5)$	−0.0800				
		−0.1038	6.[−3]		
$He^+(4)$	−0.1250				
				−0.1848[b]	0.0432[b]
$He^+(3)$	−0.2222				
Ps(1)	−0.2500				
				−0.3544[b]	0.178[b]
$He^+(2)$	−0.5000				

[a]Reference [4].
[b]Reference [3].

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APPENDIX: RELATION BETWEEN THE TIME-DELAY MATRIX AND THE EIGENPHASE SUM

Here, we prove Eq. (1) in the main text, which relates the trace of the time-delay matrix $Q(E)$ to the eigenphase sum $\delta(E)$. We assume *no particular functional form* of $\delta(E)$ in this proof. A special case of an *S*-matrix pole at a complex energy $E=E_r-i\Gamma/2$ is also discussed.

A wave-packet analysis reveals that the delay time associated with a quantum-mechanical single-channel collision may be described in terms of the derivative of the scattering phase shift $\eta(E)$ with respect to the collision energy E as [18,19]

$$\Delta t = 2\hbar\frac{d\eta}{dE} = i\hbar S\frac{dS^*}{dE} = -i\hbar\frac{dS}{dE}S^*. \tag{A1}$$

Here, $S=\exp(2i\eta)$ is the single-channel *S* matrix. Smith [9] generalized Eq. (A1) for multichannel scattering by introducing a lifetime matrix, or time-delay matrix, $Q(E)$, which is associated with the open channels only, just as the *S* matrix is. He showed that $Q(E)$ satisfies a relation

$$Q(E) = i\hbar S\frac{dS^\dagger}{dE} = -i\hbar\frac{dS}{dE}S^\dagger = Q^\dagger(E). \tag{A2}$$

The matrix $Q(E)$ is seen to be Hermitian. The eigenvalues and eigenvectors of the time-delay matrix were discussed previously (see, for example, Refs. [9,13]), in particular, in relation to the Breit-Wigner resonance formula [20]. In this Appendix, they are discussed in term of the eigenvalues and eigenvectors of the *S* matrix without assuming the Breit-Wigner approximation.

The *S* matrix is first diagonalized by a unitary matrix *U* as

$$USU^\dagger = \Lambda. \tag{A3}$$

Each element $\Lambda_{\alpha\alpha}$ of the diagonal matrix Λ is expressible as $\exp(2i\delta_\alpha)$ in terms of an eigenphase δ_α, the corresponding eigenvector representing an eigenchannel. We consider the diagonal eigenphase matrix Φ defined by the diagonal elements $\Phi_{\alpha\alpha}=\delta_\alpha$. It immediately follows that

$$2\hbar\frac{d\Phi}{dE} = i\hbar\Lambda\frac{d\Lambda^\dagger}{dE}. \tag{A4}$$

Clearly, the right-hand side of Eq. (A4) is not equal to $UQU^\dagger$ in general since *U* depends on the energy *E* in general [9]. If it were equal to $UQU^\dagger$, then the present proof would be unnecessary. We note that

$$\frac{d\Lambda^\dagger}{dE} = U\frac{dS^\dagger}{dE}U^\dagger + \frac{dU}{dE}S^\dagger U^\dagger + US^\dagger\frac{dU^\dagger}{dE}, \tag{A5}$$

so that

$$2\hbar\frac{d\Phi}{dE} = i\hbar\left(US\frac{dS^\dagger}{dE}U^\dagger + USU^\dagger\frac{dU}{dE}S^\dagger U^\dagger + U\frac{dU^\dagger}{dE}\right), \tag{A6}$$

where the unitarity of *U* and *S* has been used. Since the trace of a matrix is unchanged by a unitary transformation, the trace of Eq. (A6) may be written as

$$\mathrm{Tr}\left(2\hbar\frac{d\Phi}{dE}\right) = i\hbar\,\mathrm{Tr}\left(S\frac{dS^\dagger}{dE}\right) + i\hbar\,\mathrm{Tr}\left(U^\dagger\frac{dU}{dE} + U\frac{dU^\dagger}{dE}\right). \tag{A7}$$

The first term on the right-hand side is Tr *Q*. The second term can be reduced to the form

$$i\hbar\,\mathrm{Tr}\left(UU^\dagger\frac{dU}{dE}U^\dagger + U\frac{dU^\dagger}{dE}\right) = i\hbar\,\mathrm{Tr}\frac{d(UU^\dagger)}{dE} = 0. \tag{A8}$$

Therefore, it follows that

$$\mathrm{Tr}\ Q(E) = 2\hbar\,\mathrm{Tr}\frac{d\Phi}{dE} = 2\hbar\frac{d\delta}{dE}, \tag{A9}$$

where δ is the eigenphase sum $\Sigma_\alpha\delta_\alpha$. This is Eq. (1) in the main text.

Equation (A9) is seen to be a generalization of the single-channel formula (A1) for multichannel problems. So far, no

assumption has been made as to the functional form of $S(E)$ or $\delta_\alpha(E)$. The formulation has been quite general. It would be interesting, however, to examine the case of an isolated resonance.

Macek [21] derived a simple relation

$$E - E_r = \sum_{\alpha'} (\Gamma_{\alpha'}/2)\cot[\delta^0_{\alpha'}(E) - \delta_\alpha(E)], \qquad \text{(A10)}$$

for each eigenchannel α, valid in the presence of an S-matrix pole at $E = E_r - i\Gamma/2$ close to the real energy axis, the background eigenphases $\delta^0_{\alpha'}(E)$ varying slowly with energy E. The sum of the partial widths $\Gamma_{\alpha'}$ is the total width Γ. Equation (A10) determines the functional form of each eigenphase $\delta_\alpha(E)$. Later, Hazi [12] showed that the eigenphase sum satisfies an even simpler Breit-Wigner-type formula

$$E - E_r = (\Gamma/2)\cot[\delta^0(E) - \delta(E)], \qquad \text{(A11)}$$

with a slowly varying background eigenphase sum $\delta^0(E)$. Then, according to Eq. (A9) applied to Eq. (A11), the trace of the time-delay matrix is expressible as

$$\mathrm{Tr}\, Q(E) = \frac{\hbar\Gamma}{(E - E_r)^2 + (\Gamma/2)^2} + 2\hbar\frac{d\delta^0}{dE}. \qquad \text{(A12)}$$

By substituting the Breit-Wigner formula [20]

$$S_{ij} \simeq \exp\{i(\phi_i + \phi_j)\}\left(\delta_{ij} - \frac{i\Gamma_i^{1/2}\Gamma_j^{1/2}}{E - E_r + i\sum \Gamma_k/2}\right), \qquad \text{(A13)}$$

for the S-matrix elements directly into Eq. (A2) and by assuming $\{\phi_i\}$ and $\{\Gamma_i\}$ to be constants independent of the energy, it is straightforward to derive Eq. (A12) without the second term on the right-hand side; see, for example, Ref. [13]. In this approximation, it also follows that only one eigenvalue of $Q(E)$ is different from zero, and that the trace is equal to this eigenvalue [13]. Indeed, Burke *et al.* [22] found numerically that only one eigenvalue of $Q(E)$ grows large in the energy region of a resonance.

It should be added finally that, for broad resonances, the Breit-Wigner form with constant parameters E_r, $\{\Gamma_i\}$, and $\{\phi_i\}$ may no longer be a good approximation. Then, Eq. (A9) should be used directly, instead of Eq. (A12).

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