

Identification of the Beutler-Fano formula in eigenphase shifts and eigentime delays near a resonance

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Eigenphase shifts and eigentime delays near a resonance for a system of one discrete state and two continua are shown to be functionals of the Beutler-Fano formula using appropriate dimensionless energy units and line profile indices. Parameters responsible for the avoided crossing of eigenphase shifts and eigentime delays are identified. Similarly, parameters responsible for the eigentime delays due to a frame change are identified. With the help of new parameters, an analogy with the spin model is pursued for the S matrix and time delay matrix Q . The S matrix is found to be put into $\exp[i(a+b\vec{\sigma}\cdot\hat{n})]$. The time delay matrix Q is shown to be given as $Q = \frac{1}{2}\tau_r(1 + \vec{P}_a\cdot\vec{\sigma} + \vec{P}_f\cdot\vec{\sigma})$, where the first term is the time delay due to resonance, the second term is the one due to avoided crossing interaction, and the last term is the one due to a frame change. It is found that $P_a^2 + P_f^2 = 1$. [S1050-2947(98)06812-7]

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I. INTRODUCTION

Resonances observed in the energy dependence of atomic and molecular processes often correspond to the autoionization or predissociation observed in photoabsorption, i.e., to the excitation of a quasibound state in a continuum region [1,2]. Their spectra are characterized by rich profiles providing a wealth of information on the atomic and molecular dissociation or ionization processes. Beutler's early observation of rare-gas levels autoionizing into a single continuum with angular-momentum conservation was reproduced by Fano through the formula [3]

$$\sigma(\epsilon) = \sigma_0 \frac{(\epsilon - q)^2}{1 + \epsilon^2}, \quad (1)$$

where ϵ is the reduced energy defined by $2(E - E_0)/\Gamma$, E_0 and \hbar/Γ represent the resonance energy and the mean lifetime of the quasibound state, respectively, σ_0 represents the photofragmentation cross section to the continuum state, and q is an index that characterizes the line profile (here $-q$ is employed instead of the usual q). An extension of the Beutler-Fano formula to the dissociation into multichannels was obtained by Combet-Farnoux [4]. The energy dependence of the S matrix near an isolated resonance for such predissociation or autoionization into multichannels was obtained long ago and is well known [5]. By diagonalizing the S matrix, eigenphase shifts δ_i ($i=1,2,\dots,n$) are obtained from its eigenvalues as

$$S = U e^{2i\delta\vec{U}} \quad (2)$$

and are utilized frequently as a tool for analyzing the resonances [6,7]. Eigenphase shifts and the corresponding eigenchannels are also extensively used in various forms in multichannel quantum-defect theory, which is regarded as one of the most general and powerful theories of resonance [1].

In contrast to photofragmentation cross sections and the S matrix, the analytical formulas for eigenphase shifts in mul-

tichannel processes are not known. According to the numerical studies, eigenphase shifts in the multichannel system are known as showing complicated behaviors near a resonance due to the avoided crossing between curves of eigenphase shifts along the energy [6,8]. Such a phenomenon of the avoided crossing along the energy is not conspicuous in the case of the formulas for photodissociation cross sections and S matrices. We report here detailed studies on the behaviors of eigenphase shifts and also times delayed by collision [9,10] for the system of one discrete state and two continua, which turn out to be described by functionals of the Beutler-Fano formula. Their behaviors in the system of one discrete state and one continuum have already been studied [3]. If one more continuum is added to that system, new phenomena of the avoided crossing between curves of eigenphase shifts and eigentimes delayed and of times delayed due to the frame change along the energy besides the resonance behavior enter. The avoided crossing interactions between eigenphase shifts along the energy always take place near a resonance if they are not excluded for symmetry reasons, as we will see later. The addition of more continua may simply introduce more avoided crossings among the newly added eigenphase shifts. In this sense, the current system of one discrete state and two continua may serve as a prototypical system for the study of the effects of avoid crossings between eigenphase shifts and times delayed due to the frame change on the resonance phenomena.

The import of the current work may be in the findings of the new parameters for the avoided crossing interaction, where the S matrix can be put into a form of e^{iH} , with H the Hermitian, and the time delay matrix (or lifetime matrix, as called by Smith [10]) can be put into a form of $1 + \vec{P}\cdot\vec{\sigma}$, where \vec{P} is a polarization vector and $\vec{\sigma}$ is the Pauli matrix. The analogy with the spin system under a magnetic field is exploited to find further properties of the S matrix and time delay matrix.

Section II describes the known properties of eigenphase shifts. Section III describes the form of the S matrix near a resonance and the equation for eigenphase shifts. It also dis-

discusses some special cases and general characteristics of eigenphase shifts and eigentime delays. Section IV obtains the formulas of eigenphase shifts as functionals of the Beutler-Fano formula for the system of one discrete state and two continua. Section V obtains the formulas of eigentime delays as functionals of the Beutler-Fano formula. Section VI summarizes the results.

II. KNOWN PROPERTIES OF EIGENPHASE SHIFTS

It is well known that for an isolated resonance in single channel scattering, the energy dependence of a phase shift $\delta(E)$ is described by the formula [1]

$$\tan[\delta(E) - \delta^0] = \frac{\Gamma}{2(E_0 - E)} = -\frac{1}{\epsilon}, \quad (3)$$

where δ^0 , E_0 , and Γ denote the background phase shift, the energy, and the width of the resonance, respectively. The second equality in Eq. (3) defines the dimensionless energy. It can be deduced from Eq. (3) that $\delta(E)$ increases slowly except for the narrow energy range around E_0 where its value undergoes a rapid change and is eventually increased by π as energy varies from $-\infty$ to ∞ . Due to the property of tangent function, $\delta(E)$ can be determined only up to $n\pi$ (n an integer). It is usually taken to be δ^0 at $E \rightarrow -\infty$. Then it becomes $\delta^0 + \pi$ at $E \rightarrow \infty$. In the absence of resonance, δ is equal to δ^0 . The background phase shift δ^0 is a slowly varying function of energy and is usually taken to be constant as a good approximation. Thus the increase of $\delta(E)$ around E_0 comes solely from the resonance. Let us denote the difference between $\delta(E)$ and δ^0 by $\delta_r(E)$. With this notation, Eq. (3) becomes $\tan \delta_r(E) = \tan \bar{\delta}_r(\epsilon) = -1/\epsilon$ and with the above-mentioned phase convention of setting $\delta(E)$ to δ^0 at $E = -\infty$, it can be transformed as

$$e^{i\bar{\delta}_r(\epsilon)} = \frac{-\epsilon + i}{\sqrt{\epsilon^2 + 1}}. \quad (4)$$

Macek [8] generalized Eq. (3) to multichannel processes as

$$2(E - E_0) = \sum_{k=1}^n \Gamma_k \cot[\delta_k^0 - \delta_m(E)], \quad m = 1, \dots, n, \quad (5)$$

where $\delta_m(E)$ is the eigenphase shift defined in Eq. (2), δ_k^0 is the background phase shifts in channel k , and Γ_k is the partial decay width to channel k . Hazi [11] also showed that the eigenphase sum, which will be denoted as $\delta_\Sigma(E)$, satisfies the ‘‘single-channel’’ formula

$$\delta_\Sigma(E) \equiv \sum_{k=1}^n \delta_k(E) = \delta_\Sigma^0 + \tan^{-1} \frac{\Gamma}{2(E_0 - E)} = \delta_\Sigma^0 - \tan^{-1} \frac{1}{\epsilon}, \quad (6)$$

where Γ is the total width of the resonance, i.e., $\Gamma = \sum_{m=1}^n \Gamma_m$, and δ_Σ^0 is the sum of the background eigenphase, i.e., $\delta_\Sigma^0 = \sum_{m=1}^n \delta_m^0$. The reduced energy ϵ is the one defined in Eq. (3), except that Γ now denotes the total width.

