Geometrical Construction of the *S* Matrix and Multichannel Quantum Defect Theory for the two Open and One Closed Channel System

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The multichannel quantum defect theory (MQDT) is reformulated into the form of the configuration mixing (CM) method using the geometrical construction of the ***S*** matrix developed for the system involving two open and one closed channels. The reformulation is done by the phase renormalization method of Giusti-Suzor and Fano. The rather unconventional short-range reactance matrix K whose diagonal elements are not zero is obtained though the Lu-Fano plot becomes symmetrical. The reformulation of MQDT yields the partial cross section formulas analogous to Fano's resonance formula, which has not easily been available in other's work.

Keywords : MQDT, Resonance, Configuration interaction theory.

Introduction

I recently made a geometrical construction of the ***S*** matrix for the system involving two continua and one discrete state[1,2] in the context of the configuration-mixing (CM) method of Fano.[3] In this paper, I will apply this newly developed geometrical method to the reformulation of the multichannel quantum defect theory (MQDT)[4] into the form of the CM one for the system involving two open and one closed channels. The configuration-mixing method and the multichannel quantum defect theory are two widely used resonance theories and have their own advantages and disadvantages. The configuration-mixing method assumes the presence of discrete states from the outset, which has an advantage of treating the background and resonance contributions directly but making it impossible to treat the whole spectrum including bound states and continua in a unified manner. Multichannel quantum defect theory overcomes this limitation by not explicitly assuming the presence of discrete states. However, as resonances are handled indirectly, it is not obvious how to identify the resonance terms from the background ones or to show the resonance structures transparently in formulas for observables. Therefore, it is worth reformulating MQDT so that it has all the traits of both theories.

The first piece of work on this line was done by Giusti-Suzor and Fano[5] for a two channel system. They noticed that the usual Lu-Fano plot often obscures the symmetry of the plot. If the origin of the plot is moved to its center of symmetry by the use of the phase-shifted base pair as

$$(f, g) \rightarrow (f\cos \pi\mu - g \sin \pi\mu, g \cos \pi\mu + f \sin \pi\mu), \quad (1)$$

the diagonal elements of a short-range reactance matrix K become zero so that there remains only the coupling strength between open and closed channels. In this way, resonance structures are separated from background ones and their properties are easily studied in the new representation.

The generalizations of their method to the general system involving arbitrary numbers of open and closed channels were done by Cooke and Cromer,[6] Lecomte,[7] Ueda,[8] Giusti-Suzor and Lefebvre-Brion,[9] Wintgen and Fridrich,[10] and Cohen.[11] All the generalizations utilize the simplifications and the transparent resonance structures in the formulations derived from the zeros of diagonal blocks of the short-range reactance matrices. Only total cross section formulas for photoionization processes have been dealt in their work.

In this paper, we will adopt a different approach in which we seek the MQDT formulation identical to the one of the CM theory by comparing their physical scattering matrices. Transforming the ***S*** matrix of the MQDT formulation into the form of the CM theory can be done with the phase renormalization by Giusti-Suzor and Fano without the need of utilizing the more powerful transformation considered by Lecomte and Ueda.[7,8] Dealing the effects of the phase renormalization on ***S*** or equivalently on the phase shift matrix[12] Δ defined by $S = \exp(-2i\Delta)$ is not a simple task for systems involving more than two channels since eigenchannels for the phase renormalization and the ones for ***S*** or Δ are of different characters. If only two open channels are involved, it can be studied with the geometrical method developed in Ref. [1, 2]. By making use of the phase renormalization and the geometrical method together, we will find in this paper the representation in which MQDT gives the identical form of scattering matrix with the CM one and thus we will eventually relate the elements of the short-range reactance matrix K to the geometrical parameters of the CM theory. The reformulation will allow us to obtain the simple formula for the time delay due to the presence of closed channels and the partial cross section formulas analogous to Fano's resonance formula which has not easily been available in other's work.

Section 2 briefly describes the multichannel quantum defect theory. Then the phase renormalization is described in Section 3. Section 4 summarizes the construction of the ***S*** matrix by

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the geometrical method in the CM theory. Reformulation of the MQDT formulation into the one of the CM theory is considered in Section 5. Section 6 considers the contribution of the closed channels and Section 7 derives the partial photofragmentation cross section formulas. Finally, the summary and discussion are given in Section 8.

The Brief Introduction of the Multichannel Quantum Defect Theory

In the multichannel quantum defect theory, the fragmentation coordinate R is divided into two regions $R < R_0$ and $R > R_0$, the inner and outer regions, respectively. In the inner region, transfers in energy, momentum, angular momentum, spin, or the formation of a transient complex occur due to the presence of the strong interaction between the colliding partners there. In the outer region, channels are decoupled and the motion of a system is governed by the ordinary second-order differential equations and described by the superposition of the regular and irregular solutions for each channel, say $f_j(R)$ and $g_j(R)$, for the j-th channel. For the N-channel system, the N independent solutions in the outer region can be taken as

$$\Psi_i(R, \omega) = \sum_j \Phi_j(\omega)\,[f_j(R)\delta_{ji} - g_j(R)K_{ji}],\ (j = 1, ..., N) \quad (2)$$

where R is the coordinate for the relative motion of colliding partners and $\Phi_j(\omega)$ are the channel basis functions for the remaining coordinate space (notice that Ψ_i are not orthogonal functions but used more widely than the orthonormal ones[13]). The corresponding N independent solutions describing the motion in the inner region are described by

$$\Psi_i(R, \omega) = \sum_j \Phi_j(\omega)\,\chi_{ji}(R), \quad (3)$$

where the radial functions are obtained by solving, for example, close-coupled equations starting from the origin. By imposing the condition that the values of the wavefunctions are zero in the origin, solutions are ensured to be the regular ones. The wavefunctions (2) in the outer region are then determined by the continuous conditions of $\Psi_i(R, \omega)$ and their first derivatives at the matching radius R_0. The base pair $f_j(R)$ and $g_j(R)$ can be given by analytic formulas for the long-range potentials like Coulomb or dipole ones. But for the zero field, the pair can only be obtained numerically, for example, by the Milne method proposed in Ref. [14].

Though motions are decoupled in the outer region, closed channels are still effective and remained in the summation of Eq. (2). But in the asymptotic region, the system can no longer stay in the closed channels and the contribution of the exponentially rising term should be zero. The number of independent solutions which remain finite in the whole space will be equal to the number of open channels. Let us denote the independent solutions as $\mathbf{\Psi}_\rho$. They can be expressed into the linear combinations of the N independent standing wave solutions (2) as

$$\mathbf{\Psi}_\rho = \sum_{i\in P} \Psi_i Z_{i\rho}\cos\delta_\rho + \sum_{i\in Q} \Psi_i Z_{i\rho}\cos\beta_i, \quad (4)$$

where P and Q denote the sets of open and closed channels, respectively, δ_ρ are the eigenphase shifts for the $\boldsymbol{K}$ matrix which will be defined later in Eq. (13), and β_i is the accumulated phase shift in the i-th closed channel defined in Ref. [14]. The factor $\cos\delta_\rho$ is introduced in two respects: to make $Z_{i\rho}$ ($i \in P$) orthonormal and to normalize Ψ_i in energy. The factor $\cos\beta_i$ plays the similar role. Substituting the asymptotic forms of the regular and irregular base pair for the open channels given by

$$f_i(R) \to \sqrt{\frac{2m_i}{\pi k_i}}\sin(k_iR + \eta_i),$$
$$g_i(R) \to -\sqrt{\frac{2m_i}{\pi k_i}}\cos(k_iR + \eta_i), \quad (5)$$

and for the closed channels given by[14]

$$f_i(R) \to \sqrt{\frac{m_i}{\pi\kappa_i}}(\sin\beta_iD_i^{-1}e^{\kappa_iR} - \cos\beta_iD_ie^{-\kappa_iR}),$$
$$g_i(R) \to -\sqrt{\frac{m_i}{\pi\kappa_i}}(\cos\beta_iD_i^{-1}e^{\kappa_iR} + \sin\beta_iD_ie^{-\kappa_iR}). \quad (6)$$

into Eq. (2) and setting the coefficient of the exponentially rising term in Eq. (4) to zero, we get

$$\sum_{i\in Q}(K_{ji} + \tan\beta_j\delta_{ji})Z_{i\rho}\cos\beta_i + \sum_{i\in P}K_{ji}Z_{i\rho}\cos\delta_\rho = 0, \quad (j \in Q). \quad (7)$$

Parameters m_i, $\hbar k_i$, and η_i in Eq. (5) denote the reduced mass for the relative motion of photofragments along R when the core is in the i-th channel state, the momentum, and the phase shifted in that relative motion, respectively. The parameters $i\kappa_i$ in Eq. (6) is the analytical continuation of k_i in closed channels. For the definition of D_i in the same equation, see Ref. [14]. From the asymptotic form of $\mathbf{\Psi}_\rho$:

$$\mathbf{\Psi}_\rho \to \sum_{j\in P}\sqrt{\frac{2m_j}{\pi k_j}}\Phi_jT_{j\rho}\sin(K_jR + \eta_j + \delta_\rho), \quad (8)$$

we have

$$Z_{j\rho} = T_{j\rho},$$
$$\sum_{i\in P}(K_{ji} - \tan\delta_\rho\delta_{ji})Z_{i\rho}\cos\delta_\rho + \sum_{i\in Q}K_{ji}Z_{i\rho}\cos\beta_i = 0, \quad (j \in P). \quad (9)$$

Eqs. (7) and (9) have a nontrivial solution only when the equation

$$\begin{vmatrix} K^{oo} - \tan\delta_\rho & K^{oc} \\ K^{co} & K^{cc} + \tan\beta \end{vmatrix} = 0 \quad (10)$$

is satisfied. The formulas for $Z^c_{i\rho}$ are obtained from Eq. (7) as

$$Z^{c}_{i\rho}\cos\beta_i = -\sum_{j\in Q,k\in P}(K^{cc}+\tan\beta)^{-1}_{ij}K^{co}_{jk}T_{k\rho}\cos\delta_\rho. \quad (11)$$

where super-indices are added to indicate to which of open and closed channels the row and column indices of the K matrix and Z belong. Substituting Eq. (11) for $Z^{c}_{i\rho}$ and after some manipulations, Eq. (9) can be written into an eigenvalue equation for $\boldsymbol{K}$:

$$\sum_{i\in P}\boldsymbol{K}_{ji}T_{i\rho}\cos\delta_\rho = \tan\delta_\rho T_{j\rho}\cos\delta_\rho, \quad (12)$$

where the $\boldsymbol{K}$ matrix denotes

$$\boldsymbol{K} = K^{oo} - K^{oc}(K^{cc}+\tan\beta)^{-1}K^{co}. \quad (13)$$

The asymptotic form Ψ_ρ is obtained as $\sum_{i,j\in P}\Phi_i(f_i\delta_{ji} - g_i\boldsymbol{K}_{ji})T_{i\rho}\cos\delta_\rho$, showing that $\boldsymbol{K}$ is the reactance matrix in the asymptotic region.

In the multichannel quantum defect theory, the complex resonance spectra occurring in the photofragmentation and collision processes are explained in terms of only a few parameters, the energy-insensitive short-range K matrix, or its eigenphase shifts and eigenvectors μ_α and $U_{i\alpha}$, and the long-range quantum defect parameters η_i and β_i. The complicated behaviors of the spectra are brought about by the boundary conditions in the asymptotic region. These spectra are described by the incoming wavefunctions $\Psi^{(-)}_j$ (j = 1, ..., N_o) whose forms in the asymptotic region are given by

$$\Psi^{(-)}_j \to \frac{1}{2i}\sum_{i\in P}\sqrt{\frac{2m_i}{\pi k_j}}\Phi_i(f^{+}_i\delta_{ij} - f^{-}_i\boldsymbol{S}_{ij}) \quad (14)$$

and can be obtained by the linear combination of the fragmentation eigenchannels Ψ_ρ. In Eq. (14), $f_i^{\pm}$ denote $\exp(\pm ik_ir)$.

