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 $\Gamma$ 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, $\text{Tr} \, Q(E)$, 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 $\delta$ due to the large $\Gamma$. This work uses a general relation $\text{Tr} \, Q(E) = 2h(\delta\delta'/DE)$, 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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PACS number(s): 34.85.+x, 36.10.Dr, 03.65.Nk
obtain the $S$ matrix, the eigenphases $\delta_a$, and state-to-state partial-wave cross sections $\sigma_{if}(i\rightarrow f)$.

**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 $\delta_a$, or the eigenphase sum $\delta(E)$, follows the Breit-Wigner one-level formula in a good approximation [12], and increases nearly by $\pi$ radians in an energy region having a width of the order of $\Gamma$.

Resonances may also be analyzed by observing the time-delay or lifetime matrix $Q(E) = i\hbar S(S'\Gamma/dE)$ [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

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

(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 $\text{Tr} \ Q(E)$ behaves as

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

(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 $\Gamma$. 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 $\pi$ 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 $\text{Tr} \ Q(E)$ 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 HSNC values of $\text{Tr} \ Q(E)$ to this equation in a limited energy range $\Delta E$ around the peak center. With a choice $\Delta E=0.1$ a.u., the fit was fairly accurate and it yielded parameters $(E_c, \Gamma)=(-0.371, 0.136)$ 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 $\Delta E$, 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 $\Delta E (<1)$. 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 $\text{Tr } Q(E)$ 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 decreases drastically between the thresholds of He$^+(n=3)$ and He$^+(n=4)$, which seems to wash out any appreciable effects of the $S$-matrix pole on $\delta(E)$ in Fig. 2(a). By monitoring $\text{Tr } Q(E)$, 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 $E_r = -0.07539$ and reported in Ref. [6] as extremely narrow ($\Gamma = 10^{-12}$ a.u.) was corrected in Ref. [8] as $\Gamma = 5.3 \times 10^{-4}$ a.u. This broader $\Gamma$ 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$(n=2) + \text{He}^+$ 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 $\Gamma$ 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 $e^+e^+\text{He}^+$ 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 hydrogen-like 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.

### 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>
<thead>
<tr>
<th>Energy level $\text{He}^+(n=4) + e^+$</th>
<th>HSCC</th>
<th>CRM</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_r$ (a.u.)</td>
<td>$</td>
<td>\Gamma</td>
</tr>
<tr>
<td>Ps$(3)$</td>
<td>-0.02778</td>
<td>-0.03264</td>
</tr>
<tr>
<td>He$^+(8)$</td>
<td>-0.03125</td>
<td>-0.03512</td>
</tr>
<tr>
<td>He$^+(7)$</td>
<td>-0.03742</td>
<td>3.1[−4]</td>
</tr>
<tr>
<td>He$^+(6)$</td>
<td>-0.04082</td>
<td>-0.04755</td>
</tr>
<tr>
<td>Ps$(2)$</td>
<td>-0.05556</td>
<td>-0.06431</td>
</tr>
<tr>
<td>He$^+(5)$</td>
<td>-0.06742</td>
<td>7.3[−4]</td>
</tr>
<tr>
<td>He$^+(4)$</td>
<td>-0.07539</td>
<td>-0.07540</td>
</tr>
<tr>
<td>He$^+(3)$</td>
<td>-0.08000</td>
<td>7.3[−4]</td>
</tr>
<tr>
<td>Ps$(1)$</td>
<td>-0.12500</td>
<td>-0.1039</td>
</tr>
<tr>
<td>He$^+(2)$</td>
<td>-0.1856</td>
<td>0.0393</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Energy level $\text{He}^+(n=3) + e^+$</th>
<th>HSCC</th>
<th>CRM</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_r$ (a.u.)</td>
<td>$</td>
<td>\Gamma</td>
</tr>
<tr>
<td>He$^+(2)$</td>
<td>-0.3705</td>
<td>0.1294</td>
</tr>
</tbody>
</table>

$^a$Reference [4].
$^b$Reference [3].
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. \(\Gamma\): total width. \(x_0=10^8\).

<table>
<thead>
<tr>
<th>Energy level</th>
<th>HSCC</th>
<th>CRM</th>
</tr>
</thead>
<tbody>
<tr>
<td>(E_r) (a.u.)</td>
<td>(\Gamma) (a.u.)</td>
<td>(E_r) (a.u.)</td>
</tr>
<tr>
<td>Ps(3)</td>
<td>(-0.0278)</td>
<td></td>
</tr>
<tr>
<td>He(^*)(8)</td>
<td>(-0.03125)</td>
<td></td>
</tr>
<tr>
<td>He(^*)(7)</td>
<td>(-0.04082)</td>
<td>(-0.0474)</td>
</tr>
<tr>
<td>He(^*)(6)</td>
<td>(-0.05556)</td>
<td></td>
</tr>
<tr>
<td>Ps(2)</td>
<td>(-0.0625)</td>
<td>(-0.06313)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(-0.06395)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(-0.06430)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(-0.06715)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(-0.07484)</td>
</tr>
<tr>
<td>He(^*)(5)</td>
<td>(-0.0800)</td>
<td>(-0.1038)</td>
</tr>
<tr>
<td>He(^*)(4)</td>
<td>(-0.1250)</td>
<td>(-0.1848) (^b)</td>
</tr>
<tr>
<td>He(^*)(3)</td>
<td>(-0.2222)</td>
<td></td>
</tr>
<tr>
<td>Ps(1)</td>
<td>(-0.2500)</td>
<td>(-0.3544) (^b)</td>
</tr>
<tr>
<td>He(^*)(2)</td>
<td>(-0.5000)</td>
<td></td>
</tr>
</tbody>
</table>

\(^a\)Reference [4].
\(^b\)Reference [3].