III. EQUATIONS FOR EIGENPHASE SHIFTS IN THE NEIGHBORHOOD OF RESONANCE

The form of the S matrix in the neighborhood of an isolated resonance in multichannel processes is well known and has been repeatedly derived in the past using various resonance theories [2,5]. Though its form is basically the same for all resonance theories, its detailed expressions may look different from theory to theory. Here Fano’s configuration interaction theory is adopted for the treatment of the resonance [3]. In the configuration interaction theory, an isolated resonance in the multichannel system is treated as regarding the system as composed of one discrete state ϕ and many continuum wave functions $\psi_E^{-(j)}$. The latter are taken to pre-diagonalize H . In other words, it is assumed that continuum wave functions are unable to interact directly with each other. They can, however, interact with each other indirectly via their interactions with the discrete state ϕ if the integrals

$$V_{jE} = (\psi_E^{-(j)} | H | \phi) \quad (7)$$

are not zero. This means that H is no longer diagonalized in the combined space spanned by the basis set $\{\phi, \psi_E^{-(j)}\}$. Eigenfunctions $\Psi_E^{-(j)}$ of H in the space spanned by $\{\phi, \psi_E^{-(j)}\}$ can be obtained analytically as shown by Fano [3,4]. By applying the incoming wave boundary conditions to those eigenfunctions as

$$\Psi_E^{-(j)} \rightarrow \sum_{j'} \phi_{j'}(\omega) \sqrt{\frac{m}{2\pi k_j}} (e^{ik_j'R} \delta_{j'j} - e^{-ik_j'R} S_{j'j}), \quad (8)$$

The S matrix may be obtained [4] as

$$S_{j'j} = \sum_{j''} S_{j'j''}^0 \left(\delta_{j''j} + 2\pi i \frac{V_{j''E} V_{jE}^*}{E - E_0 - i\pi \sum_k |V_{kE}|^2} \right), \quad (9)$$

where $S_{j'j''}^0$ is the S matrix of the background scattering. Equation (9) is different from that of the outgoing wave in that i is replaced by $-i$. The incoming wave, instead of the outgoing one, is employed here as our interests are in the photodissociation processes.

As stated in Ref. [3], $2\pi \sum_k |V_{kE}|^2$ is the spectral width of the resonance peak and is denoted as Γ . According to Refs. [5,8], Eq. (9) may be rewritten as

$$S_{j'j} = \sum_{j''} U_{j'j''}^0 (e^{-2i\delta_{j''}^0} \delta_{j''j} + ic_{j''} c_{j''m}) \tilde{U}_{j''j}^0. \quad (10)$$

In matrix notation, Eq. (10) becomes

$$S = U^0 (e^{-2i\delta^0} + ic\tilde{c}) \tilde{U}^0 \equiv U^0 A \tilde{U}^0, \quad (11)$$

where c is the column vector and its k th element is defined by

$$c_k \equiv e^{-i\delta_k^0} \sqrt{\frac{\Gamma_k}{E - E_0 - i\Gamma/2}}. \quad (12)$$

Γ_k is the partial resonance decay width to the background eigenchannel k .

Let us consider obtaining eigenphase shifts δ by the diagonalization of the S matrix

$$S = U e^{-2i\delta} \tilde{U}. \quad (13)$$

If $A = e^{-2i\delta^0} + ic\tilde{c}$ is diagonalized as

$$\begin{vmatrix} e^{-2i\delta_1^0} + ic_1^2 - x & ic_1c_2 & ic_1c_3 & \cdots \\ ic_2c_1 & e^{-2i\delta_2^0} + ic_2^2 - x & ic_2c_3 & \cdots \\ ic_3c_1 & ic_3c_2 & e^{-2i\delta_3^0} + ic_3^2 - x & \cdots \\ \vdots & \vdots & \vdots & \cdots \\ \vdots & \vdots & \vdots & \cdots \end{vmatrix} = 0. \quad (16)$$

If we divide the first row of the above determinant by ic_1 , the second row by ic_2 , and the k th row by ic_k , in general, and if we introduce x_k defined by

$$x_k \equiv \frac{e^{-2i\delta_k^0} + ic_k^2 - x}{ic_k} \quad \left(\text{or } x_k - c_k = \frac{e^{-2i\delta_k^0} - x}{ic_k} \right), \quad (17)$$

the secular equation becomes

$$\begin{vmatrix} x_1 & c_2 & c_3 & \cdots \\ c_1 & x_2 & c_3 & \cdots \\ c_1 & c_2 & x_3 & \cdots \\ \vdots & \vdots & \vdots & \cdots \\ \vdots & \vdots & \vdots & \cdots \end{vmatrix} = 0. \quad (18)$$

The above equation for the system of n continua can be transformed into Sardi's form [12]

$$\prod_{k=1}^n (x_k - c_k) + \sum_{k=1}^n \left[c_k \frac{\partial}{\partial x_k} \prod_{m=1}^n (x_m - c_m) \right] = 0. \quad (19)$$

By dividing Eq. (19) by its first term, one obtains

$$\sum_{k=1}^n \frac{c_k}{c_k - x_k} = 1. \quad (20)$$

By substitution of Eqs. (12) and (17), Eq. (20) becomes

$$i \sum_{k=1}^n \frac{\Gamma_k}{e^{-2i(\delta - \delta_k^0)} - 1} = E - E_0 - i \frac{\Gamma}{2}. \quad (21)$$

Equating the real and imaginary parts, Eq. (21) yields two relations: One is Macek's formula and the other is $\sum_k \Gamma_k = \Gamma$. This derivation of Macek's formula is simpler than the original one. Sardi's form is given as a polynomial of order n

$$A = V e^{-2i\delta} \tilde{V}, \quad (14)$$

$$S = U^0 V e^{-2i\delta} \tilde{V} U^0. \quad (15)$$

From Eqs. (13) and (15), $U = U^0 V$.

Let x denote the eigenvalue $e^{-2i\delta}$ of A . Then the eigenvalue of $A = e^{-2i\delta^0} + ic\tilde{c}$ can be obtained by solving the secular equation

and is more convenient than Macek's formula in obtaining the solution. In particular it shows explicitly that the number of roots of Macek's formula is the same as the number of continua n . We will use it in Sec. IV to obtain the solution for the system of one discrete state and two continua. Before doing that, let us comment on the general properties of eigenphase shifts obtainable from Macek's formula.

From Macek's formula we could draw two properties of eigenphase shifts. First, their differentiation with respect to energy yields

$$\frac{d\delta_m}{dE} = 2 \left[\sum_{k=1}^n \frac{\Gamma_k}{\sin^2(\delta_k^0 - \delta_m)} \right]^{-1} > 0, \quad m = 1, \dots, n. \quad (22)$$

This equation tells us that the first derivatives of eigenphase shifts with respect to energy near a resonance are positive. Second, the asymptotic values of the eigenphase shifts [at $|2(E - E_0)/\Gamma| \rightarrow \infty$] are given as $\delta_1^0, \delta_2^0, \delta_3^0, \dots, \delta_n^0$ up to multiples of π .

Let us assume that $\delta_1^0 < \delta_2^0 < \dots < \delta_n^0$ and that they are all in the range $[0, \pi]$, for simplicity, which can be always done without losing generality by Hazi's formula (6). Then the above two properties of eigenphase shifts tell us that eigenphase shifts vary between two asymptotic values of their abscissas given by $[\delta_1^0, \delta_2^0], [\delta_2^0, \delta_3^0], \dots, [\delta_{n-1}^0, \delta_n^0]$. If δ_n^0 becomes larger than π , it is shifted by $-\pi$ and increases again toward δ_1^0 . Since the sum of the eigenphase shifts shows the resonance behavior and increases by π around resonance, each eigenphase shift should similarly show the resonance behavior between two consecutive asymptotes of the abscissas $[\delta_i^0, \delta_{i+1}^0]$ ($i = 1, \dots, n$). When the consecutive eigenphase shifts are the same, let us say $\delta_i^0 = \delta_{i+1}^0$, then one of the two corresponding eigenphase shifts remains constant while the other one shows the resonance behavior between two asymptotes $[\delta_i^0, \delta_{i+2}^0]$.