The Phase Renormalization

Intra- and inter-channel couplings are usually entangled in solutions of Eqs. (7) and (9), or equivalently, of the secular equation (10), which makes the identification of the resonance structures in the solutions difficult. Giusti-Suzor and Fano[5] used the transformation, called the phase renormalization, originally considered by Eissner and Seaton[15] for the different purpose, to separate out an inter-channel coupling from the intra-ones by making the diagonal elements of the reactance matrix K zero and thus were able to identify the resonance structures clearly. Their work was extended by Cooke and Cromer,[6] Lecomte,[7] Ueda,[8] Giusti-Suzor and Lefebvre-Brion,[9] Wintgen and Fridrich,[10] and Cohen.[11] Though their work, especially the one by Lecomte and Ueda, is essential in investigating full resonance structures in the MQDT formulation, the phase renormalization is enough for the purpose of the present work, *i.e.*, of reformulating the MQDT into the form of the CM theory. Phase renormalization utilizes the freedom we have in defining basis pairs used in Eq. (2). The pair of functions obtained by shifting phases in a basis pair defined in the outer region can still be used as a basis pair in the same region. The phase renormalization may be regarded as being caused by the change of potential in the inner region. The potential used as a reference in the inner region to define the basis pair in the outer region is considered by Mies and named as the reference potential.[16] If the potential is not taken zero in the inner region, the base pair contains the contributions from the short-range potentials and the long- and short-range contributions are no longer treated separately in the MQDT formulation. But still the long-range contributions are absent in the short-range K matrix. The change in reference potentials brings about the changes in the phase shifts η_i and β_j, defined in Eqs. (5) and (6), by $\pi\mu_j$ as

$$\tilde{\eta}_j = \eta_j + \pi\mu_j \quad \text{for} \quad j\in P,$$
$$\tilde{\beta}_j = \beta_j + \pi\mu_j \quad \text{for} \quad j\in Q, \quad (15)$$

where the tilde is used to denote new phase shifts. The transformations (15) of phase shifts correspond to the transformations of the base pairs as

$$\tilde{f}_j = f_j\cos\pi\mu_j - g_j\sin\pi\mu_j,$$
$$\tilde{g}_j = f_j\sin\pi\mu_j + g_j\cos\pi\mu_j, \quad (16)$$

and of the N independent standing wavefunctions as

$$\Psi_i = \sum_j\Phi_j(f_j\delta_{ji} - g_jK_{ji}),$$
$$\tilde{\Psi}_i = \sum_j\Phi_j(\tilde{f}_j\delta_{ji} - \tilde{g}_j\tilde{K}_{ji}). \quad (17)$$

The K matrices and standing wavefunctions are similarly transformed as

$$\tilde{K} = (K\sin\pi\mu + \cos\pi\mu)^{-1}(K\cos\pi\mu - \sin\pi\mu), \quad (18)$$
$$\tilde{\Psi} = \Psi(\cos\pi\mu - \sin\pi\mu\tilde{K}), \quad (19)$$

respectively. Transformation between fragmentation eigenchannels Ψ_ρ and $\tilde{\Psi}_\rho$ in the asymptotic region defined by

$$\Psi_\rho = \sum_{j\in P}\Phi_jT_{j\rho}(f_j\cos\delta_\rho - g_j\sin\delta_\rho),$$
$$\tilde{\Psi}_\rho = \sum_{j\in P}\Phi_j\tilde{T}_{j\rho}(\tilde{f}_j\cos\tilde{\delta}_\rho - \tilde{g}_j\sin\tilde{\delta}_\rho) \quad (20)$$

will not be considered as it is irrelevant to the present work.

Finally, let us consider the transformation relations between $\boldsymbol{S}$ and $\tilde{\boldsymbol{S}}$ matrices. For this purpose, it is convenient to define a little different incoming wavefunction $\Psi(\eta)^{(-)}_j$ whose asymptotic form is given by

$$\Psi(\eta)^{(-)}_j \to \frac{1}{2i}\sum_{i\in P}\Phi_i\sqrt{\frac{2m_i}{\pi k_j}}(e^{i(k_iR+\eta_i)}\delta_{ij} - e^{-i(k_iR+\eta_i)}\boldsymbol{S}(\eta)_{ij}) \quad (21)$$

instead of the usual $\Psi_j^{(-)}$ whose asymptotic form is given by Eq. (14). The usual $\Psi_j^{(-)}$ can be written as $\boldsymbol{\Psi}(0)_j^{(-)}$ in this definition and $\boldsymbol{S}$ as $\boldsymbol{S}(0)$. If we consider $\boldsymbol{\Psi}(\tilde{\eta})_j^{(-)}$ corresponding to a new reference potential, its asymptotic form will be given by

$$\boldsymbol{\Psi}(\tilde{\eta})_j^{(-)} \rightarrow \frac{1}{2i}\sum_{i\in P}\Phi_i\sqrt{\frac{2m_i}{\pi k_i}}\left(e^{i(k_iR+\tilde{\eta}_i)}\delta_{ij}-e^{-i(k_iR+\tilde{\eta}_i)}\boldsymbol{S}(\tilde{\eta})_{ij}\right)$$

$$=\frac{1}{2i}\sum_{i\in P}\Phi_i\sqrt{\frac{2m_i}{\pi k_i}}\left(e^{ik_iR}\delta_{ij}-e^{-ik_iR}e^{-i\tilde{\eta}_i}\boldsymbol{S}(\tilde{\eta})_{ij}e^{-i\tilde{\eta}_j}\right)e^{i\tilde{\eta}_j} \quad (22)$$

$$=\boldsymbol{\Psi}(0)_j^{(-)}e^{i\tilde{\eta}_j} \quad (23)$$

Eq. (22) yields the transformation relations among various scattering matrices

$$\boldsymbol{S}(0)_{ij}=e^{i\tilde{\eta}_i}\boldsymbol{S}(\tilde{\eta})_{ij}e^{i\tilde{\eta}_j}=e^{i\eta_i}\boldsymbol{S}(\eta)_{ij}e^{i\eta_j}, \quad (24)$$

and the corresponding ones for these incoming wavefunctions from Eq. (23) as

$$\Psi(0)_j^{(-)}=\Psi(\tilde{\eta})_j^{(-)}e^{i\tilde{\eta}_j}=\Psi(\eta)_j^{(-)}e^{i\eta_j}. \quad (25)$$

If we restrict the number of open channels to two, the simplicity of SU(2) algebra allows us to deal with the transformation relations among various phase shift matrices, the generators of scattering matrices, instead of scattering matrices as a whole as will be seen in the next subsection.

A. The transformation of the S matrix by the phase renormalization in the two open channel system.

$\boldsymbol{K}$ in Eq. (13) is defined in terms of the submatrices of the short-range K matrix which, in turn, is defined with respect to the basis pair f_j, g_j in Eq. (17), indicating that it corresponds to $\boldsymbol{K}(\eta)$. It shares the eigenvectors with $\boldsymbol{S}(\eta)$. From Eq. (12), the latter can be expressed as

$$\boldsymbol{S}(\eta)_{ij}=\sum_{\rho}T_{i\rho}e^{2i\delta_\rho}T_{\rho j}^{(T)}. \quad (26)$$

If we restrict the number of open channels to two, the T matrix can be parametrized with one mixing angle, say θ, by

$$T=e^{-i\frac{\theta}{2}\sigma_y}. \quad (27)$$

For two open channel systems, the diagonal matrix exp $(-2i\delta)$ can be expressed in terms of the Pauli matrices as

$$e^{-2i\delta}=\begin{pmatrix} e^{-2i\delta_1} & 0 \\ 0 & e^{-2i\delta_2}\end{pmatrix}=e^{-i(\delta_\Sigma 1+\Delta\delta\sigma_z)}. \quad (28)$$

Substituting Eqs. (27) and (28) for T and $\exp(-2i\delta)$, respectively, Eq. (26) becomes

$$\boldsymbol{S}(\eta)=e^{i\delta_\Sigma}e^{i\frac{\theta}{2}\sigma_y}e^{i\Delta\delta\sigma_z}e^{i\frac{\theta}{2}\sigma_y}=e^{i\delta_\Sigma}e^{i\Delta\delta\boldsymbol{\sigma}\cdot\boldsymbol{n}}, \quad (29)$$

where $\boldsymbol{n}$ is defined as $R_y(\theta)z$ and equal to $z\cos\theta + x\sin\theta$. $\boldsymbol{S}(0)$ is calculated from Eq. (24) by substituting Eq. (29) for $\boldsymbol{S}(\eta)$ and the expression for $\exp(-i\eta)$ similar to that for exp $(-2i\delta)$ as

$$\boldsymbol{S}(0)=e^{i(\delta_\Sigma-\eta_\Sigma)}e^{i\frac{\Delta\eta}{2}\sigma_z}e^{i\Delta\delta\boldsymbol{\sigma}\cdot\boldsymbol{n}}e^{i\frac{\Delta\eta}{2}\sigma_z}$$

$$=e^{i(\delta_\Sigma-\eta_\Sigma)}e^{i\Delta\delta\boldsymbol{\sigma}\cdot\boldsymbol{n}'}e^{i\Delta\eta\sigma_z}, \quad (30)$$

where $\boldsymbol{n}'$ denotes $R_z(\Delta\eta)\boldsymbol{n}$. In the same way, $\boldsymbol{S}(0)$ is obtained from $\boldsymbol{S}(\tilde{\eta})$ as

$$\boldsymbol{S}(0)=e^{-i(\tilde{\delta}_\Sigma+\tilde{\eta}_\Sigma)}e^{i\Delta\tilde{\delta}\boldsymbol{\sigma}\cdot\tilde{\boldsymbol{n}}'}e^{i\Delta\tilde{\eta}\sigma_z}, \quad (31)$$

where $\tilde{\boldsymbol{n}}'$ denotes $R_z(\Delta\tilde{\eta})\tilde{\boldsymbol{n}}$ with $\tilde{\boldsymbol{n}}$ given by $R_y(\tilde{\theta})z$ with the mixing angle $\tilde{\theta}$ defined as $\tilde{T}$ = $\exp(-i\tilde{\theta}\sigma_y/2)$. Let us rewrite the relations between $\tilde{\eta}_i$ and η_i in Eq. (15) as the relations between their respective sums and differences as

$$\tilde{\eta}_\Sigma=\eta_\Sigma+\pi\mu_\Sigma,$$

$$\Delta\tilde{\eta}=\Delta\eta+\pi\Delta\mu. \quad (32)$$

Equating two equations (30) and (31), we obtain

$$e^{-i(\delta_\Sigma+\eta_\Sigma)}e^{-i\Delta\delta\boldsymbol{\sigma}\cdot\boldsymbol{n}'}e^{-i\Delta\eta\sigma_z}=e^{-i(\tilde{\delta}_\Sigma+\tilde{\eta}_\Sigma)}e^{-i\Delta\tilde{\delta}\boldsymbol{\sigma}\cdot\tilde{\boldsymbol{n}}'}e^{-i\Delta\tilde{\eta}\sigma_z}. \quad (33)$$

Taking the trace of both sides of the above matrix equation yields

$$\delta_\Sigma+\eta_\Sigma=\tilde{\delta}_\Sigma+\tilde{\eta}_\Sigma, \quad (34)$$

which shows that the sum of the eigenphase shifts are invariant under the change of the reference potentials. From Eq. (34), $\tilde{\delta}_\Sigma$ is related to δ_Σ as

$$\tilde{\delta}_\Sigma=\delta_\Sigma-\pi\mu_\Sigma. \quad (35)$$

The remaining anisotropic part becomes

$$e^{i\Delta\delta\boldsymbol{\sigma}\cdot\boldsymbol{n}'}=e^{i\Delta\tilde{\delta}\boldsymbol{\sigma}\cdot\tilde{\boldsymbol{n}}'}e^{i\pi\Delta\mu\sigma_z}. \quad (36)$$

With $\boldsymbol{\sigma}\cdot\boldsymbol{n}'$ $\boldsymbol{\sigma}\cdot[R_z(\pi\Delta\eta)\boldsymbol{n}]$ = $\exp(-i\pi\Delta\eta\sigma_z/2)\boldsymbol{\sigma}\cdot\boldsymbol{n}$ exp $(i\pi\Delta\eta\sigma_z/2)$ and $\Delta\tilde{\eta}$ = $\Delta\eta+\pi\Delta\mu$. Eq. (36) can be rewritten after some manipulations as

$$e^{-i\Delta\delta\boldsymbol{\sigma}\cdot\boldsymbol{n}''}=e^{-i\Delta\tilde{\delta}\boldsymbol{\sigma}\cdot\tilde{\boldsymbol{n}}}e^{-i\pi\Delta\mu\sigma_z}. \quad (37)$$

where $\boldsymbol{n}''$ represents $R_z(-\pi\Delta\mu)\boldsymbol{n}$. Eq. (36) or (37) tells us that the new phase shift difference $\Delta\tilde{\delta}$, which is caused by the anisotropic influence of the reference potentials in two eigenchannels, cannot be obtained as a simple translation of the old $\Delta\delta$ by $\pi\Delta\mu$ as in Eq. (35) for the eigenphase sum. This derives from the fact that the eigenchannels for $\boldsymbol{S}(\eta)$ and the ones for $\exp(i\pi\Delta\mu)$ are of different character. The combining rule of $\Delta\delta$ and $\pi\Delta\mu$ for $\Delta\tilde{\delta}$ can be obtained at first by expressing Eq. (37) into the spherical triangle shown in Figure 1 following the rule described in Ref. [2]. Then, from the laws of spherical trigonometry, the formulas for the