ACKNOWLEDGMENTS

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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 \(\Delta t=2h\frac{d\eta}{dE}=i\hbar S^*\frac{dS}{dE}=-i\hbar \frac{dS}{dE}S^*\). (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

\[
Q(E) = i\hbar S^\dagger \frac{dS}{dE} = -i\hbar \frac{dS}{dE} S^\dagger = Q^\dagger(E).
\] (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 terms 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

\[
SU^\dagger = \Lambda.
\] (A3)

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

\[
2\hbar \frac{d\Phi}{dE} = i\hbar \frac{d\Lambda}{dE} = \Lambda.
\] (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

\[
\frac{d\Lambda}{dE} = U\frac{dS}{dE}S^\dagger U^\dagger + U S^\dagger U^\dagger \frac{dU}{dE} + U S^\dagger \frac{dU}{dE} S^\dagger U^\dagger + U \frac{dU}{dE},
\] (A5)

so that

\[
2\hbar \frac{d\Phi}{dE} = i\hbar \left(U S^\dagger \frac{dS}{dE} U^\dagger + US^\dagger \frac{dU}{dE} S^\dagger U^\dagger + U \frac{dU}{dE} \right).
\] (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

\[
\text{Tr} \left(2\hbar \frac{d\Phi}{dE}\right) = i\hbar \left(\text{Tr} \left(S^\dagger \frac{dS}{dE}\right) + \text{Tr} \left(U^\dagger \frac{dU}{dE} + U \frac{dU}{dE}\right)\right).
\] (A7)

The first term on the right-hand side is \(\text{Tr} Q\). The second term can be reduced to the form

\[
i\hbar \text{Tr} \left(U U^\dagger \frac{dU}{dE} U^\dagger + U \frac{dU}{dE}\right) = i\hbar \text{Tr} \left(\frac{d(UU^\dagger)}{dE}\right) = 0.
\] (A8)

Therefore, it follows that

\[
\text{Tr} Q(E) = 2\hbar \frac{d\Phi}{dE} = 2\hbar \frac{d\delta}{dE}.
\] (A9)

where \(\delta\) 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 $\delta_0(E)$. 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

$$E - E_r = \sum_{\alpha'} (\Gamma_{\alpha'}/2) \cot[\delta_{\alpha'}(E) - \delta_0(E)],$$

(A10)

for each eigenchannel $\alpha$, 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 $\delta_{\alpha'}(E)$ varying slowly with energy $E$. The sum of the partial widths $\Gamma_{\alpha'}$ is the total width $\Gamma$. Equation (A10) determines the functional form of each eigenphase $\delta_0(E)$. Later, Hazi [12] showed that the eigenphase sum satisfies an even simpler Breit-Wigner-type formula

$$E - E_r = (\Gamma/2) \cot[\delta(E) - \delta_0(E)],$$

(A11)

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

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

(A12)

By substituting the Breit-Wigner formula [20]

$$S_{ij} = \exp[i(\phi_i + \phi_j)] \left( \frac{\delta_{ij} - \frac{i(\Gamma_i/2)^2}{E - E_r + i \sum\Gamma_j/2}}{E - E_r + i \sum\Gamma_j/2} \right),$$

(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).

[9] F. T. Smith, Phys. Rev. 118, 349 (1960). In fact, this paper refers to the matrix $Q$, introduced there, as the lifetime matrix, and discusses its difference from what may be more appropriately called the delay-time matrix, introduced in Eisenbud's unpublished thesis. In the later literature, however, $Q$ is more often referred to as time-delay matrix.
[11] The 20-channel $S$-wave close-coupling calculation in Ref. [7] at a collision energy of 47.25 eV [0.37 eV below the $\text{Ps}(1s)$ threshold], including only one $\text{Ps}$ channel and many $\text{He}^+$ pseudochannels, reportedly yielded results in disagreement with the 24-channel HSCC results of Ref. [6] at 47.62 eV [0.0025 eV above $\text{Ps}(1s)$]. The “elastic cross section” $\bar{\sigma}_0(1s \rightarrow 1s)$ excluding the contribution from the Coulomb potential was about half the HSCC result (though the definition of the “elastic cross section” in Ref. [7] is unclear to us), and the excitation cross section $\sigma_0(1s \rightarrow n = 2)$ was about a factor of 5 smaller than the HSCC result. The present 42-channel $S$-wave HSCC calculation reduced $\bar{\sigma}_0(1s \rightarrow 1s)$ by $\sim$15%, which is unimportant since $\bar{\sigma}_0(1s \rightarrow 1s)$ is only $\sim$1% of the true $S$-wave cross section $\sigma_0(1s \rightarrow 1s)$ including the Coulomb contribution. Note that the elastic cross section is known to diverge if summed over all partial waves. The excitation cross section $\sigma_0(1s \rightarrow n = 2)$, which is smaller than $\sigma_0(1s \rightarrow 1s)$ by five orders of magnitude, is harder to calculate accurately. The present result differs from that in Ref. [7] by only $\sim$30%, if compared at the same energy. The eigenphase sum is merely shifted by 0.05 to 0.1 radians if the He($1s$) channel is removed artificially from the HSCC calculation.
[18] D. Bohm, Quantum Mechanics (Prentice-Hall, New York, 1951), Chap. 11