IV. EIGENPHASE SHIFTS FOR THE SYSTEM OF ONE DISCRETE STATE AND TWO CONTINUA

Let us now consider the system of one discrete state and two continua. For this system Eq. (19) becomes

$$[(x_1 - c_1)(x_2 - c_2) + c_1(x_2 - c_2) + c_2(x_1 - c_1)] = 0. \quad (23)$$

Substituting Eq. (17) into Eq. (23), we obtain

$$x^2 - (e^{-2i\delta_1^0} + ic_1^2 + e^{-2i\delta_2^0} + ic_2^2)x + (e^{-2i\delta_1^0} + ic_1^2)(e^{-2i\delta_2^0} + ic_2^2) + c_1^2c_2^2 = 0. \quad (24)$$

The roots of the quadratic equation (24) are obtained as

$$x = e^{-2i\delta_{\pm}(E)} = \frac{e^{-i(\delta_1^0 + \delta_2^0)}}{\Gamma} \left((E - E_0) \cos \Delta_{12}^0 + \frac{\Delta\Gamma}{2} \sin \Delta_{12}^0 \right. \\ \left. \pm i \left[\Gamma_1 \Gamma_2 + \left((E - E_0) \sin \Delta_{12}^0 - \frac{\Delta\Gamma}{2} \cos \Delta_{12}^0 \right)^2 \right]^{1/2} \right), \quad (25)$$

where $\Gamma = \Gamma_1 + \Gamma_2$, $\Delta\Gamma = \Gamma_1 - \Gamma_2$, and $\Delta_{12}^0 = \delta_1^0 - \delta_2^0$. If we introduce a dimensionless energy ϵ_r (taken differently from the usual notation ϵ in order to avoid the confusion with another dimensionless energy ϵ_a , which will be defined later) as

$$\epsilon_r \equiv \frac{E - E_0}{\Gamma/2}, \quad (26)$$

Equation (25) becomes

$$e^{-2i\bar{\delta}_{\pm}(\epsilon_r)} = \frac{e^{-i(\delta_1^0 + \delta_2^0)}}{\epsilon_r - i} \left\{ \epsilon_r \cos \Delta_{12}^0 + \frac{\Delta\Gamma}{\Gamma} \sin \Delta_{12}^0 \right. \\ \left. \pm i \left[\frac{4\Gamma_1\Gamma_2}{\Gamma^2} + \left(\epsilon_r \sin \Delta_{12}^0 - \frac{\Delta\Gamma}{\Gamma} \cos \Delta_{12}^0 \right)^2 \right]^{1/2} \right\}, \quad (27)$$

where $\bar{\delta}$ is used instead of δ in order to emphasize that the eigenphase shifts are now functions of ϵ_r instead of E . An analysis of the eigenphase shifts in Eq. (27) is done in the next subsection by introducing phase shifts due to the resonance and avoided crossing interaction.

A. Phase shifts due to resonance and avoided crossing interaction

Equation (27) can be decomposed into the product of two terms of unit modulus [13]

$$e^{-i\bar{\delta}_r(\epsilon_r)} = \frac{-\sqrt{\epsilon_r^2 + 1}}{\epsilon_r - i}, \quad (28)$$

$$e^{\pm i\bar{\delta}_a(\epsilon_r)} = \frac{-1}{\sqrt{\epsilon_r^2 + 1}} \left\{ \epsilon_r \cos \Delta_{12}^0 + \frac{\Delta\Gamma}{\Gamma} \sin \Delta_{12}^0 \right. \\ \left. \mp i \left[\frac{4\Gamma_1\Gamma_2}{\Gamma^2} + \left(\epsilon_r \sin \Delta_{12}^0 - \frac{\Delta\Gamma}{\Gamma} \cos \Delta_{12}^0 \right)^2 \right]^{1/2} \right\} \quad (29)$$

(the notations $\bar{\delta}_r$ and $\bar{\delta}_a$ without the bar are also used elsewhere if it is desired to express them in terms of E instead of ϵ_r). The phase shift $\bar{\delta}_r$ in the first term is the one due to the resonance as in Eq. (4). In single-channel scattering, it is the only term besides the background phase shift contributing to the eigenphase shifts near a resonance. In two-channel scattering, there enters another phase shift $\bar{\delta}_a$ defined by the second term due to the indirect coupling of two continua via a quasibound state near a resonance.

The functional dependence of $\bar{\delta}_a(\epsilon_r)$ on energy may be best seen by considering its cotangent like $\cot \bar{\delta}_r = -\epsilon_r$ as in single-channel scattering:

$$\cot \bar{\delta}_a(\epsilon_r) = \frac{-\left(\epsilon_r \cos \Delta_{12}^0 + \frac{\Delta\Gamma}{\Gamma} \sin \Delta_{12}^0 \right)}{\left[\left(\epsilon_r \sin \Delta_{12}^0 - \frac{\Delta\Gamma}{\Gamma} \cos \Delta_{12}^0 \right)^2 + \frac{4\Gamma_1\Gamma_2}{\Gamma^2} \right]^{1/2}}. \quad (30)$$

Let us first rewrite Eq. (30) as

$$\cot \bar{\delta}_a(\epsilon_r) \\ = -\cot \Delta_{12}^0 \frac{\frac{\Gamma \sin \Delta_{12}^0}{2\sqrt{\Gamma_1\Gamma_2}} \left(\epsilon_r + \frac{\Delta\Gamma}{\Gamma} \tan \Delta_{12}^0 \right)}{\left[\frac{\Gamma \sin \Delta_{12}^0}{2\sqrt{\Gamma_1\Gamma_2}} \left(\epsilon_r - \frac{\Delta\Gamma}{\Gamma} \cot \Delta_{12}^0 \right) \right]^2 + 1}^{1/2}. \quad (31)$$

The term inside the square brackets in the denominator of Eq. (31) can be transformed as

$$\frac{\Gamma \sin \Delta_{12}^0}{2\sqrt{\Gamma_1\Gamma_2}} \left(\epsilon_r - \frac{\Delta\Gamma}{\Gamma} \cot \Delta_{12}^0 \right) = \frac{\sin \Delta_{12}^0}{\sqrt{\Gamma_1\Gamma_2}} \left(E - E_0 \right. \\ \left. - \frac{\Delta\Gamma}{2} \cot \Delta_{12}^0 \right). \quad (32)$$

This suggests that we can introduce a new energy unit Γ_a ,

$$\Gamma_a \equiv \frac{2\sqrt{\Gamma_1\Gamma_2}}{\sin \Delta_{12}^0} = \frac{\sqrt{\Gamma^2 - \Delta\Gamma^2}}{\sin \Delta_{12}^0}. \quad (33)$$

For simplicity, let us also introduce a new parameter E_a ,

$$E_a \equiv E_0 + \frac{\Delta\Gamma}{2} \cot \Delta_{12}^0 \quad (34)$$

(later it will be shown that E_a is the avoided crossing point energy and Γ_a is the strength of the avoided crossing interaction).

With these parameters, Eq. (32) becomes $2(E - E_a)/\Gamma_a$, which may be considered as a new dimensionless energy and will be denoted as ϵ_a :

$$\epsilon_a \equiv \frac{2(E - E_a)}{\Gamma_a}. \quad (35)$$

By substituting Eqs. (32) and (35) into Eq. (31) we obtain

$$\cot \tilde{\delta}_a(\epsilon_a) = -\cot \Delta_{12}^0 \frac{\epsilon_a - q_a}{\sqrt{\epsilon_a^2 + 1}}, \quad (36)$$

where $\tilde{\delta}_a(\epsilon_a)$ is used instead of $\tilde{\delta}_a(\epsilon_r)$ in order to emphasize that it is now a function of ϵ_a and q_a is a new parameter defined by

$$q_a \equiv \frac{-\Delta\Gamma}{\sqrt{\Gamma^2 - \Delta\Gamma^2 \cos \Delta_{12}^0}}. \quad (37)$$

Equation (36) is a functional of the Beutler-Fano function defined by

$$f_{\text{BF}}(\epsilon, q) \equiv \frac{(\epsilon - q)^2}{1 + \epsilon^2} \quad (38)$$

and can be rewritten as

$$\cot \tilde{\delta}_a(\epsilon_a) = \begin{cases} \cot \Delta_{12}^0 \sqrt{f_{\text{BF}}(\epsilon_a, q_a)} & \text{when } \epsilon_a < q_a \\ -\cot \Delta_{12}^0 \sqrt{f_{\text{BF}}(\epsilon_a, q_a)} & \text{when } \epsilon_a \geq q_a. \end{cases} \quad (39)$$

Equation (36) or (39) tells us that the phase shift δ_a due to the avoided crossing interaction takes its simplest form when it is parametrized in terms of ϵ_a and q_a . Since we want Γ_a to be positive, it will be assumed that $\sin \Delta_{12}^0 \geq 0$, which can always be achieved by the appropriate choice of 1 and 2 for δ_1^0 and δ_2^0 . With this convention in mind, Γ_a will be written as $2\sqrt{\Gamma_1\Gamma_2}/|\sin \Delta_{12}|$ hereinafter.

With the above phase shifts, eigenphase shifts are obtained as

$$2\delta_{\pm}(E) = \delta_1^0 + \delta_2^0 + \delta_r(E) \pm \delta_a(E) \quad (40)$$

(for the choice of the sign see [13]). It is interesting to note that phase shifts of different origins are added up linearly to eigenphase shifts.