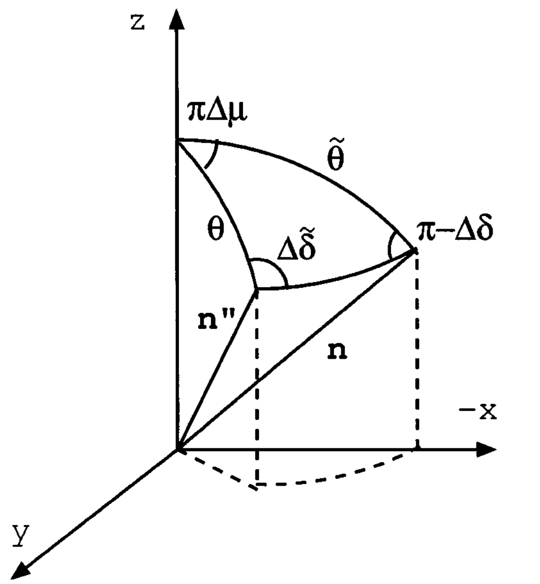

Figure 1. The diagram showing the relation between $\Delta\delta$ and its transformed $\Delta\tilde{\delta}$ due the change of reference potentials.

new $\Delta\tilde{\delta}$ and $\tilde{\theta}$ in terms of the old ones are obtained as

$$\cos\Delta\tilde{\delta} = \cos\Delta\delta\cos\pi\Delta\mu + \sin\Delta\delta\sin\pi\Delta\mu\cos\theta,$$

$$\cot\tilde{\theta} = \frac{1}{\sin\theta}(\cos\theta\cos\pi\Delta\mu - \sin\pi\Delta\mu\cot\Delta\delta). \quad (38)$$

Geometrical Description of the *S* matrix for the System with two Continua and One Discrete State in the CM Theory

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.[17] For the system composed of one discrete state ϕ and many continuum wavefunctions $\psi_j^{(-)}(E)$, the *S* matrix defined by Eq. (14) may be obtained[17] as

$$S_{j'j} = \sum_{j''\in P} S^0_{j'j''}\left(\delta_{j''j} + 2\pi i\frac{V_{j''E}V^*_{jE}}{E - E_0 - i\pi\Sigma_k|V_{kE}|^2}\right). \quad (39)$$

where V_{jE} denotes $(\psi_j^{(-)}(E)|H|\phi)$ and $S^0_{j'j''}$ is the background scattering matrix. Eq. (39) is different from that of outgoing wave in that i is replaced by $-i$ and adopted here as our interests are in the photodissociation processes. $2\pi\Sigma_k|V_{kE}|^2$ is the spectral width of the resonance peak and will be denoted as Γ. Eq. (39) can be greatly simplified by introducing Fano's 'a' state, $\psi^{(a)}(E)$, defined as

$$|\psi^{(a)}(E)\rangle = \sqrt{\frac{2\pi}{\Gamma}}\sum_j|\psi_j^{(-)}\rangle V_{jE}, \quad (40)$$

and the projection operator $\Pi_a = |\psi^{(a)}\rangle\langle\psi^{(a)}|$ whose (i, j) element is given by

$$(\Pi_a)_{ij} = \langle\psi_i^{(-)}|\psi^{(a)}\rangle\langle\psi^{(a)}|\psi_j^{(-)}\rangle = \frac{2\pi}{\Gamma}V_{iE}V^*_{jE}. \quad (41)$$

With Eq. (41) and $\cot\delta_r = -2(E-E_0)/\Gamma$, Eq. (39) becomes in matrix form as

$$S = S^0 + (e^{2i\delta_r} - 1)S^0\Pi_a = S^0[1 + (e^{2i\delta_r} - 1)\Pi_a] = S^0e^{2i\delta_r\Pi_a}. \quad (42)$$

Let us restrict the number of open channels to two. Let the background S^0 matrix in Eq. (39) be diagonalized by the similarity transformation as $S^0 = U^0e^{-2i\delta^0}(U^0)^{(T)}$ where U^0 is a real orthogonal matrix as the unitary S^0 matrix is symmetric. The S^0 matrix may be expressed in terms of Pauli matrices as

$$S^0 = U^0\begin{pmatrix} e^{2i\delta_1^0} & 0 \\ 0 & e^{2i\delta_2^0}\end{pmatrix}(U^0)^{(T)}$$

$$= e^{\frac{i}{2}\theta_0\sigma_y}e^{i(\delta_\Sigma^0 1 + \Delta_{12}^0\sigma_z)}e^{\frac{i}{2}\theta_0\sigma_y} = e^{i(\delta_\Sigma^0 1 - \Delta_{12}^0\boldsymbol{\sigma}\cdot\boldsymbol{n}_0)} \quad (43)$$

where $\boldsymbol{n}_0 = R_y(\theta_0)\boldsymbol{z}$, $\delta_\Sigma^0 \equiv \delta_1^0 + \delta_2^0$, and $\Delta_{12}^0 \equiv \delta_1^0 - \delta_2^0$. If we denote the m-th eigenchannels of S^0 as ψ_m, U^0_{im} may be considered as the transformation matrix from $\psi_i^{(-)}$ to ψ_m. The interaction matrices $(\psi_m | H | \phi)$ are real and can always be taken to be positive by choosing appropriately the sign of ψ_m at the origin. Let $(\psi_m | H | \psi) = \sqrt{\Gamma_m/2\pi}$. Notice that $\Gamma_1 + \Gamma_2$ is equal to the previously defined Γ. Then, we have

$$(U^0)^{(T)}e^{2i\delta_r\Pi_a}U^0 = e^{i(\delta_r 1 - \delta_r\boldsymbol{\sigma}\cdot\boldsymbol{n}_r)}, \quad (44)$$

where $\boldsymbol{n}_r$ is defined by

$$\boldsymbol{n}_r = R_z(-\Delta_{12}^0)R_y(\theta_r)\boldsymbol{z}$$
$$= (\sin\theta_r\cos\Delta_{12}^0, -\sin\theta_r\sin\Delta_{12}^0, \cos\theta_r) \quad (45)$$

with

$$\cos\theta_r \equiv \frac{\Gamma_1 - \Gamma_2}{\Gamma},$$

$$\sin\theta_r \equiv \frac{2\sqrt{\Gamma_1\Gamma_2}}{\Gamma}. \quad (46)$$

Ref. [1] obtained

$$e^{-i\Delta_{12}^0\sigma_z}e^{-i\delta_r\boldsymbol{\sigma}\cdot\boldsymbol{n}_r} = e^{-i\delta_a\boldsymbol{\sigma}\cdot\boldsymbol{n}_a}, \quad (47)$$

where $\boldsymbol{n}_a$ and δ_a are defined by

$$\boldsymbol{n}_a = R_y(\theta_a)\boldsymbol{z}, \quad (48)$$

$$\cot\delta_a = -\cot\Delta_{12}^0\frac{\varepsilon_a - q_a}{\sqrt{\varepsilon_a^2 + 1}}, \quad (49)$$

respectively, with $q_a = -\cot\theta_r/\cos\Delta_{12}^0$ and

$$\varepsilon_a \equiv -\cot\theta_a = \frac{\sin\Delta_{12}^0}{\sin\theta_r}(\varepsilon_r - \cot\Delta_{12}^0\cos\theta_r). \quad (50)$$

With Eq. (47), the $\boldsymbol{S}$ matrix becomes

$$\boldsymbol{S} = e^{i(\delta_\Sigma^0 + \delta_r)} U^0 e^{i\delta_- \boldsymbol{\sigma}\cdot\boldsymbol{n}_y} (U^0)^{(T)} = e^{i(\delta_\Sigma^0 - \delta_r)} e^{i\delta_- \boldsymbol{\sigma}\cdot\boldsymbol{n}'_a}, \tag{51}$$

where $\boldsymbol{n}'_a = R_y(\theta_0)\boldsymbol{n}_a$. In Ref. [2], all the procedures described so far are shown to be neatly fitted into the construction of the spherical triangle shown in Figure 2.

The Solution of MQDT for the System with two Open and One Closed Channels

Let us now consider obtaining the solution of the compatibility equation (10) for the system involving two open and one closed channels, where the compatibility equation is reduced to

$$\begin{vmatrix} K_{11} - \tan\delta & K_{12} & K_{13} \\ K_{12} & K_{22} - \tan\delta & K_{23} \\ K_{13} & K_{23} & K_{33} + \tan\beta \end{vmatrix} = 0 \tag{52}$$

and can be written as a quadratic equation for $\tan\delta$ as

$$(\tan\beta + K^{cc})\tan^2\delta - (\tan\beta + K^{cc})\mathrm{tr}\boldsymbol{K}\tan\delta + |K^{oo}|\tan\beta + |K| = 0. \tag{53}$$

Eq. (13) becomes for this three-channel system as

$$\boldsymbol{K} = K^{oo} - \frac{K^{oc}K^{co}}{\tan\beta + K^{cc}} \tag{54}$$

and its trace and determinant are obtained as

$$\mathrm{tr}\boldsymbol{K} = \mathrm{tr}K^{oo} - \frac{K_{13}^2 + K_{23}^2}{\tan\beta + K^{cc}},$$
$$|\boldsymbol{K}| = \frac{\tan\beta|K^{oo}| + |K|}{\tan\beta + K^{cc}}. \tag{55}$$

Substituting Eq. (55) for the corresponding terms in Eq. (53), we obtain

$$\tan^2\delta - \mathrm{tr}\boldsymbol{K}\tan\delta + |\boldsymbol{K}| = 0. \tag{56}$$

The two solutions denoted as $\tan\delta_+$ and $\tan\delta_-$ are obtained with the discriminant D [$= (\mathrm{tr}\boldsymbol{K})^2 - 4|\boldsymbol{K}|$] as

$$\tan\delta_\pm = \frac{\mathrm{tr}\boldsymbol{K} \pm \sqrt{D}}{2}, \tag{57}$$

whereby

$$\tan\delta_+ - \tan\delta_- = \sqrt{D},$$
$$\tan\delta_+ + \tan\delta_- = \mathrm{tr}\boldsymbol{K},$$
$$\tan\delta_+ \cdot \tan\delta_- = |\boldsymbol{K}|. \tag{58}$$

As is well known cite.[18,19] the behavior of the eigenphase sum $\delta_\Sigma (= \delta_+ + \delta_-)$ should be simpler than those of individual eigenphase shifts. Let us consider the tangent functions of the sum and difference of eigenphase shifts:

$$\tan\delta_\Sigma = \frac{\mathrm{tr}\boldsymbol{K}}{1 - |\boldsymbol{K}|} = \frac{K^{cc}\mathrm{tr}K^{oo} - \mathrm{tr}(K^{oc}K^{co}) + \mathrm{tr}K^{oo}\tan\beta}{K^{cc} - |K| + (1 - |K^{oo}|)\tan\beta}, \tag{59}$$

$$\tan\Delta\delta = \frac{\sqrt{D}}{1 + |\boldsymbol{K}|}. \tag{60}$$

The eigenphase sum δ_Σ of Eq. (59) does not show the typical resonance structure. By changing the reference potentials, we want it to be given as the form $\tan\tilde{\delta}_\Sigma = -\xi^2/\tan\tilde{\beta}$, which shows the typical resonance behavior as described in Appendix A. The corresponding equation to Eq. (59) for the new reference potential becomes this form when its elements satisfy

$$\mathrm{tr}\tilde{K}^{oo} = 0, \quad \tilde{K}^{cc} = |\tilde{K}|. \tag{61}$$

In this case,

$$\tan\tilde{\delta}_\Sigma = -\xi^2/\tan\tilde{\beta}, \tag{62}$$

where ξ is defined by

$$\xi^2 = \frac{\mathrm{tr}(\tilde{K}^{oc}\tilde{K}^{co})}{1 - |\tilde{K}^{oo}|}. \tag{63}$$

From $\mathrm{tr}\tilde{K}^{oo} = 0$, we have

$$\tilde{K}_{11} = -\tilde{K}_{22},$$
$$|\tilde{K}^{oo}| = -(|\tilde{K}_{11}|^2 + |\tilde{K}_{12}|^2) < 0 \tag{64}$$

and the square of ξ becomes

$$\xi^2 = \frac{\tilde{K}_{13}^2 + \tilde{K}_{23}^2}{1 + \tilde{K}_{11}^2 + \tilde{K}_{12}^2} > 0, \tag{65}$$

where its positive-ness is shown explicitly.

A. The Extraction of CM Parameters from MQDT Formulas.

As explained in Appendix A, if $\tilde{\delta}_\Sigma$ satisfies $\tan\tilde{\delta}_\Sigma = -\xi^2/\tan\tilde{\beta}$, it shows the identical behavior with the resonance eigenphase shift δ_r and may be regarded as identical to δ_r:

$$\tilde{\delta}_\Sigma = \delta_r. \tag{66}$$

For convenience, let us call the reference potential in which $\tilde{\delta}_\Sigma$ satisfies Eq. (62) the resonance-centered reference potential and the representation the resonance-centered representation. Let us now examine how other CM parameters are assigned to the elements of the $\tilde{K}$ matrix in the resonance-centered representation as the result of the assignment of δ_r to $\tilde{\delta}_\Sigma$. For this purpose, let us utilize the equality of $\boldsymbol{S}(0)$ given by (51) in the CM theory and given by Eq. (31) in MQDT:

$$e^{i(\delta_\Sigma^0-\delta_r)}e^{i\delta_a\boldsymbol{\sigma}\cdot\boldsymbol{n}'_a}=e^{i(\tilde{\delta}_\Sigma-\tilde{\eta}_\Sigma)}e^{-i\Delta\tilde{\delta}\boldsymbol{\sigma}\cdot\tilde{\boldsymbol{n}}'}e^{i\Delta\tilde{\eta}\sigma_z}. \quad (67)$$

The above matrix equation holds when isotropic and anisotropic parts of both sides are equal, respectively, as can be easily seen by equating the traces of its left- and right-hand sides:

$$\delta_\Sigma^0+\delta_r=\tilde{\delta}_\Sigma+\tilde{\eta}_\Sigma, \quad (68)$$

$$e^{-i\delta_a\boldsymbol{\sigma}\cdot\boldsymbol{n}'_a}=e^{i\Delta\tilde{\delta}\boldsymbol{\sigma}\cdot\tilde{\boldsymbol{n}}'}e^{-i\Delta\tilde{\eta}\sigma_z}. \quad (69)$$

Because of the equality (66), Eq. (68) yields

$$\delta_\Sigma^0=\tilde{\eta}_\Sigma. \quad (70)$$

Since the left-hand side of Eq. (69) has two parameters, *i.e.*, θ'_a for $\boldsymbol{n}'_a$ and δ_a while the right-hand side has three parameters $\Delta\tilde{\delta}$, $\Delta\tilde{\eta}$, and $\tilde{\theta}'$ for $\tilde{\boldsymbol{n}}'$ there will be an infinite number of ways of making both sides equal. The simplest of all will be the one that makes one of two exponential matrices on the left-hand side a unit matrix, which can be achieved here by setting

$$\Delta\tilde{\eta}=0. \quad (71)$$

In this setting, $\tilde{\boldsymbol{n}}'$ which is defined as $R_z(\Delta\tilde{\eta})\tilde{\boldsymbol{n}}$ becomes equal to $\tilde{\boldsymbol{n}}$. The right hand side of Eq. (69) is now simplified as

$$e^{i\delta_a\boldsymbol{\sigma}\cdot\boldsymbol{n}'_a}=e^{-i\Delta\tilde{\delta}\boldsymbol{\sigma}\cdot\tilde{\boldsymbol{n}}}. \quad (72)$$

Eq. (72) holds when

$$\boldsymbol{n}'_a=\tilde{\boldsymbol{n}}, \quad (73)$$

$$\delta_a=\Delta\tilde{\delta}. \quad (74)$$

Since vectors $\boldsymbol{n}'_a$ and $\tilde{\boldsymbol{n}}$ are obtained from the z axis by rotating about the y axis by θ'_a and $\tilde{\theta}$, respectively, the equality of two vectors is produced when $\theta'_a=\tilde{\theta}$. If we recall that a projection operator of type $(1+\boldsymbol{\sigma}\cdot\boldsymbol{n})/2$ generates an eigenchannel of $\boldsymbol{\sigma}\cdot\boldsymbol{n}$, Eq. (73) indicates that both $\boldsymbol{S}(0)$ and $\boldsymbol{S}(\tilde{\eta})$ have the identical eigenchannels.

From Eq. (60), $\tan\Delta\tilde{\delta}$ is given in terms of the elements of the $\tilde{K}$ matrix as $\sqrt{\tilde{D}}/(1+|\tilde{\boldsymbol{K}}|)$ and since $\Delta\tilde{\delta}$ is equal to δ_a from Eq. (74), we should be able to write $\sqrt{\tilde{D}}/(1+|\tilde{\boldsymbol{K}}|)$ into the form in Eq. (49). In order to do this, let us start from rewriting the discriminant $\tilde{D}$ using Eq. (55) as

$$\tilde{D}=\frac{[\mathrm{tr}(\tilde{K}^{oc}\tilde{K}^{co})]^2-4(|\tilde{K}^{oo}|\tan\tilde{\beta}+|\tilde{K}|)(\tan\tilde{\beta}+|\tilde{K}|)}{(\tan\tilde{\beta}+|\tilde{K}|)^2}. \quad (75)$$

Let D denote $\tilde{D}\,(\tan\tilde{\beta}+|\tilde{K}|)^2$. D may be rewritten as

$$\mathrm{D}=-4|\tilde{K}^{oo}|\left(\tan\tilde{\beta}+\frac{1+|\tilde{K}^{oo}|}{2|\tilde{K}^{oo}|}|\tilde{K}|\right)^2+\frac{(1-|\tilde{K}^{oo}|)^2}{|\tilde{K}^{oo}|}|\tilde{K}|^2$$
$$+[\mathrm{tr}(\tilde{K}^{oc}\tilde{K}^{co})]^2. \quad (76)$$

Using the relation

$$\frac{(1-|\tilde{K}^{oo}|)^2}{|\tilde{K}^{oo}|}|\tilde{K}|^2+[\mathrm{tr}(\tilde{K}^{oc}\tilde{K}^{co})]^2=-\frac{1}{|\tilde{K}^{oo}|}[(\tilde{K}_{13}^2-\tilde{K}_{23}^2)\tilde{K}_{12}-2\tilde{K}_{11}\tilde{K}_{13}\tilde{K}_{23}]^2, \quad (77)$$

it becomes

$$\begin{aligned}\mathrm{D}&=-\frac{1}{|\tilde{K}^{oo}|}\left\{4|\tilde{K}^{oo}|^2\left(\tan\tilde{\beta}+\frac{1+|\tilde{K}^{oo}|}{2|\tilde{K}^{oo}|}|\tilde{K}|\right)^2+[(\tilde{K}_{13}^2-\tilde{K}_{23}^2)\tilde{K}_{12}-2\tilde{K}_{11}\tilde{K}_{13}\tilde{K}_{23}]^2\right\}\\&=\frac{[(\tilde{K}_{13}^2-\tilde{K}_{23}^2)\tilde{K}_{12}-2\tilde{K}_{11}\tilde{K}_{13}\tilde{K}_{23}]^2}{\tilde{K}_{11}^2+\tilde{K}_{12}^2}\times\left[\frac{4(\tilde{K}_{11}^2+\tilde{K}_{12}^2)^2}{[(\tilde{K}_{13}^2-\tilde{K}_{23}^2)\tilde{K}_{12}-2\tilde{K}_{11}\tilde{K}_{13}\tilde{K}_{23}]^2}\times\left(\tan\tilde{\beta}+\frac{1+|\tilde{K}^{oo}|}{2|\tilde{K}^{oo}|}|\tilde{K}|\right)^2+1\right]\\&=\frac{[(\tilde{K}_{13}^2-\tilde{K}_{23}^2)\tilde{K}_{12}-2\tilde{K}_{11}\tilde{K}_{13}\tilde{K}_{23}]^2}{\tilde{K}_{11}^2+\tilde{K}_{12}^2}(\varepsilon_a^2+1),\end{aligned} \quad (78)$$

where ε_a is given by

$$\begin{aligned}\varepsilon_a&=-\frac{2(\tilde{K}_{11}^2+\tilde{K}_{12}^2)}{(\tilde{K}_{13}^2-\tilde{K}_{23}^2)\tilde{K}_{12}-2\tilde{K}_{11}\tilde{K}_{13}\tilde{K}_{23}}\times\left(\tan\tilde{\beta}-\frac{(1+|\tilde{K}^{oo}|)|\tilde{K}|}{2(\tilde{K}_{11}^2+\tilde{K}_{12}^2)}\right)\\&=\frac{2(\tilde{K}_{11}^2+\tilde{K}_{12}^2)(\tilde{K}_{13}^2+\tilde{K}_{23}^2)}{[(\tilde{K}_{13}^2-\tilde{K}_{23}^2)\tilde{K}_{12}-2\tilde{K}_{11}\tilde{K}_{13}\tilde{K}_{23}](1+\tilde{K}_{11}^2+\tilde{K}_{12}^2)}\times\left[\varepsilon_r-\frac{1-\tilde{K}_{11}^2-\tilde{K}_{12}^2}{2(\tilde{K}_{11}^2+\tilde{K}_{12}^2)}\frac{(\tilde{K}_{13}^2-\tilde{K}_{23}^2)\tilde{K}_{11}+2\tilde{K}_{12}\tilde{K}_{13}\tilde{K}_{23}}{\tilde{K}_{13}^2+\tilde{K}_{23}^2}\right]\end{aligned} \quad (79)$$

In Eqs. (78) and (79), ε_a and ε_r are used as convenient notations for $-\cot\theta_a$ and $-\cot\delta_r$, respectively. In the CM theory, they are reduced energy parameters and can vary from $-\infty$ to ∞ only once while in MQDT they undergo such a variation repeatedly every time θ_a or δ_r increase by π. By giving up the meanings of ε_a and ε_r as energies and replacing them with $-\cot\theta_a$ and $-\cot\delta_r$, respectively, the same CM formulas for an isolated resonance can be used for all resonances belonging to the same threshold by extending the ranges of θ_a and δ_r from $[0,\pi]$ to $[-\infty,\infty]$. Then each interval $[(n-1)\pi, n\pi]$ corresponds to one resonance. Equating Eqs. (79) and (50), we obtain

$$\frac{\sin\Delta_{12}^{0}}{\sin\theta_r} = -\frac{2(\tilde{K}_{11}^2+\tilde{K}_{12}^2)(\tilde{K}_{13}^2+\tilde{K}_{23}^2)}{[(\tilde{K}_{13}^2-\tilde{K}_{23}^2)\tilde{K}_{12}-2\tilde{K}_{11}\tilde{K}_{13}\tilde{K}_{23}](1+\tilde{K}_{11}^2+\tilde{K}_{12}^2)} \,. \quad (80)$$

$$\cot\Delta_{12}^{0}\cos\theta_r = \frac{1-\tilde{K}_{11}^2-\tilde{K}_{12}^2}{2(\tilde{K}_{11}^2+\tilde{K}_{12}^2)}\frac{(\tilde{K}_{13}^2-\tilde{K}_{23}^2)\tilde{K}_{11}+2\tilde{K}_{12}\tilde{K}_{13}\tilde{K}_{23}}{\tilde{K}_{13}^2+\tilde{K}_{23}^2}. \quad (81)$$

Both signs are possible for the right-hand side of Eq. (80). But the positive sign is not taken as it yields the inconsistent result.