Using Eq. (6), Eq. (40) may be expressed in terms of the eigenphase sum $\delta_{\Sigma}(E)$

$$2\delta_{\pm}(E) = \delta_{\Sigma}(E) \pm \delta_a(E). \quad (41)$$

The eigenphase sum $\delta_{\Sigma}(E)$ consists of the background eigenphase sum δ_{Σ}^0 and the phase shift $\delta_r(E)$ due to the resonance. The phase shifts due to the resonance contribute positively from zero to π as energy varies around a resonance. The phase shift is positive since particles are attracted and bound temporarily near a resonance. The \pm sign in front of $\delta_a(E)$ in Eq. (40) tells us that the phase shift due to the

avoided crossing interaction in one eigenchannel increases at the expense of the phase shift of the other eigenchannel and vice versa. If it increases in one eigenchannel due to attraction, it decreases in the other one due to repulsion. They are exactly canceled out and do not contribute to the eigenphase sum. The study of δ_a as a function of ϵ_a shows that δ_a has an extremum of $\cot^{-1}(\sqrt{q_a^2 + 1} \cot \Delta_{12}^0)$ at $\epsilon_a = -1/q_a$ (a minimum when $q_a > 0$, a maximum when $q_a < 0$). From its definition, the limiting behavior of $\tilde{\delta}_a$ at off resonance is obtained as

$$\tilde{\delta}_a(\epsilon_a) \rightarrow \begin{cases} \Delta_{12}^0 & \text{when } \epsilon_a \rightarrow -\infty \\ \pi - \Delta_{12}^0 & \text{when } \epsilon_a \rightarrow \infty \end{cases} \quad (42)$$

[note that $0 \leq \Delta_{12}^0 \leq \pi/2$ according to the convention mentioned below Eq. (39)]. $\tilde{\delta}_a$ increases around resonance by $\pi - 2\Delta_{12}^0$. Thus the phase shift due to the avoided crossing interaction varies most around resonance when $\Delta_{12}^0 = 0$ and least when $\Delta_{12}^0 = \pi/2$. It passes the middle $\pi/2$ of two asymptotes of the abscissas in Eq. (42) when $\epsilon_a = q_a$. Since the avoided crossing point energy E_a corresponds to the zero of ϵ_a [see the discussion below Eq. (45)], q_a indicates that the avoided crossing point energy is away from the middle of two asymptotes of the abscissas. Such a separation is a measure of the asymmetry of the curves of $\tilde{\delta}_a(\epsilon_a)$. Figure 1 shows the variations in the behaviors of δ_a and δ_{\pm} as q_a varies.

So far, we have obtained eigenvalues of S matrix for two open channels near a resonance and decomposed them into contributions from the background, resonance, and avoided crossing interactions. Let us now consider obtaining the eigenvectors of the S matrix, which are usually called eigenchannels. The S matrix is diagonalized in two steps. It is first transformed to A by U^0 , which diagonalizes the S^0 matrix, i.e., $S = U^0 A \tilde{U}^0$ ($S^0 = U^0 e^{-2i\delta^0} \tilde{U}^0$). A is then diagonalized as in Eq. (14) by the V matrix, which is composed of two eigenvectors v_+ and v_- corresponding to δ_+ and δ_- as

$$V = (v_+ \quad v_-). \quad (43)$$

After a lengthy derivation, eigenvectors are obtained as

$$v_+ = \begin{bmatrix} \cos\left(\frac{\theta_a}{2}\right) \\ \sin\left(\frac{\theta_a}{2}\right) \end{bmatrix}, \quad v_- = \begin{bmatrix} -\sin\left(\frac{\theta_a}{2}\right) \\ \cos\left(\frac{\theta_a}{2}\right) \end{bmatrix}, \quad (44)$$

with θ_a defined by

$$\cos \theta_a \equiv -\frac{\epsilon_a}{\sqrt{1 + \epsilon_a^2}}, \quad \sin \theta_a \equiv \frac{1}{\sqrt{1 + \epsilon_a^2}}. \quad (45)$$

It is interesting to note that eigenvectors are independent of q_a . They depend only on ϵ_a . As ϵ_a varies from $-\infty$ through zero to ∞ , θ_a varies from zero through $\pi/2$ to π and v_+ varies from $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ through $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ to $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$. Thus, at $\epsilon_a = 0$ or at $E = E_0 + (\Delta\Gamma/2)\cot \Delta_{12}^0$, two background channels are mixed equally, indicating that two eigenphase shifts are avoided most. For this reason $\epsilon_a = 0$ is considered as the

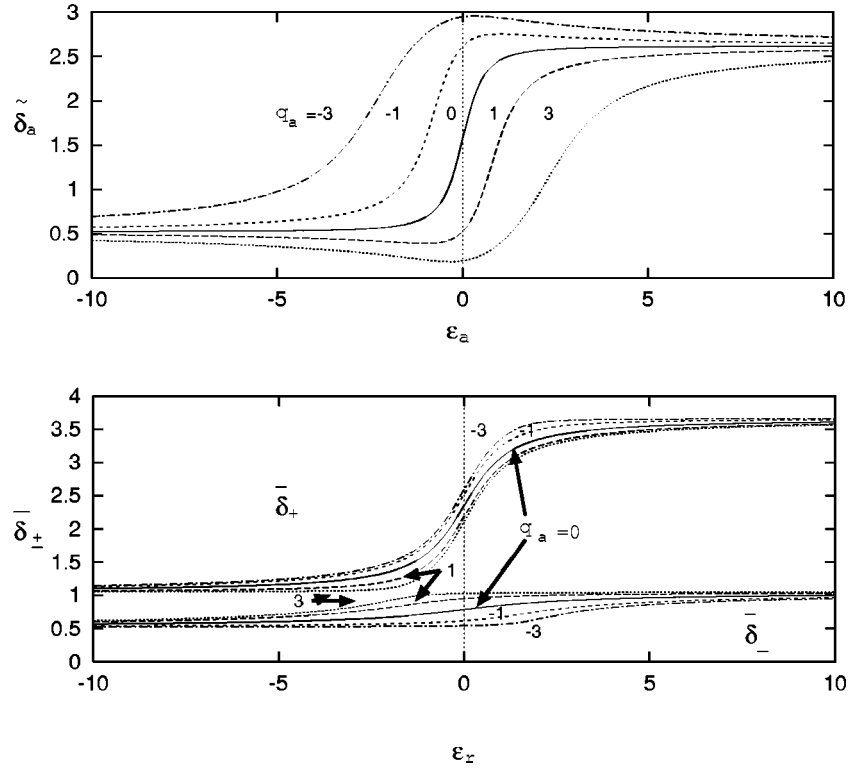


FIG. 1. $\tilde{\delta}_a(E)$ vs ϵ_a and $\tilde{\delta}_\pm(\epsilon_r)$ vs ϵ_r are plotted for $q_a = 0, \pm 1$, and ± 3 . The values for δ_1^0 and δ_2^0 are $\pi/3$ and $\pi/6$, respectively.

avoided crossing point energy. (Another way to see that $\epsilon_a = 0$ is the avoided crossing point energy might be to remove the cause of the avoidance of two eigenphase shift curves, let them cross each other, and see whether the crossing point is $\epsilon_a = 0$. This was done and $\epsilon_a = 0$ was confirmed to be the crossing point.)

Let us parametrize the U^0 matrix as

$$U^0 = \begin{pmatrix} \cos \theta^0 & -\sin \theta^0 \\ \sin \theta^0 & \cos \theta^0 \end{pmatrix}, \quad (46)$$

where θ^0 may be considered the angle by which the frame for background eigenchannels is rotated from the frame for background asymptotic channels. By calculating the multiplication of $U = U^0 V$ and by noting that the U matrix is composed of eigenvectors u_+ and u_- of the S matrix as

$$U = (u_+ \quad u_-), \quad (47)$$

the eigenvectors of the S matrix are obtained as

$$u_+ = \begin{bmatrix} \cos\left(\frac{\theta'_a}{2}\right) \\ \sin\left(\frac{\theta'_a}{2}\right) \end{bmatrix}, \quad u_- = \begin{bmatrix} -\sin\left(\frac{\theta'_a}{2}\right) \\ \cos\left(\frac{\theta'_a}{2}\right) \end{bmatrix}, \quad (48)$$

where θ'_a is defined by

$$\theta'_a \equiv \theta_a + 2\theta^0. \quad (49)$$

B. S matrix in terms of new parameters

Let us now express the S matrix in terms of the parameters introduced in the preceding subsection. Reassembling by using its eigenvalues $e^{-2i\delta_+}$ and $e^{-2i\delta_-}$ ($\delta_\pm = \delta_\Sigma \pm \delta_a$) and eigenvectors (44), A becomes

$$A = \begin{pmatrix} v_+ & v_- \end{pmatrix} \begin{pmatrix} e^{-2i\delta_+} & 0 \\ 0 & e^{-2i\delta_-} \end{pmatrix} \begin{pmatrix} \tilde{v}_+ \\ \tilde{v}_- \end{pmatrix} = e^{-i\delta_\Sigma} \begin{pmatrix} \cos \delta_a - i \sin \delta_a \cos \theta_a & -i \sin \delta_a \sin \theta_a \\ -i \sin \delta_a \sin \theta_a & \cos \delta_a + i \sin \delta_a \cos \theta_a \end{pmatrix}. \quad (50)$$

From the relation $S = U^0 A \tilde{U}^0$ with U^0 matrix defined in Eq. (46), the S matrix is obtained as

$$S = e^{-i\delta_\Sigma} \begin{pmatrix} \cos \delta_a - i \sin \delta_a \cos \theta'_a & -i \sin \delta_a \sin \theta'_a \\ -i \sin \delta_a \sin \theta'_a & \cos \delta_a + i \sin \delta_a \cos \theta'_a \end{pmatrix}, \quad (51)$$

where θ'_a is defined in Eq. (49). Using Pauli matrices, it can be transformed into an invariant form

$$S = e^{-i\delta_\Sigma} \{ \cos \delta_a - i \sin \delta_a [\sigma_z \cos \theta'_a + \sigma_x \sin \theta'_a] \} \quad (52)$$

$$= e^{-i\delta_\Sigma} (\cos \delta_a - i \sin \delta_a \vec{\sigma} \cdot \hat{n}_{\theta'_a}), \quad (53)$$

where the unit vector $\hat{n}_{\theta'_a}$ is defined as

$$\hat{n}_{\theta'_a} \equiv \hat{z} \cos \theta'_a + \hat{x} \sin \theta'_a. \quad (54)$$

Since

$$\cos \delta_a - i \sin \delta_a \vec{\sigma} \cdot \hat{n}_{\theta'_a} = e^{-i\delta_a \vec{\sigma} \cdot \hat{n}_{\theta'_a}}, \quad (55)$$

it is simplified into the form of e^{iH} (H Hermitian):

$$S = e^{-i(\delta_\Sigma + \delta_a \vec{\sigma} \cdot \hat{n}_{\theta'_a})}. \quad (56)$$

Since $(\vec{\sigma} \cdot \hat{n}_{\theta'_a})^2 = 1$, $\vec{\sigma} \cdot \hat{n}_{\theta'_a}$ has two eigenvalues ± 1 . u_+ and u_- in Eq. (48) are their corresponding eigenvectors. In this case, it is well known [14] that the vectors $\pm \hat{n}_{\theta'_a}$ equal the expectation values of the Pauli spin operator ($u_\pm | \vec{\sigma} | u_\pm$) and are called the polarization vectors that correspond to the eigenstates u_\pm , respectively. We can obtain the change in the direction of the polarization axis as a function of energy by differentiating Eq. (54) with respect to ϵ_a :

$$\frac{d\hat{n}_{\theta'_a}}{d\epsilon_a} = \hat{y} \times \hat{n}_{\theta'_a} \frac{d\theta'_a}{d\epsilon_a}. \quad (57)$$

Since $\tan \theta_a = -1/\epsilon_a$,

$$\frac{d\theta'_a}{d\epsilon_a} = \frac{d\theta_a}{d\epsilon_a} = \frac{1}{1 + \epsilon_a^2}. \quad (58)$$

Equations (57) and (58) also appear in the spin model for the adiabatic analysis of collisions [15].

V. TIMES DELAYED BY A COLLISION NEAR A RESONANCE

A. Time delay matrix and eigentime delays

For a single-channel system, times delayed by a collision τ are obtained by the first derivatives of phase shifts

$$\tau(E) = 2\hbar \frac{d\delta(E)}{dE}. \quad (59)$$

For a multichannel system, we may consider the time delay matrix Q defined by [9,10]

$$Q = i\hbar \left(S^\dagger \frac{dS}{dE} \right). \quad (60)$$

The unitarity of the S matrix ensures that the time delay matrix Q is Hermitian. Let us now consider the time delay matrix for the system of one discrete state and two continua. Using Eq. (53) for the S matrix expressed in terms of the

Pauli matrices, the first derivative of the S matrix with respect to energy is calculated as

$$\begin{aligned} \frac{dS}{dE} &= -i \frac{d\delta_\Sigma}{dE} S + e^{-i\delta_\Sigma} (-\sin \delta_a - i \cos \delta_a \vec{\sigma} \cdot \hat{n}_{\theta'_a}) \\ &\times \frac{d\delta_a}{dE} + e^{-i\delta_\Sigma} \left(-i \sin \delta_a \vec{\sigma} \cdot \frac{d\hat{n}_{\theta'_a}}{dE} \right). \end{aligned} \quad (61)$$

Now the time delay matrix Q is obtained as

$$\begin{aligned} i\hbar S^\dagger \frac{dS}{dE} &= \hbar \frac{d\delta_\Sigma}{dE} + \vec{\sigma} \cdot \hat{n}_{\theta'_a} \hbar \frac{d\delta_a}{dE} \\ &+ \sin \delta_a \vec{\sigma} \cdot [\hat{y} \times \hat{n}_{\theta'_a} \cos \delta_a - \hat{y} \sin \delta_a] \left(\hbar \frac{d\theta'_a}{dE} \right). \end{aligned} \quad (62)$$

Since $\hat{n}_{\theta'_a} \times \hat{y}$ and \hat{y} are perpendicular to $\hat{n}_{\theta'_a}$, their linear combination is also perpendicular to $\hat{n}_{\theta'_a}$. Let us introduce a vector

$$\hat{n}_{\theta'_a}^\perp \equiv \hat{y} \times \hat{n}_{\theta'_a} \cos \delta_a - \hat{y} \sin \delta_a, \quad (63)$$

perpendicular to $\hat{n}_{\theta'_a}$ and making an angle δ_a with $\hat{n}_{\theta'_a} \times \hat{y}$, and also define the quantities

$$\tau_r \equiv 2\hbar \frac{d\delta_r}{dE}, \quad \tau_a \equiv 2\hbar \frac{d\delta_a}{dE}, \quad \tau_f \equiv 2\hbar \sin \delta_a \frac{d\theta'_a}{dE}. \quad (64)$$

The last three quantities correspond to the time delay due to the resonance, the avoided crossing interaction, and the change of the direction of the eigenvectors $\hat{n}_{\theta'_a}$ of the S matrix, usually termed the frame change, as a function of energy, respectively. Then the time delay matrix Q may be written as

$$Q = \frac{1}{2} (\tau_r + \vec{\sigma} \cdot \hat{n}_{\theta'_a} \tau_a + \vec{\sigma} \cdot \hat{n}_{\theta'_a}^\perp \tau_f). \quad (65)$$

Since the observable properties of a particle with spin $\frac{1}{2}$ can be represented as a function of its spin polarization \vec{P} and the states of all the two-level (two-continua here) systems can be mapped onto the states of orientation of a particle with spin $\frac{1}{2}$, Q may be rewritten in terms of the polarization vectors as

$$Q = \frac{1}{2} \tau_r (1 + \vec{P}_a \cdot \vec{\sigma} + \vec{P}_f \cdot \vec{\sigma}), \quad (66)$$

where polarization vectors are defined as

$$\vec{P}_a \equiv \frac{\tau_a}{\tau_r} \hat{n}_{\theta'_a}, \quad \vec{P}_f \equiv \frac{\tau_f}{\tau_r} \hat{n}_{\theta'_a}^\perp. \quad (67)$$

The degrees of polarization $|\vec{P}_a|$ and $|\vec{P}_f|$ will be denoted simply as P_a and P_f . They are positive by definition (the

term polarization may not be adequate for the time delay matrix; we will return to this point later). Let us introduce a new unit vector

$$\hat{n}_t = \hat{n}_{\theta'_a} \frac{\tau_a}{\sqrt{\tau_a^2 + \tau_f^2}} + \hat{n}_{\theta'_a}^\perp \frac{\tau_f}{\sqrt{\tau_a^2 + \tau_f^2}}. \quad (68)$$