Thus far, we considered the numerator of the formula for $\tan\Delta\tilde{\delta}$. Let us next consider its denominator given by $1+|\tilde{\boldsymbol{K}}|$:

$$1+|\tilde{\boldsymbol{K}}| = -\frac{(1+|\tilde{K}^{oo}|)\tan\tilde{\beta}+2|\tilde{K}|}{\tan\tilde{\beta}+|\tilde{K}|}$$

$$= \frac{1-\tilde{K}_{11}^2-\tilde{K}_{12}^2}{2(\tilde{K}_{11}^2+\tilde{K}_{12}^2)}[(\tilde{K}_{13}^2-\tilde{K}_{23}^2)\tilde{K}_{12}-2\tilde{K}_{11}\tilde{K}_{13}\tilde{K}_{23}]\frac{\varepsilon_a-q_a}{\tan\tilde{\beta}+|\tilde{K}|}, \quad (82)$$

where q_a is given by

$$q_a = -\frac{\cot\theta_r}{\cos\Delta_{12}^{0}} = \frac{1+\tilde{K}_{11}^2+\tilde{K}_{12}^2}{(1-\tilde{K}_{11}^2-\tilde{K}_{12}^2)}\frac{(\tilde{K}_{13}^2-\tilde{K}_{23}^2)\tilde{K}_{11}+2\tilde{K}_{12}\tilde{K}_{13}\tilde{K}_{23}}{(\tilde{K}_{13}^2-\tilde{K}_{23}^2)\tilde{K}_{12}-2\tilde{K}_{11}\tilde{K}_{13}\tilde{K}_{23}}. \quad (83)$$

From Eqs. (78) and (82), we obtain

$$\cot\Delta\tilde{\delta} = -\frac{1-\tilde{K}_{11}^2-\tilde{K}_{12}^2}{2\sqrt{\tilde{K}_{11}^2+\tilde{K}_{12}^2}}\frac{\varepsilon_a-q_a}{\sqrt{\varepsilon_a^2+1}} \quad (84)$$

whereby

$$\cos\Delta_{12}^{0} = \frac{1-\tilde{K}_{11}^2-\tilde{K}_{12}^2}{2\sqrt{\tilde{K}_{11}^2+\tilde{K}_{12}^2}}. \quad (85)$$

The sign of the right-hand side of Eq. (84) is not uniquely determined as it is obtained by taking the square root of the discriminant $\tilde{D}$ but is taken as minus in order to obtain $\cot\Delta_{12}^{0}$ in the form of Eq. (85) so that the self-consistency is obtained with the convention that $\sin\Delta_{12}^{0}$ is positive. From the convention that $\sin\Delta_{12}^{0}$ is positive for small magnitudes of K matrix elements, we have

$$\sin\Delta_{12}^{0} = \frac{2\sqrt{\tilde{K}_{11}^2+\tilde{K}_{12}^2}}{1+\tilde{K}_{11}^2+\tilde{K}_{12}^2}, \quad (86)$$

$$\cos\Delta_{12}^{0} = \frac{1-\tilde{K}_{11}^2-\tilde{K}_{12}^2}{1+\tilde{K}_{11}^2+\tilde{K}_{12}^2}. \quad (87)$$

From Eqs. (80) and (86), $\sin\theta_r$ is obtained as

$$\sin\theta_r = -\frac{(\tilde{K}_{13}^2-\tilde{K}_{23}^2)\tilde{K}_{12}-2\tilde{K}_{11}\tilde{K}_{13}\tilde{K}_{23}}{\sqrt{\tilde{K}_{11}^2+\tilde{K}_{12}^2}(\tilde{K}_{13}^2+\tilde{K}_{23}^2)} \quad (88)$$

and $\cos\theta_r$ is obtained from Eqs. (81) and (85) as

$$\cos\theta_r = \frac{(\tilde{K}_{13}^2-\tilde{K}_{23}^2)\tilde{K}_{11}+2\tilde{K}_{12}\tilde{K}_{13}\tilde{K}_{23}}{\sqrt{\tilde{K}_{11}^2+\tilde{K}_{12}^2}(\tilde{K}_{13}^2+\tilde{K}_{23}^2)} \quad (89)$$

So far, we found the formulas for the CM parameters δ_r, δ_Σ^0, and etc. in terms of the elements of the short-range $\tilde{K}$ matrix and the long-range parameters $\tilde{\eta}_\Sigma$ and $\tilde{\beta}$. Though it does not appear explicitly in the formulas of the CM theory, θ_0 is a CM parameter which should be included in the theoretical derivation and still remains to be expressed in terms of short-range MQDT parameters. This connection can be achieved by considering the $\tilde{K}$ matrix without including the elements related to the closed channel, which will be denoted as $\tilde{K}^0$ and is given by

$$\tilde{K}^0 = \begin{pmatrix} \tilde{K}_{11} & \tilde{K}_{12} \\ \tilde{K}_{12} & \tilde{K}_{22} \end{pmatrix} = \begin{pmatrix} \tilde{K}_{11} & \tilde{K}_{12} \\ \tilde{K}_{12} & -\tilde{K}_{11} \end{pmatrix}. \quad (90)$$

Its eigenvalues denoted by $\tan\tilde{\delta}_1^0$ and $\tan\tilde{\delta}_2^0$ are easily obtained as

$$\tan\tilde{\delta}_1^0 = \sqrt{\tilde{K}_{11}^2+\tilde{K}_{12}^2},$$
$$\tan\tilde{\delta}_2^0 = -\sqrt{\tilde{K}_{11}^2+\tilde{K}_{12}^2} \quad (91)$$

revealing that $\tilde{\delta}_1^0 = -\tilde{\delta}_2^0$. Therefore we have

$$\tilde{\delta}_\Sigma^0 = 0, \quad \Delta\tilde{\delta}^0 = 2\tilde{\delta}_1^0. \quad (92)$$

Following the previous convention, its eigenvectors may be parametrized as $(\cos\tilde{\theta}_0/2, \sin\tilde{\theta}_0/2)$ and $(-\sin\tilde{\theta}_0/2, \cos\tilde{\theta}_0/2)$ with

$$\cos\frac{\tilde{\theta}^0}{2} = \mathrm{sign}(\tilde{K}_{12})\left(\frac{\sqrt{\tilde{K}_{11}^2+\tilde{K}_{12}^2}+\tilde{K}_{11}}{2\sqrt{\tilde{K}_{11}^2+\tilde{K}_{12}^2}}\right)^{1/2},$$

$$\sin\frac{\tilde{\theta}^0}{2} = \left(\frac{\sqrt{\tilde{K}_{11}^2+\tilde{K}_{12}^2}-\tilde{K}_{11}}{2\sqrt{\tilde{K}_{11}^2+\tilde{K}_{12}^2}}\right)^{1/2}, \quad (93)$$

where $\mathrm{sign}(\tilde{K}_{12})$ is 1 for positive $\tilde{K}_{12}$ and −1 for negative $\tilde{K}_{12}$. Let us consider the $\tilde{\boldsymbol{S}}^0$ matrix corresponding to $\tilde{K}^0$. Similar to Eq. (29), it can be written as

$$\tilde{\boldsymbol{S}}^0 = e^{i\tilde{\delta}_\Sigma^0}e^{-i\Delta\tilde{\delta}^0\boldsymbol{\sigma}\cdot\tilde{\boldsymbol{n}}} = e^{-i\Delta\tilde{\delta}^0\boldsymbol{\sigma}\cdot\tilde{\boldsymbol{n}}}, \quad (94)$$

where $\tilde{\delta}_\Sigma^0 = 0$ is used. Inserting $\tilde{\delta}_\Sigma^0$, $\Delta\tilde{\eta}0$, and $\tilde{\boldsymbol{n}}'=\tilde{\boldsymbol{n}}$ into the background form of Eq. (31) and then equating it with the one in Eq. (43), we have

$$\boldsymbol{S}^0(0) = e^{-i\delta_\Sigma^0} e^{-i\Delta_{12}^0 \boldsymbol{\sigma}\cdot\boldsymbol{n}_0} = e^{-i\tilde{\eta}_\Sigma} e^{i\Delta\tilde{\delta}^0 \boldsymbol{\sigma}\cdot\tilde{\boldsymbol{n}}}. \tag{95}$$

The equality of the trace of both sides of the matrix equation (95), which is isotropic to channel interaction and given by $\delta_\Sigma^0 = \tilde{\eta}_\Sigma$, is consistent with the previous (70) and, from the remaining anisotropic part to channel interaction, we obtain

$$\Delta_{12}^0 = \Delta\tilde{\delta}^0 = 2\tilde{\delta}_1^0, \tag{96}$$

$$\theta_0 = \tilde{\theta}_0. \tag{97}$$

In terms of Pauli matrices, eigenphase shifts, and mixing angles, $\tilde{K}^0$ can be rewritten as

$$\tilde{K}^0 = \tan\tilde{\delta}_1^0 \boldsymbol{\sigma}\cdot[R_y(\tilde{\theta}_0)z] = \tan\frac{\Delta_{12}^0}{2}\boldsymbol{\sigma}\cdot[R_y(\theta_0)z], \tag{98}$$

from which we have

$$\tilde{K}_{11} = -\tilde{K}_{22} = \tan\frac{\Delta_{12}^0}{2}\cos\theta_0,$$
$$\tilde{K}_{12} = \tan\frac{\Delta_{12}^0}{2}\sin\theta_0. \tag{99}$$

Eqs. (93) and (97) yield

$$\cos\theta_0 = \frac{\tilde{K}_{11}}{\sqrt{\tilde{K}_{11}^2 + \tilde{K}_{12}^2}},$$
$$\sin\theta_0 = \frac{\tilde{K}_{12}}{\sqrt{\tilde{K}_{11}^2 + \tilde{K}_{12}^2}}. \tag{100}$$

Substituting Eq. (100) into Eqs. (89) and (88), we obtain

$$\cos\theta_r = \frac{\tilde{K}_{13}^2 - \tilde{K}_{23}^2}{\tilde{K}_{13}^2 + \tilde{K}_{23}^2}\cos\theta_0 + \frac{2\tilde{K}_{13}\tilde{K}_{23}}{\tilde{K}_{13}^2 + \tilde{K}_{23}^2}\sin\theta_0,$$
$$\sin\theta_r = -\frac{\tilde{K}_{13}^2 - \tilde{K}_{23}^2}{\tilde{K}_{13}^2 + \tilde{K}_{23}^2}\sin\theta_0 + \frac{2\tilde{K}_{13}\tilde{K}_{23}}{\tilde{K}_{13}^2 + \tilde{K}_{23}^2}\cos\theta_0 \tag{101}$$

and accordingly

$$\frac{\tilde{K}_{13}^2 - \tilde{K}_{23}^2}{\tilde{K}_{13}^2 + \tilde{K}_{23}^2} = \cos(\theta_r + \theta_0), \quad \frac{2\tilde{K}_{13}\tilde{K}_{23}}{\tilde{K}_{13}^2 + \tilde{K}_{23}^2} = \sin(\theta_r + \theta_0) \tag{102}$$

and finally

$$\frac{\tilde{K}_{13}}{\sqrt{\tilde{K}_{13}^2 + \tilde{K}_{23}^2}} = \cos\frac{1}{2}(\theta_r + \theta_0), \quad \frac{\tilde{K}_{23}}{\sqrt{\tilde{K}_{13}^2 + \tilde{K}_{23}^2}} = \sin\frac{1}{2}(\theta_r + \theta_0) \tag{103}$$

are obtained. Substituting Eq. (65) and $\tilde{K}_{11}^2 + \tilde{K}_{12}^2 = \tan^2\Delta_{12}^0/2$ obtained from (99) into Eq. (103), $\tilde{K}_{13}$ and $\tilde{K}_{23}$ are expressed completely in terms of CM parameters as

$$\tilde{K}_{13} = \frac{\xi}{\cos\frac{\Delta_{12}^0}{2}}\cos\frac{1}{2}(\theta_r + \theta_0), \quad \tilde{K}_{23} = \frac{\xi}{\cos\frac{\Delta_{12}^0}{2}}\sin\frac{1}{2}(\theta_r + \theta_0). \tag{104}$$

Only $\tilde{K}_{33}$ among the elements of the $\tilde{K}$ matrix remains unexpressed in terms of CM parameters while expressions for the others are given by Eqs. (99) and (104). Its expression is easily obtained from $\tilde{K}_{33} = |\tilde{K}|$ as follows

$$|\tilde{K}| = \frac{(\tilde{K}_{13}^2 - \tilde{K}_{23}^2)\tilde{K}_{11} + 2\tilde{K}_{12}\tilde{K}_{13}\tilde{K}_{23}}{1 + \tilde{K}_{11}^2 + \tilde{K}_{12}^2} = \xi^2\tan\frac{\Delta_{12}^0}{2}\cos\theta_r. \tag{105}$$

The final expression for the short-range $\tilde{K}$ matrix can be written as

$$\tilde{K} = \begin{pmatrix} \tan\frac{\Delta_{12}^0}{2}\cos\theta_0 & \tan\frac{\Delta_{12}^0}{2}\sin\theta_0 & \frac{\xi}{\cos\frac{\Delta_{12}^0}{2}}\cos\frac{1}{2}(\theta_r + \theta_0) \\ \tan\frac{\Delta_{12}^0}{2}\sin\theta_0 & -\tan\frac{\Delta_{12}^0}{2}\cos\theta_0 & \frac{\xi}{\cos\frac{\Delta_{12}^0}{2}}\sin\frac{1}{2}(\theta_r + \theta_0) \\ \frac{\xi}{\cos\frac{\Delta_{12}^0}{2}}\cos\frac{1}{2}(\theta_r + \theta_0) & \frac{\xi}{\cos\frac{\Delta_{12}^0}{2}}\sin\frac{1}{2}(\theta_r + \theta_0) & \xi^2\tan\frac{\Delta_{12}^0}{2}\cos\theta_r \end{pmatrix}. \tag{106}$$

Originally 6 parameters are needed to describe the short-range K matrix due to its symmetric nature. The two conditions (61) for the resonance-centered representation restrict the number of independent parameters to 4. In Eq. (106), three CM parameters Δ_{12}^0, θ_0, θ_r and one short-range parameter ξ represent those four independent parameters.