Then Eqs. (65) and (67) become

$$Q = \frac{1}{2} (\tau_r + \vec{\sigma} \cdot \hat{n}_t \sqrt{\tau_a^2 + \tau_f^2}) = \frac{1}{2} \tau_r (1 + \vec{P}_t \cdot \vec{\sigma}), \quad (69)$$

where

$$\vec{P}_t \equiv \sqrt{P_a^2 + P_f^2} \hat{n}_t. \quad (70)$$

Now eigenvalues of the time delay matrix Q or eigentime delays, which will be denoted as τ_\pm , are easily obtained as

$$\tau_\pm = \frac{1}{2} (\tau_r \pm \sqrt{\tau_a^2 + \tau_f^2}) = \frac{1}{2} \tau_r (1 \pm P_t). \quad (71)$$

Notice that τ_a and τ_f are added up incoherently to eigentime delays. Also, because $\text{tr}(\sigma_i) = 0$ ($i = x, y, z$),

$$\text{tr } Q = \tau_+ + \tau_- = \tau_r, \quad (72)$$

that is, the eigentime delay sum has the same form as that of the eigentime delay in the single-channel scattering [16].

B. Explicit formulas of time delays

The time delay due to the resonance, the first term of Eq. (71), is obtained by differentiating $\tan \bar{\delta}_r = -1/\epsilon_r$ with respect to ϵ_r as

$$\bar{\tau}_r(\epsilon_r) \equiv 2\hbar \frac{d\bar{\delta}_r(\epsilon_r)}{d\epsilon_r} = \frac{2\hbar}{1 + \epsilon_r^2}. \quad (73)$$

It takes the Lorentzian form and is thus always positive or delayed as it is kept temporarily by the quasibound state.

The form of the time delay due to avoidance, the second term of Eq. (71), is rather complex:

$$\tau_a(E) = 2\hbar \frac{d\delta_a}{dE} = \frac{-2\hbar \left[\frac{1}{2} \Delta \Gamma (E - E_0) \sin \Delta_{12}^0 - \left(\frac{\Gamma}{2} \right)^2 \cos \Delta_{12}^0 \right]}{\left[(E - E_0)^2 + \left(\frac{\Gamma}{2} \right)^2 \right] \left\{ \Gamma_1 \Gamma_2 + \left[(E - E_0) \sin \Delta_{12}^0 - \frac{1}{2} \Delta \Gamma \cos \Delta_{12}^0 \right]^2 \right\}^{1/2}}. \quad (74)$$

By changing the independent variable from E to ϵ_r , considering the reduced time delays $\bar{\tau}_a [= 2\hbar(d\delta_a/d\epsilon_r)]$, and introducing the new parameters r^2 and q_τ defined by

$$r^2 \equiv \frac{\Gamma^2 - \Delta \Gamma^2}{\Delta \Gamma^2}, \quad (75)$$

$$q_\tau \equiv \frac{\Gamma}{\Delta \Gamma} \cot \Delta_{12}^0, \quad (76)$$

Eq. (74) is simplified as

$$\bar{\tau}_a(\epsilon_r) = -\bar{\tau}_r(\epsilon_r) \frac{\epsilon_r - q_\tau}{\sqrt{(\epsilon_r - q_\tau)^2 + r^2(1 + \epsilon_r^2)}}. \quad (77)$$

The factor multiplying $\bar{\tau}_r(\epsilon_r)$ in Eq. (77) can be transformed to the functional of the Beutler-Fano formula [the Lorentzian shape of $\bar{\tau}_r(\epsilon_r)$ may be regarded as a Beutler-Fano shape]

$$\bar{\tau}_a(\epsilon_r) = \begin{cases} \bar{\tau}_r(\epsilon_r) \frac{1}{\sqrt{1 + r^2} \frac{1 + \epsilon_r^2}{(\epsilon_r - q_\tau)^2}} & \text{when } \epsilon_r \leq q_\tau \\ -\bar{\tau}_r(\epsilon_r) \frac{1}{\sqrt{1 + r^2} \frac{1 + \epsilon_r^2}{(\epsilon_r - q_\tau)^2}} & \text{when } \epsilon_r > q_\tau \end{cases} = \begin{cases} \bar{\tau}_r(\epsilon_r) \sqrt{\frac{f_{\text{BF}}(\epsilon_r, q_\tau)}{f_{\text{BF}}(\epsilon_r, q_\tau) + r^2}} & \text{when } \epsilon_r \leq q_\tau \\ -\bar{\tau}_r(\epsilon_r) \sqrt{\frac{f_{\text{BF}}(\epsilon_r, q_\tau)}{f_{\text{BF}}(\epsilon_r, q_\tau) + r^2}} & \text{when } \epsilon_r > q_\tau \end{cases} \equiv \bar{\tau}_r(\epsilon_r) g_a(\epsilon_r). \quad (78)$$

Interestingly, $\bar{\tau}_a$ takes the Beutler-Fano formula in the energy scale of ϵ_r instead of ϵ_a in contrast to the case of $\bar{\delta}_a$, though the former is obtained as the derivative of the latter. Notice that the absolute value of g_a is the polarization P_a considered in Sec. V A:

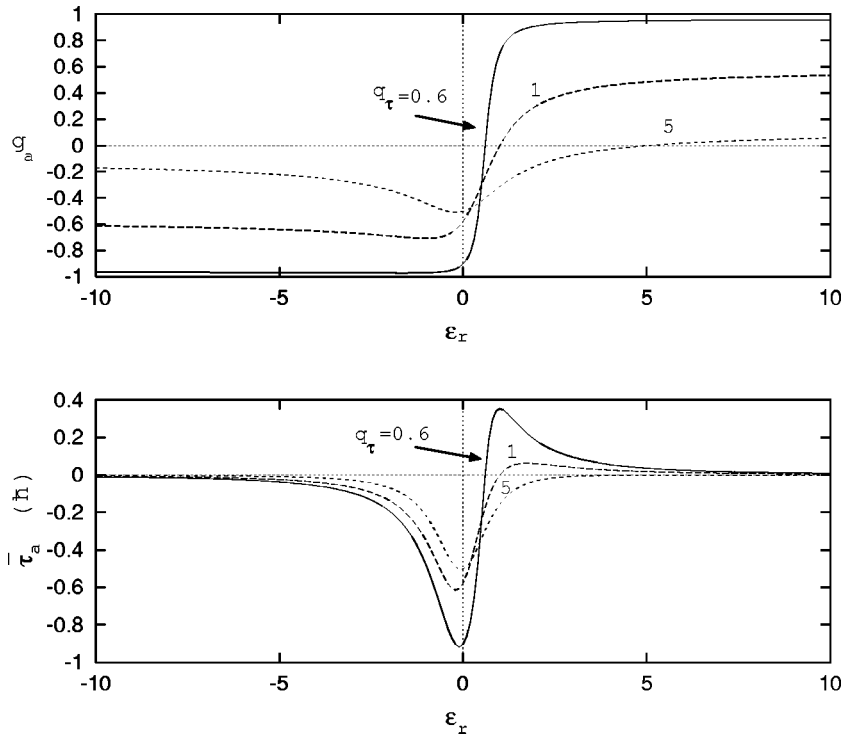


FIG. 2. $g_a(\epsilon_r)$ and $\bar{\tau}_a(\epsilon_r)$ vs ϵ_r are plotted for three different profile indices $q_\tau=0.6, 1,$ and 5 with $\Delta_{12}^0=\pi/3$.

$$P_a = \sqrt{\frac{f_{BF}(\epsilon_r, q_\tau)}{f_{BF}(\epsilon_r, q_\tau) + r^2}} \quad (79)$$

g_a changes its sign at $\epsilon_r = q_\tau$; so does the polarization vector \vec{P}_a at the same energy. The study of P_a as a function of ϵ_r shows that P_a has a maximum of $\sqrt{(1+q_\tau^2)/(1+q_\tau^2+r^2)}$ at $\epsilon_r = -1/q_\tau$ and a minimum of 0 at $\epsilon_r = q_\tau$ (which corresponds to $\epsilon_a = -1/q_a$ where δ_a has an extremum). Figure 2 shows the variations in the behaviors of $g_a(\epsilon_r)$ and $\bar{\tau}_a(\epsilon_r)$ as functions of ϵ_r at three different profile indices q_τ with Δ_{12}^0 fixed (the value of q_τ is restricted by $|q_\tau/\cot \Delta_{12}^0| \geq 1$).

Recalling that $f_{BF}(\epsilon_r, q_\tau) \geq 0$, Eq. (79) tells us that the magnitude of $P_a(\epsilon_r)$ is smaller than or equal to unity and has the effect of making the absolute magnitude of the time delay $\bar{\tau}_a$ due to an avoidance smaller than or equal to that of the time delay $\bar{\tau}_r$ due to a resonance:

$$\bar{\tau}_r(\epsilon_r) \geq |\bar{\tau}_a(\epsilon_r)|, \quad (80)$$

which ensures that $\bar{\tau}_r(\epsilon_r) \pm \bar{\tau}_a$ are positive. The inequality (80) may be obtained without knowing the explicit functional dependences of τ_r and τ_a as functions of energy. Notice that

$$\tau_r \pm \tau_a = 2\hbar \frac{d(\delta_r \pm \delta_a)}{dE} = 2\hbar \frac{d\delta_\pm}{dE}. \quad (81)$$

Because of the inequality (22), Eq. (81) should be larger than or equal to zero, which proves Eq. (80). This inequality is the manifestation of the physical fact that eigenphase shifts are increasing functions of energy in the neighborhood of a reso-

nance as colliding particles are kept bound temporarily around a resonance (attractive forces make positive phase shifts).

The above inequality restricts the magnitude of P_a to $0 \leq P_a \leq 1$. The magnitude of P_a causes the difference between two eigentime delays. Equation (79) tells us that the degree of difference in the two eigentime delays is governed by r^2 . Let us consider r^2 as a function of $x = \Gamma_1/\Gamma$ ($0 \leq x \leq 1$). Then, since r^2 is symmetric with respect to $x = \frac{1}{2}$ and its values are zero at $x=0$ and 1 and infinity at $x = \frac{1}{2}$, the magnitudes of P_a are 1 at $x=0$ and 0 at $x = \frac{1}{2}$. Since the avoided crossing interaction is strongest at $x = \frac{1}{2}$, the difference in two eigentimes delayed due to an avoided crossing completely disappears when the avoided crossing interaction is strongest.

Let us now consider obtaining the explicit formula of the times delayed due to a frame change. By substituting Eq. (58) and

$$\sin \delta_a = \frac{\Gamma_a}{\Gamma} \sin \Delta_{12}^0 \sqrt{\frac{\epsilon_a^2 + 1}{\epsilon_r^2 + 1}} \quad (82)$$

into Eq. (64), the time delay τ_f due to the frame change is obtained as

$$\tau_f = \tau_r \sin \Delta_{12}^0 \sqrt{\frac{\epsilon_r^2 + 1}{\epsilon_a^2 + 1}} \equiv \tau_r g_f. \quad (83)$$

The absolute value of g_f is the same as P_f ,

$$P_f = |\sin \Delta_{12}^0| \sqrt{\frac{\epsilon_r^2 + 1}{\epsilon_a^2 + 1}} \quad (84)$$

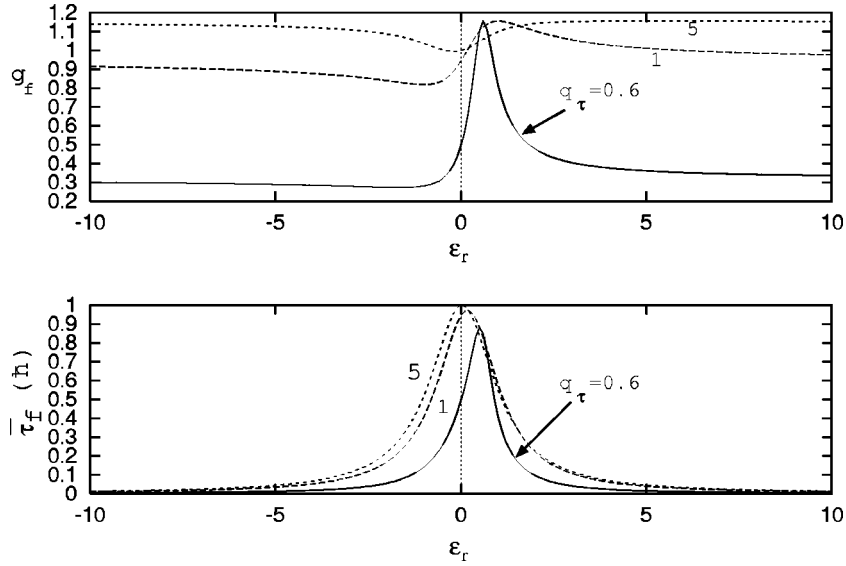


FIG. 3. $g_f(\epsilon_r)$ and $\bar{\tau}_f(\epsilon_r)$ vs ϵ_r are plotted for three different profile indices $q_\tau=0.6, 1,$ and 5 with $\Delta_{12}^0=\pi/6$.

[actually $g_f=P_f$ in the convention mentioned below Eq. (33)]. Figure 3 shows the variations in the behaviors of $P_f(\epsilon_r)$ and $\bar{\tau}_f(\epsilon_r)$ as functions of energy at three different profile indices q_τ with Δ_{12}^0 fixed.

As in the case of τ_a , P_f is smaller than or equal to unity. This can be proved by examining the behavior of the graph of P_f as a function of ϵ_r . P_f can be easily transformed as a function of ϵ_r by substituting

$$\epsilon_a = \frac{\Gamma}{\Gamma_a} \left(\epsilon_r - \frac{\Delta\Gamma}{\Gamma} \cot \Delta_{12}^0 \right) \quad (85)$$

for ϵ_a into Eq. (83). It is then differentiated with respect to energy to yield the roots of the first derivative of $\bar{\tau}_f(\epsilon_r)$ at $\epsilon_r = -1/q_\tau$ and q_τ . From this, it is found that P_f has the minimum of $\sin \Delta_{12}^0 \sqrt{1 - (\Delta\Gamma/\Gamma)^2}$ at $-1/q_\tau$ and the maximum of unity at q_τ . Its values become $\sqrt{1 - (\Delta\Gamma/\Gamma)^2}$ at $\epsilon_r \rightarrow \pm\infty$. This proves $0 \leq P_f \leq 1$.

Now let us consider the magnitude of the total polarization vector $P_t = \sqrt{P_a^2 + P_f^2}$. In order to obtain this, let us further transform Eq. (85) using the definition (33) of Γ_a and $\Delta\Gamma/\Gamma = \cot \Delta_{12}^0/q_\tau$ as

$$\epsilon_a = \frac{|\sin \Delta_{12}^0|}{\sqrt{1 - \left(\frac{\cot \Delta_{12}^0}{q_\tau}\right)^2}} \left(\epsilon_r - \frac{\cot^2 \Delta_{12}^0}{q_\tau} \right). \quad (86)$$

Also after some manipulation, we obtain the relation

$$(\epsilon_r - q_\tau)^2 + r^2(\epsilon_r^2 + 1) = \left(\frac{q_\tau}{\cot \Delta_{12}^0} \right)^2 \left[\left(\epsilon_r - \frac{\cot^2 \Delta_{12}^0}{q_\tau} \right)^2 + \frac{1 - \left(\frac{\cot \Delta_{12}^0}{q_\tau} \right)^2}{\sin^2 \Delta_{12}^0} \right]. \quad (87)$$

Using Eq. (86) to calculate $\epsilon_a^2 + 1$ and comparing the latter with the right-hand side of Eq. (87), we obtain

$$\epsilon_a^2 + 1 = \frac{\sin^2 \Delta_{12}^0}{r^2} [(\epsilon_r - q_\tau)^2 + r^2(\epsilon_r^2 + 1)], \quad (88)$$

where $r^2 = (q_\tau/\cot \Delta_{12}^0)^2 - 1$ is used. Substituting Eq. (88) into Eq. (84), P_f can be put into a functional of the Beutler-Fano formula

$$P_f = \frac{r}{\sqrt{f_{\text{BF}}(\epsilon_r, q_\tau) + r^2}}. \quad (89)$$

From Eqs. (89) and (79) we obtain the surprising result

$$P_a^2 + P_f^2 = 1. \quad (90)$$

This means that eigentime delays for the system of one discrete state and two continua are zero and $\tau_r(\epsilon_r)$. Though time delays due to the avoided crossing interaction and frame change are asymmetric with respect to the resonance energy and therefore the energy of the longest lifetime is not matched with the resonance energy, the energy of the longest overall eigentime delays is exactly matched with the resonance energy.