Long-range parameters $\tilde{\eta}$ and $\tilde{\beta}$ are related to the CM parameters as

$$\Delta\tilde{\eta} = 0,$$
$$\tilde{\eta}_\Sigma = \delta_\Sigma^0,$$
$$\tan\tilde{\beta} = -\frac{\xi^2}{\tan\delta_r}. \tag{107}$$

In the above, we obtained the representation, called the resonance-centered representation, where behaviors of eigenphase shifts show those of the eigenphase shifts in the configuration mixing theory, such as $-\cot\delta_\Sigma = \tan\tilde{\beta}/\xi^2$ and $\cot\Delta\delta = -\cot\Delta_{12}^0(\varepsilon_a - q_a)/\sqrt{\varepsilon_a^2 + 1}$. So far, we did not mention about how we can obtain this representation from the given representation using the transformation (15), *i.e.*, what are the values of μ_1, μ_2, and μ_3 or equivalently μ_Σ, $\Delta\mu$, and μ_3 which give the resonance-centered representation. One of them, $\Delta\mu$, is obtained as $-\Delta\eta/\pi$ from $\Delta\tilde{\eta} = 0$ and $\Delta\tilde{\eta} = \Delta\eta + \pi\Delta\mu$. The procedure of obtaining the remaining μ_3 and μ_Σ is lengthy and given in Appendix B. The results are reproduced here

$$\tan 2\pi\mu_3 = \frac{2\{\mathrm{tr}K^{\cdot oo}[K^{\cdot cc}\mathrm{tr}K^{\cdot oo} - \mathrm{tr}(K^{\cdot oc}K^{\cdot co})] + (1-|K^{\cdot oo}|)(K^{\cdot cc} - |K|)\}}{(\mathrm{tr}K^{\cdot oo})^2 - [K^{\cdot cc}\mathrm{tr}K^{\cdot oo} - \mathrm{tr}(K^{\cdot oc}K^{\cdot co})]^2 + (1-|K^{\cdot oo}|)^2 - (K^{\cdot cc} - |K|)^2}, \tag{108}$$

$$\tan 2\pi\mu_\Sigma = \frac{2\{(1-|K^{\cdot oo}|)\mathrm{tr}K^{\cdot oo} + [K^{\cdot cc}\mathrm{tr}K^{\cdot oo} - \mathrm{tr}(K^{\cdot oc}K^{\cdot co})] \times (K^{\cdot cc} - |K|)\}}{(1-|K^{\cdot oo}|)^2 + (K^{\cdot cc} - |K|)^2 - (\mathrm{tr}K^{\cdot oo})^2 - [K^{\cdot cc}\mathrm{tr}K^{\cdot oo} - \mathrm{tr}(K^{\cdot oc}K^{\cdot co})]^2} \tag{109}$$

The origin of the Lu-Fano plot of (β, δ_Σ) is moved to a new position by the shifts given by $(\pi\mu_3, \pi\mu_\Sigma)$ in Eq. (109) so that the plot $(\tilde{\beta}, \tilde{\delta}_\Sigma)$ becomes symmetrical in the new coordinate system.

The contribution of the closed channels

When the system is in the ρ-th fragmentation eigenchannel, the system is described by the wavefunction $\Psi_\rho = \Sigma_{i\in P}\Psi_i Z_{i\rho}\cos\beta_\rho$, where $Z_{i\rho}$ is the probability amplitude that the system is found in the i-th stationary state Ψ_i and $\cos\delta_\rho$ normalizes Ψ_i per unit energy. The probability amplitude that the system is in the i-th open channels is described by $T_{i\rho}$. Since $T_{i\rho}$ is orthogonal, the flux of particles in collision is conserved. This should be so as the wavefunctions describing closed channels become zero at the asymptotic region. Though the presence of the closed channels do not affect the flux, it affects the collision by delaying the process as the particles are trapped there for some time. Here we want to find out how long the collision system will stay in closed channels when the system is in the ρ-th fragmentation eigenchannel.

The probability amplitudes $Z_{i\rho}$ for the system in the closed channels are given by Eq. (11). In the present case, only one closed and two open channels are involved. If we use indices 1 and 2 for the open channels and 3 for the closed one, the probability amplitudes are simplified as:

$$\tilde{Z}_{3\rho}\cos\tilde{\beta} = -\sum_k \tilde{K}_{3k}\tilde{T}_{k\rho}\frac{\cos\tilde{\delta}_\rho}{\tan\tilde{\beta} + |\tilde{K}|}. \tag{110}$$

From Eq. (105) and $\tan\tilde{\beta} = \xi^2\varepsilon_r$, the denominator of the right-hand side of Eq. (110) becomes

$$\tan\tilde{\beta} + |\tilde{K}| = \xi^2\left(\varepsilon_r + \tan\frac{1}{2}\Delta^0_{12}\cos\theta_r\right). \tag{111}$$

If we substitute $\varepsilon_a \sin\theta_r/\sin\Delta^2_{12} + \cot\Delta^2_{12}\cos\theta_r$ for ε_r and make use of $\varepsilon_a = -\cot\theta_a$, Eq. (110) becomes

$$\tan\tilde{\beta} + |\tilde{K}| = \frac{\xi^2}{\sin\Delta^2_{12}\sin\theta_a}\sin(\theta_a - \theta_r). \tag{112}$$

(ε_r and ε_a are not the usual energy parameters but are used here as convenient notations as mentioned before). When Eq. (112) is substituted, the last factor of the right-hand side of Eq. (110) becomes

$$\frac{\cos\tilde{\delta}_\rho}{\tan\tilde{\beta} + |\tilde{K}|} = \frac{\sin\Delta^0_{12}\sin\theta_a}{\xi^2\sin(\theta_a - \theta_r)}\begin{cases}\cos\frac{1}{2}(\delta_r + \delta_a) & \text{for } \rho=1, \\ \cos\frac{1}{2}(\delta_r - \delta_a) & \text{for } \rho=2.\end{cases} \tag{113}$$

By Delambre's analogies among the half-angle formula of spherical trigonometry,[20] we have

$$\cos\frac{1}{2}(\delta_r + \delta_a) = -\frac{\sin\frac{1}{2}(\theta_a - \theta_r)}{\sin\frac{1}{2}\theta_f}\cos\frac{1}{2}\Delta^0_{12},$$

$$\cos\frac{1}{2}(\delta_r - \delta_a) = \frac{\cos\frac{1}{2}(\theta_a - \theta_r)}{\cos\frac{1}{2}\theta_f}\cos\frac{1}{2}\Delta^0_{12}. \tag{114}$$

Entering Eq. (114), Eq. (113) becomes

$$\frac{\cos\tilde{\delta}_\rho}{\tan\tilde{\beta} + |\tilde{K}|} = \frac{\cos\frac{1}{2}\Delta^0_{12}\sin\Delta^0_{12}\sin\theta_a}{\xi^2\sin(\theta_a - \theta_r)}\begin{cases}-\dfrac{\sin\frac{1}{2}(\theta_a - \theta_r)}{\sin\frac{1}{2}\theta_f} & \text{for } \rho=1, \\ \dfrac{\cos\frac{1}{2}(\theta_a - \theta_r)}{\cos\frac{1}{2}\theta_f} & \text{for } \rho=2.\end{cases}$$

$$= \frac{\cos\frac{1}{2}\Delta^0_{12}\sin\Delta^0_{12}\sin\theta_a}{\xi^2\sin\theta_f}\begin{cases}-\dfrac{\cos\frac{1}{2}\theta_f}{\cos\frac{1}{2}(\theta_a - \theta_r)} & \text{for } \rho=1, \\ \dfrac{\sin\frac{1}{2}\theta_f}{\sin\frac{1}{2}(\theta_a - \theta_r)} & \text{for } \rho=2.\end{cases}$$

$$= \frac{\sin\delta_r\cos\frac{1}{2}\Delta^0_{12}}{\xi^2}\begin{cases}-\dfrac{\cos\frac{1}{2}\theta_f}{\cos\frac{1}{2}(\theta_a - \theta_r)} & \text{for } \rho=1, \\ \dfrac{\sin\frac{1}{2}\theta_f}{\sin\frac{1}{2}(\theta_a - \theta_r)} & \text{for } \rho=2.\end{cases} \tag{115}$$

By Eq. (104) and $\tilde{T} = \exp[-i(\theta_a + \theta_0)\sigma_y/2]$, the first factor of the right-hand side of Eq. (110) becomes

$$\sum_k \tilde{K}_{3k}\tilde{T}_{k\rho} = \frac{\xi}{\cos\frac{1}{2}\Delta^0_{12}}\begin{cases}\cos\frac{1}{2}(\theta_a - \theta_r) & \text{for } \rho=1, \\ -\sin\frac{1}{2}(\theta_a - \theta_r) & \text{for } \rho=2.\end{cases} \tag{116}$$

Using Eqs. (115) and (116), Eq. (110) is simplified as

$$\tilde{Z}_{3\rho}\cos\tilde{\beta} = \frac{\sin\delta_r}{\xi}\begin{cases}\cos\frac{1}{2}\theta_f & \text{for } \rho=1,\\ \sin\frac{1}{2}\theta_f & \text{for } \rho=2.\end{cases} \tag{117}$$

From Eq. (62), we obtain easily

$$\frac{\sin\delta_r}{\xi} = \left(\frac{d\delta_r}{d\tilde{\beta}}\right)^{1/2}\cos\tilde{\beta} \tag{118}$$

(the convention that δ_r increases from zero as $\tilde{\beta}$ increases from $-\pi/2$ is adopted here, which implies that $\sin\delta_r\cos\tilde{\beta} > 0$ or $\cos\delta_r\sin\tilde{\beta} < 0$). Entering Eq. (118) into Eq. (117), we obtain the formula for $\tilde{Z}_{3\rho}$:

$$\tilde{Z}_{3\rho} = \left(\frac{d\delta_r}{d\tilde{\beta}}\right)^{1/2}\begin{cases}\cos\frac{1}{2}\theta_f & \text{for } \rho=1,\\ \sin\frac{1}{2}\theta_f & \text{for } \rho=2,\end{cases} \tag{119}$$

and the following equation is easily derived:

$$\sum_\rho \tilde{Z}_{3\rho}^2 = \frac{d\delta_r}{d\tilde{\beta}}. \tag{120}$$

Eq. (120) shows that though the interaction becomes complicated as the number of involved channels changes from one open and one closed channels to two open and one closed channels, the total time for which the system stays in a close channel remains the same. The total time delay due to a closed channel does not depend on the characteristics of systems. The characteristics of systems appear when we consider the branching ratio of the probability amplitudes for a closed channel to decompose into open channels. This ratio is determined by the transformation matrix between fragmentation eigenchannels and resonance ones described by the mixing angle θ_f defined in the spherical triangle of Figure 2. That is, it is purely determined by geometry.

Photofragmentation cross section formulas

In the photofragmentation processes, the final state is described by the incoming wavefunctions. Let us denote them as $\tilde{\Psi}_j^{(-)}$. They are obtained from the fragmentation eigenchannel wavefunctions $\tilde{\boldsymbol{\Psi}}_\rho$ or from the short-range standing-wave channel wavefunctions $\tilde{\Psi}_i$ as

$$\tilde{\boldsymbol{\Psi}}_j^{(-)} = \sum_\rho \tilde{\boldsymbol{\Psi}}_\rho e^{-i\tilde{\delta}_\rho}\tilde{T}_{\rho j}^{(T)} = \sum_{i\in P}\tilde{\Psi}_i[\tilde{T}\cos\tilde{\delta}e^{-i\tilde{\delta}}\tilde{T}^{(T)}]_{ij} + \sum_{i\in Q}\tilde{\Psi}_i[\cos\tilde{\beta}\tilde{Z}e^{-i\tilde{\delta}}\tilde{T}^{(T)}]_{ij}. \tag{121}$$

We note the following matrix relations

$$\tilde{T}\cos\tilde{\delta}e^{-i\tilde{\delta}}\tilde{T}^{(T)} = (1 + i\tilde{\boldsymbol{K}})^{-1},$$

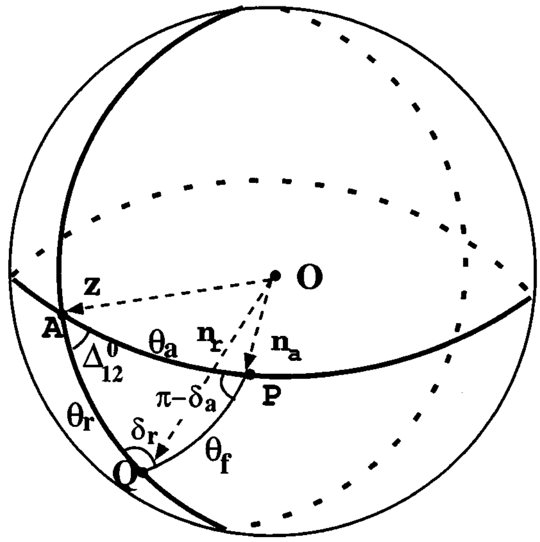

Figure 2. The spherical triangle formed by the three vectors $\boldsymbol{z}$, $\boldsymbol{n}_r$ and $\boldsymbol{n}_a$.

$$\cos\tilde{\beta}\tilde{Z}e^{-i\tilde{\delta}}\tilde{T}^{(T)} = -(\tan\tilde{\beta} + \tilde{K}^{cc})^{-1}\tilde{K}^{co}(1 + i\tilde{\boldsymbol{K}})^{-1}. \tag{122}$$

It may be more natural to expand physical incoming wavefunctions with incoming-wave channel basis functions. Using the transformation relation

$$\tilde{\Psi}_i = \sum_k \tilde{\Psi}_k^{(-)}(1 + i\tilde{K})_{ki} \tag{123}$$

between the short-range incoming- and standing-wave channel basis functions and after some manipulations, we get

$$\tilde{\Psi}_j^{(-)} = \tilde{\Psi}_j^{(-)} + \sum_{k\in Q}\tilde{\Psi}_k^{(-)}(\tan\tilde{\beta} + i)(\tan\tilde{\beta} + \tilde{\kappa}^{cc})^{-1} \times \tilde{K}^{co}(-i + \tilde{K}^{oo})^{-1}, \tag{124}$$

where $\tilde{\kappa}^{cc}$ is defined by

$$\tilde{\kappa}^{cc} = \tilde{K}^{cc} - \tilde{K}^{co}(-i + \tilde{K}^{oo})^{-1}\tilde{K}^{oc}, \tag{125}$$

which is the one considered by Lecomte but differs from his by complex conjugation.[7] Let us now limit the discussion to the two open and one closed channel case. Then $\tilde{\kappa}^{cc}$ becomes $-i\xi^2$ and we have the following identity

$$\frac{\tan\tilde{\beta} + i}{\tan\tilde{\beta} - i\xi^2} = -\frac{i}{\xi}e^{-i(\tilde{\beta}+\delta_r)}\left(\frac{d\delta_r}{d\tilde{\beta}}\right)^{1/2}. \tag{126}$$

With it, Eq. (124) may be rewritten as

$$\tilde{\boldsymbol{\Psi}}_j^{(-)} = \tilde{\Psi}_j^{(-)} - \frac{i}{\xi}\tilde{\Psi}_3^{(-)}e^{-i(\tilde{\beta}+\delta_r)}\left(\frac{d\delta_r}{d\tilde{\beta}}\right)^{1/2}[\tilde{K}^{co}(-i + \tilde{K}^{oo})^{-1}]_{3j}. \tag{127}$$

Now it is convenient to introduce new short-range wavefunctions $\tilde{M}_j^{(-)}$ and $\tilde{N}_j^{(-)}$ defined by

$$\tilde{M}_j^{(-)} = \tilde{\Psi}_j^{(-)} + \tilde{\Psi}_3^{(-)}[\tilde{K}^{co}(-i+\tilde{K}^{oo})^{-1}]_{3j},$$
$$\tilde{N}_j^{(-)} = \tilde{\Psi}_j^{(-)} - \frac{1}{\xi^2}\tilde{\Psi}_3^{(-)}[\tilde{K}^{co}(-i+\tilde{K}^{oo})^{-1}]_{3j}. \quad (128)$$

With these functions, the square of the modulus of the transition dipole moment can be expressed into the Beutler-Fano formula given by

$$\left|\tilde{D}_j^{(-)}\right|^2 = \left|(\tilde{\Psi}_j^{(-)}|T|i)\right|^2 = \left|(\tilde{M}_j^{(-)}|T|i)\right|^2 \frac{\left|\tan\tilde{\beta}/\xi^2+\tilde{q}_j\right|^2}{\tan^2\tilde{\beta}/\xi^4+1}, \quad (129)$$

with the complex line profile index $\tilde{q}_j$ defined by

$$\tilde{q}_j = i\frac{(\tilde{N}_j^{(-)}|T|i)}{(\tilde{M}_j^{(-)}|T|i)}. \quad (130)$$

More detailed analysis of Eq. (129) can be done with the help of the transformation considered by Lecomte and Ueda and will be treated in the separate paper.

Summary and Discussion

We reformulated the MQDT formulation into the form of the CM theory by using the transformation considered by Giusti-Suzor and Fano in order to clearly identify the resonance structures. The transformation moves the axes of the Lu-Fano plot so that the curve ($\tilde{\beta}$, $\tilde{\delta}_\Sigma$) becomes symmetrical. But the short-range reactance matrix $\tilde{K}$ obtained is not a form considered by Giusti-Suzor and Fano, *i.e.*, its diagonal elements are not zero. It means that the intra- and inter-channel couplings are not fully separated yet though the resonance position is centered in the Lu-Fano plot. In the two channel case, to make the Lu-Fano plot symmetric is equivalent to the complete deparation of intra- and inter-channel couplings. But this is no longer true with more than two channels. In order to achieve that, we have to introduce the orthogonal transformation as well as the phase renormalization as done by Lecomte and Ueda. Therefore, this work should be regarded as a basis for the full investigation of the resonance structures in the MQDT formulation. The full investigation will be published as a separate paper.

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Appendix A: The differentiation of the phase shifts with respect to energy

Let us calculate the first derivative of Eq. (59) with respect to energy. Modifying Eq. (59) as

$$\tan\delta_\Sigma = \frac{\mathrm{tr}K^{oo}}{1-|K^{oo}|} - \frac{\mathrm{tr}K^{oo}(|K^{oo}|K^{cc}-|K|)+\mathrm{tr}(K^{oc}K^{co})(1-|K^{oo}|)}{(1-|K^{oo}|)^2\left(\tan\beta+\frac{K^{cc}-|K|}{1-|K^{oo}|}\right)} \quad (A1)$$

and differentiating with respect to β, we obtain

$$(1+\tan^2\delta_\Sigma)\frac{d\delta_\Sigma}{d\beta} = \frac{\mathrm{tr}K^{oo}(|K^{oo}|K^{cc}-|K|)+\mathrm{tr}(K^{oc}K^{co})(1-|K^{oo}|)(1+\tan^2\beta)}{(1-|K^{oo}|)^2\left(\tan\beta+\frac{K^{cc}-|K|}{1-|K^{oo}|}\right)^2}, \quad (A2)$$

where the explicit formula for the first factor of the left-hand side is given by

$$1+\tan^2\delta_\Sigma = \frac{\left(\tan\beta+\frac{K^{cc}-|K|}{1-|K^{oo}|}\right)^2 + \left[\tan\beta\frac{\mathrm{tr}K^{oo}}{1-|K^{oo}|} + \frac{K^{cc}\mathrm{tr}K^{oo}-\mathrm{tr}(K^{oc}K^{co})}{1-|K^{oo}|}\right]^2}{\left(\tan\beta+\frac{K^{cc}-|K|}{1-|K^{oo}|}\right)^2} \quad (A3)$$

The numerator of Eq. (A3), when organized with respect to $\tan\beta$, becomes

$$\frac{(1-|K^{oo}|)^2+(\mathrm{tr}K^{oo})^2}{(1-|K^{oo}|)^2}\{[\tan\beta+\Re(\kappa^{cc})]^2+[\Im(\kappa^{cc})]^2\}, \quad (A4)$$

where explicit formulas for $\Re(\kappa^{cc})$ and $\Im(\kappa^{cc})$ are given by

$$\Re(\kappa^{cc}) = \frac{(K^{cc}-|K|)(1-|K^{oo}|)+\mathrm{tr}K^{oo}[K^{cc}\mathrm{tr}K^{oo}-\mathrm{tr}(K^{oc}K^{co})]}{(1-|K^{oo}|)^2+(\mathrm{tr}K^{oo})^2}$$

$$\Im(\kappa^{cc}) = -\frac{(K^{cc}-|K|)\mathrm{tr}K^{oo}-[K^{cc}\mathrm{tr}K^{oo}-\mathrm{tr}(K^{oc}K^{co})](1-|K^{oo}|)}{(1-|K^{oo}|)^2+(\mathrm{tr}K^{oo})^2} \quad (a5)$$

Substituting Eq. (A3) for $1+\tan^2\delta_\Sigma$, Eq. (A2) becomes

$$\frac{d\delta_\Sigma}{d\beta} = -\frac{\Im(\kappa^{cc})(1+\tan^2\beta)}{[\tan\beta+\Re(\kappa^{cc})]^2+[\Im(\kappa^{cc})]^2}. \quad (A6)$$

$\Im(\kappa^{cc})$ is negative as can explicitly be shown as

$$\mathfrak{J}(\kappa^{cc}) = -\frac{(K_{11}K_{23}-K_{12}K_{13})^2 + (K_{22}K_{13}-K_{12}K_{23})^2 + K_{13}^2 + K_{23}^2}{(1-|K^{oo}|)^2 + (\mathrm{tr}K^{oo})^2} \le 0 \quad \text{(A7)}$$

and becomes equal to $-\xi^2$ of Eq. (63) when $\mathrm{tr}(K^{oo})=0$. Eq. (A6) tells us that the derivative of the eigenphase sum with respect to energy is always positive. Even individual eigenphase shift should have a positive derivative with respect to energy according to Macek's formula.[21]

Eq. (A6) can be rewritten into a Lorentzian form as

$$\frac{d\delta_\Sigma}{d\left(\frac{\tan\beta+\Re(\kappa^{cc})}{-\mathfrak{J}(\kappa^{cc})}\right)} = \frac{1}{\left(\frac{\tan\beta+\Re(\kappa^{cc})}{-\mathfrak{J}(\kappa^{cc})}\right)^2+1}. \quad \text{(A8)}$$

From Eq. (A8), the inflection point of the curve δ_Σ *vs.* $\tan\beta$ is obtained as $\tan\beta = -\Re(\kappa^{cc})$, which is different from the pole position of $\tan\delta_\Sigma$ given by $\tan\beta = -(K^{cc}-|K|)/(1-K^{oo})$ in Eq. (A1). Two positions becomes equal to $-\Re(\kappa^{cc})$ by setting $\mathrm{tr}(K^{oo})$ to zero. If we further set $\Re(\kappa^{cc})$ to zero, the graph of δ_Σ enjoys the same behavior as that of δ_r in the CM theory for isolated resonances if $\tan\beta/\xi^2$ is identified with $-1/\varepsilon_r$. Then we may set $\tilde{\delta}_\Sigma = \delta_r$ to make the MQDT formulation look like the CM one.