VI. RESULTS AND DISCUSSION

Let us summarize the results. In this paper we considered eigenphase shifts and eigentime delays near a resonance for a system of one discrete state and two continua using Fano's configuration interaction theory. The eigenphase shifts are obtained as

$$2\delta_\pm(E) = \sum_i \delta_i^0 + \delta_r(E) \pm \delta_a(E),$$

where $\delta_r(E)$ is the phase shift due to the modification of the scattering wave by the quasibound state and is given by $-\arctan(1/\epsilon_r)$, and $\delta_a(E)$ is the one due to the modification

of the scattering wave by the other wave through the indirect interaction via the quasibound state and given as a functional of the Beutler-Fano formula

$$\cot \delta_a(E) = -\cot \Delta_{12}^0 \frac{\epsilon_a - q_a}{(1 + \epsilon_a^2)^{1/2}}.$$

In the above formula, energy is expressed in units of $\Gamma_a = 2\sqrt{\Gamma_1\Gamma_2}/|\sin \Delta_{12}^0|$ and is shifted from the resonance energy E_0 by $(\Delta\Gamma/2)\cot \Delta_{12}^0$. The shape of the curve of $\delta_a(E)$ is characterized by the line profile index $q_a = -2\Delta\Gamma/(2\sqrt{\Gamma_1\Gamma_2}\cos \Delta_{12}^0)$. The strength of the avoided crossing interaction experienced by the eigenphase shifts is governed by the magnitude of Γ_a . No shift is expected when $\Gamma_1 = \Gamma_2$, where the strength of the avoided crossing interaction is strongest. The maximum shift obtains when either Γ_1 or Γ_2 is zero.

Eigenvectors v_{\pm} of A of $S = S^0A$ corresponding to eigenvalues $\delta_{\pm}(E)$ are obtained as

$$v_+ = \begin{bmatrix} \cos\left(\frac{\theta_a}{2}\right) \\ \sin\left(\frac{\theta_a}{2}\right) \end{bmatrix}, \quad v_- = \begin{bmatrix} -\sin\left(\frac{\theta_a}{2}\right) \\ \cos\left(\frac{\theta_a}{2}\right) \end{bmatrix},$$

where θ_a is defined by

$$\cos \theta_a = -\frac{\epsilon_a}{\sqrt{1 + \epsilon_a^2}}, \quad \sin \theta_a = \frac{1}{\sqrt{1 + \epsilon_a^2}}.$$

Eigenvectors are independent of q_a . They depend only on ϵ_a . Since q_a stands for the separation of the avoided crossing point energy from the middle of asymptotes of the abscissas of two eigenphase shifts, the above result means that the characteristics of the avoided crossing interactions are independent of the asymptotes of the abscissas of the eigenphase shifts. The corresponding eigenvectors of the S matrix are obtained by replacing θ_a with $\theta'_a = \theta_a + 2\theta_0$.

With the new parameters, the S matrix is found to be expressible as

$$S = e^{-i(\delta_{\Sigma} + \delta_a \vec{\sigma} \cdot \hat{n}_{\theta'_a})},$$

where $\hat{n}_{\theta'_a} = \hat{z} \cos \theta'_a + \hat{x} \sin \theta'_a$. In terms of Pauli matrices, the time delay matrix $Q = i\hbar S^\dagger (dS/dE)$ is found to consist of three terms

$$Q = \frac{1}{2}(\tau_r + \vec{\sigma} \cdot \hat{n}_{\theta'_a} \tau_a + \vec{\sigma} \cdot \hat{n}_{\theta'_a}^\perp \tau_f),$$

one due to the resonance, one due to the avoided crossing interaction, and one due to the change of frame as a function of energy. Because of the last term, the eigenfunctions of the Q matrix are different from those of the S matrix.

The time delay due to the resonance takes a symmetric Lorentzian form and the time delay due to the avoided crossing takes a form of a functional of the Beutler-Fano formula

$$\tau_a(E) = \begin{cases} -\tau_r(E) \frac{1}{\sqrt{1+r^2} \frac{1+\epsilon_r^2}{(\epsilon_r - q_r)^2}} & \text{when } \epsilon_r \leq q_r \\ \tau_r(E) \frac{1}{\sqrt{1+r^2} \frac{1+\epsilon_r^2}{(\epsilon_r - q_r)^2}} & \text{when } \epsilon_r > q_r. \end{cases}$$

The asymmetry of τ_a as a function of energy is brought about by the nonzero value of q_r , which is proportional to the shift of the avoided crossing point energy from the resonance one. Thus the asymmetry of τ_a is caused by the mismatch in the positions of the avoided crossing point and resonance energies.

The time delay due to frame change takes the form

$$\tau_f(E) = \tau_r(E) \sin \Delta_{12}^0 \sqrt{\frac{\epsilon_r^2 + 1}{\epsilon_a^2 + 1}}.$$

The above form may be understood from the fact that the changes of the frame spanned by the eigenvectors of the S matrix is governed by $1 + \epsilon_a^2$, while the time delay due to the resonance is governed by $1 + \epsilon_r^2$. Therefore, the ratio of τ_a to τ_r will be a function of $(1 + \epsilon_r^2)/(1 + \epsilon_a^2)$. $\tau_f(E)$ is also found to be transformed into a functional of the Beutler-Fano formula.

In analogy with the spin $\frac{1}{2}$ system, the time delay matrix Q may be expressed in terms of the polarization vectors and the Pauli spin matrices as

$$Q = \frac{1}{2} \tau_r (1 + \vec{P}_a \cdot \vec{\sigma} + \vec{P}_f \cdot \vec{\sigma}),$$

where the polarization vectors are defined by

$$\vec{P}_a = \frac{\tau_a}{\tau_r} \hat{n}_{\theta'_a}, \quad \vec{P}_f = \frac{\tau_f}{\tau_r} \hat{n}_{\theta'_a}^\perp.$$

Like the spin $\frac{1}{2}$ system, it is found that the absolute values of \vec{P}_a and \vec{P}_f are restricted to $0 \leq |\vec{P}_a| \leq 1$ and $0 \leq |\vec{P}_f| \leq 1$. In the present case a complete depolarization means that eigentime delays are the same regardless of eigenchannels, while a complete polarization means that eigentime delays are 0 and $\tau_r(E)$ as a function of energy. Eigenvectors for eigentime delays due to an avoided crossing interaction and due to a frame change are orthogonal to each other and contribute to the total eigentime delays as $\sqrt{\tau_a^2 + \tau_f^2} = \tau_r \sqrt{P_a^2 + P_f^2}$. It is found that $P_a^2 + P_f^2 = 1$. This means that one of the two total eigentime delays is zero while the other one is the same as the time delayed by the resonance state. Though time delays due to an avoided crossing interaction and a frame change are asymmetric with respect to the resonance energy and therefore the energy of the longest lifetime does not match the resonance energy, the energy of the longest overall eigentime delays exactly matches the resonance energy. Though this is a surprising result, it should rather be so if we recall that all the partial lifetimes obtained from the partial photo-dissociation cross sections as a function of energy are the

same in the system of one discrete state and many continua. However, the detailed study on their connection is beyond the scope of this paper.

The present work reveals the dynamical parameters that govern the behaviors of eigenphase shifts and eigentime delays for the system of one discrete state and two continua. It may be applied to the systems of more than two continua by approximating that such systems are a cascade of independent two interacting continua. In that sense, the current study may be considered as a prototypical model for the "isolated" avoided crossing interaction. For the system of one discrete state and three or four continua, Eq. (19) becomes a third- or fourth-order equation and its solution can be ob-

tained by Cartan and Ferrari's method [17]. It may be highly desirable to do similar studies on these systems.

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- $$\sin \delta_a = \frac{\Gamma_a}{\Gamma} \sin \Delta_{12}^0 \sqrt{\frac{1 + \epsilon_a^2}{1 + \epsilon_r^2}}, \quad \cos \delta_a = -\frac{\Gamma_a}{\Gamma} \cos \Delta_{12}^0 \frac{\epsilon_a - q_a}{\sqrt{1 + \epsilon_r^2}},$$
- whose forms are consistent with those for θ_a and δ_r defined in Eqs. (45) and (4).
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