Appendix B: The phase shifts which yield the resonance-centered representation

First of all, $\Delta\mu(=\mu_1-\mu_2)$ is obtained from (71) and (32) as

$$\pi\Delta\mu = -\Delta\eta. \quad \text{(B1)}$$

The remaining two parameters might be directly obtained from the relation (18) between K and $\tilde{K}$ but the easier way of obtaining them is to make use of the invariance of the functional form (59) of $\tan\delta_\Sigma$ under the change of the reference potentials. The invariance is the result that no condition on the reference potentials are applied when Eq. (59) is derived. From this invariance, $\tan\tilde{\delta}_\Sigma$ is given by

$$\tan\tilde{\delta}_\Sigma = \frac{\tilde{K}^{cc}\mathrm{tr}\tilde{K}^{oo} - \mathrm{tr}(\tilde{K}^{oc}\tilde{K}^{co}) + \mathrm{tr}\tilde{K}^{oo}\tan\tilde{\beta}}{\tilde{K}^{cc} - |\tilde{K}| + (1-|\tilde{K}^{oo}|)\tan\tilde{\beta}}. \quad \text{(B2)}$$

Using the relations $\tilde{\delta}_\Sigma = \delta_\Sigma - \pi\mu_\Sigma$ and $\tilde{\beta} = \beta + \pi\mu_3$, Eq. (B2) becomes

$$\tan(\delta_\Sigma-\pi\mu_\Sigma) = \frac{\tilde{K}^{cc}\mathrm{tr}\tilde{K}^{oo} - \mathrm{tr}(\tilde{K}^{oc}\tilde{K}^{co}) + \mathrm{tr}\tilde{K}^{oo}\tan(\beta+\pi\mu_3)}{\tilde{K}^{cc} - |\tilde{K}| + (1-|\tilde{K}^{oo}|)\tan(\beta+\pi\mu_3)}, \quad \text{(B3)}$$

which can be transformed into the following by making use of the tangent law:

$$\frac{\tan\delta_\Sigma - \tan\pi\mu_\Sigma}{1+\tan\delta_\Sigma\tan\pi\mu_\Sigma} = \frac{A+B\tan\beta}{C+D\tan\beta}, \quad \text{(B4)}$$

where A, B, C, D are defined as

$$\begin{aligned}
A &= \tilde{K}^{cc}\mathrm{tr}\tilde{K}^{oo} - \mathrm{tr}(\tilde{K}^{oc}\tilde{K}^{co}) + \mathrm{tr}\tilde{K}^{oo}\tan\pi\mu_3,\\
B &= \mathrm{tr}\tilde{K}^{oo} - [\tilde{K}^{cc}\mathrm{tr}\tilde{K}^{oo} - \mathrm{tr}(\tilde{K}^{oc}\tilde{K}^{co})]\tan\pi\mu_3,\\
C &= \tilde{K}^{cc} - |\tilde{K}| + (1-|\tilde{K}^{oo}|)\tan\pi\mu_3,\\
D &= 1-|\tilde{K}^{oo}| - (|\tilde{K}^{oo}| - |\tilde{K}|)\tan\pi\mu_3.
\end{aligned} \quad \text{(B5)}$$

When Eq. (B4) is solved for $\tan\delta_\Sigma$, it becomes

$$\tan\delta_\Sigma = \frac{(A+C\tan\pi\mu_\Sigma) + (B+D\tan\pi\mu_\Sigma)\tan\beta}{(C-A\tan\pi\mu_\Sigma) + (D-B\tan\pi\mu_\Sigma)\tan\beta}. \quad \text{(B6)}$$

Equating two equations (59) and (B6), we obtain the relations containing the proportionality constant k as

$$\begin{aligned}
&[\tilde{K}^{cc}\mathrm{tr}\tilde{K}^{oo} - \mathrm{tr}(\tilde{K}^{oc}\tilde{K}^{co})] + \mathrm{tr}\tilde{K}^{oo}\tan\pi\mu_3\\
&\quad + [\tilde{K}^{cc} - |\tilde{K}| + (1-|\tilde{K}^{oo}|)\tan\pi\mu_3]\tan\pi\mu_\Sigma\\
&= k[\tilde{K}^{cc}\mathrm{tr}\tilde{K}^{oo} - \mathrm{tr}(\tilde{K}^{oc}\tilde{K}^{co})].
\end{aligned} \quad \text{(B7)}$$

$$\begin{aligned}
&\mathrm{tr}\tilde{K}^{oo} - [\tilde{K}^{cc}\mathrm{tr}\tilde{K}^{oo} - \mathrm{tr}(\tilde{K}^{oc}\tilde{K}^{co})]\tan\pi\mu_3\\
&\quad + [1-|\tilde{K}^{oo}| - (\tilde{K}^{cc} - |\tilde{K}|)\tan\pi\mu_3]\tan\pi\mu_\Sigma = k\,\mathrm{tr}K^{oo}.
\end{aligned} \quad \text{(B8)}$$

$$\begin{aligned}
&\tilde{K}^{cc} - |\tilde{K}| + (1-|\tilde{K}^{oo}|)\tan\pi\mu_3\\
&\quad -\{[\tilde{K}^{cc}\mathrm{tr}\tilde{K}^{oo} - \mathrm{tr}(\tilde{K}^{oc}\tilde{K}^{co})] + \mathrm{tr}\tilde{K}^{oo}\tan\pi\mu_3\}\tan\pi\mu_\Sigma\\
&= k(\tilde{K}^{cc} - |K|),
\end{aligned} \quad \text{(B9)}$$

$$\begin{aligned}
&(1-|\tilde{K}^{oo}|) - (\tilde{K}^{cc} - |\tilde{K}|)\tan\pi\mu_3\\
&\quad -\{\mathrm{tr}\tilde{K}^{oo} - [\tilde{K}^{cc}\mathrm{tr}\tilde{K}^{oo} - \mathrm{tr}(\tilde{K}^{oc}\tilde{K}^{co})]\tan\pi\mu_3\}\tan\pi\mu_\Sigma\\
&= k(1-|K^{oo}|).
\end{aligned} \quad \text{(B10)}$$

If we introduce p, q, r, s for convenience as follows

$$\begin{aligned}
p &= \mathrm{tr}K^{oo} + [K^{cc}\mathrm{tr}K^{oo} - \mathrm{tr}(K^{oc}K^{co})],\\
q &= \mathrm{tr}K^{oo} - [K^{cc}\mathrm{tr}K^{oo} - \mathrm{tr}(K^{oc}K^{co})],\\
r &= 1 - |K^{oo}| + (K^{cc} - |K|),\\
s &= 1 - |K^{oo}| - (K^{cc} - |K|),
\end{aligned} \quad \text{(B11)}$$

we can express the sum and difference of Eqs. (B7) and (B8) and also the same ones for (B9) and (B10) in terms of them as

$$\begin{pmatrix} 1 & \tan\pi\mu_3 & \tan\pi\mu_\Sigma & \tan\pi\mu_3\tan\pi\mu_\Sigma \\ -\tan\pi\mu_3 & 1 & -\tan\pi\mu_3\tan\pi\mu_\Sigma & \tan\pi\mu_\Sigma \\ -\tan\pi\mu_\Sigma & -\tan\pi\mu_3\tan\pi\mu_\Sigma & 1 & \tan\pi\mu_3 \\ \tan\pi\mu_3\tan\pi\mu_\Sigma & -\tan\pi\mu_\Sigma & -\tan\pi\mu_3 & 1 \end{pmatrix}\begin{pmatrix}\tilde{p}\\ \tilde{q}\\ \tilde{r}\\ \tilde{s}\end{pmatrix} = k\begin{pmatrix}p\\ q\\ r\\ s\end{pmatrix}. \quad \text{(B12)}$$

Eq. (B12) is inverted as

$$\begin{pmatrix} \tilde{p} \\ \tilde{q} \\ \tilde{r} \\ \tilde{s} \end{pmatrix} = \begin{pmatrix} \cos\pi\mu_\Sigma e^{i\pi\mu_3\sigma_y} & -\sin\pi\mu_\Sigma e^{i\pi\mu_3\sigma_y} \\ \sin\pi\mu_\Sigma e^{i\pi\mu_3\sigma_y} & \cos\pi\mu_\Sigma e^{i\pi\mu_3\sigma_z} \end{pmatrix} k' \begin{pmatrix} p \\ q \\ r \\ s \end{pmatrix}, \tag{B13}$$

where the new proportionality constant k' is related to k as $k' = k \cos\pi\mu_3 \cos\pi\mu_\Sigma$. The proportionality constant may be determined from the relation between K and $\tilde{K}$ but the determination requires a long tedious derivation. Eventually it can be shown that k' is equal to $1/|K \sin\pi\mu + \cos\pi\mu|$.

Eq. (B13) holds for any arbitrary reference potential. In the resonance-centered representation where we have $\mathrm{tr}\tilde{K}^{oo} = 0$ and $\tilde{K}^{cc} = |\tilde{K}|$, $\tilde{p}$, $\tilde{q}$, $\tilde{r}$, and $\tilde{s}$ are related as $\tilde{p} = -\tilde{q}$, $\tilde{r} = \tilde{s}$. When the latter relations are applied to Eq. (B13), we have

$$\begin{aligned} &\cos\pi\mu_\Sigma(p\cos\pi\mu_3 - q\sin\pi\mu_3) - \sin\pi\mu_\Sigma(r\cos\pi\mu_3 - s\sin\pi\mu_3) \\ &= -\cos\pi\mu_\Sigma(p\sin\pi\mu_3 + q\cos\pi\mu_3) + \sin\pi\mu_\Sigma(r\sin\pi\mu_3 + s\cos\pi\mu_3) \end{aligned} \tag{B14}$$

and

$$\begin{aligned} &\sin\pi\mu_\Sigma(p\cos\pi\mu_3 - q\sin\pi\mu_3) + \cos\pi\mu_\Sigma(r\cos\pi\mu_3 - s\sin\pi\mu_3) \\ &= \sin\pi\mu_\Sigma(p\sin\pi\mu_3 + q\cos\pi\mu_3) + \cos\pi\mu_\Sigma(r\sin\pi\mu_3 + s\cos\pi\mu_3). \end{aligned} \tag{B15}$$

Dividing Eqs. (B14) and (B15) by $\cos\pi\mu_3$ and $\cos\pi\mu_\Sigma$, respectively, and collecting the terms for $\tan\pi\mu_\Sigma$, we obtain

$$\begin{aligned} \tan\pi\mu_\Sigma &= \frac{p(1+\tan\pi\mu_3) + q(1-\tan\pi\mu_3)}{r(1+\tan\pi\mu_3) + s(1-\tan\pi\mu_3)}, \\ \tan\pi\mu_\Sigma &= \frac{-r(1-\tan\pi\mu_3) + s(1+\tan\pi\mu_3)}{p(1-\tan\pi\mu_3) - q(1+\tan\pi\mu_3)}. \end{aligned} \tag{B16}$$

By equating the above equations for $\tan\pi\mu_\Sigma$, we obtain the formula for $\tan\pi\mu_3$ as

$$\tan 2\pi\mu_3 = \frac{2\{\mathrm{tr}\tilde{K}^{oo}[\tilde{K}^{cc}\mathrm{tr}\tilde{K}^{oo} - \mathrm{tr}(\tilde{K}^{oc}\tilde{K}^{co})] + (1-|\tilde{K}^{oo}|)(\tilde{K}^{cc} - |\tilde{K}|)\}}{(\mathrm{tr}\tilde{K}^{oo})^2 - [\tilde{K}^{cc}\mathrm{tr}\tilde{K}^{oo} - \mathrm{tr}(\tilde{K}^{oc}\tilde{K}^{co})]^2 + (1-|\tilde{K}^{oo}|)^2(\tilde{K}^{cc} - |\tilde{K}|)^2} \tag{B17}$$

In the same way, dividing Eqs. (B14) and (B15) by $\cos\pi\mu_3$ and $\cos\pi\mu_\Sigma$, respectively, and collecting the terms for $\tan\pi\mu_3$, we obtain the formula for $\tan\pi\mu_\Sigma$ as

$$\tan 2\pi\mu_\Sigma = \frac{2[(1-|\tilde{K}^{oo}|)\mathrm{tr}\tilde{K}^{oo} + (\tilde{K}^{cc}\mathrm{tr}\tilde{K}^{oo} - \mathrm{tr}(\tilde{K}^{oc}\tilde{K}^{co}))(\tilde{K}^{cc} - |\tilde{K}|)]}{(1-|\tilde{K}^{oo}|)^2 + (\tilde{K}^{cc} - |\tilde{K}|)^2 - (\mathrm{tr}\tilde{K}^{oo})^2 - [\tilde{K}^{cc}\mathrm{tr}\tilde{K}^{oo} - \mathrm{tr}(\tilde{K}^{oc}\tilde{K}^{co})]^2}. \tag{B18}$$

In the two channel system, general resonance phenomena are described by the Lu-Fano plot which can differ from system to system in the position of the inflection points described by μ_1 and μ_2 and in the amplitude of the curve determined by the interchannel coupling strength ξ. In the system with two open and one closed channels, two more parameters Δ_{12}^{0} and θ_P are needed to describe the coupling between two curves ($\tilde{\beta}$, δ_-) and ($\tilde{\beta}$, δ_+) in the Lu-Fano plot and the relative coupling strengths of two open channels with a closed channel, respectively, besides three parameters (μ_1, μ_2, ξ) in the two channel system.

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