The Lecomte-Ueda Transformation and Resonance Structure in the Multichannel Quantum Defect Theory for the Two Open and One Closed Channel System

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The transformation devised by Lecomte and Ueda for the study of resonance structures in the multichannel quantum defect theory (MQDT) is used to analyze partial photofragmentation cross section formulas in MQDT analogous to Fano's resonance formula obtained in the previous work for the system involving two open and one closed channels. Detailed comparison of the MQDT results with the configuration mixing (CM) ones is made. Resonance structures and their geometrical relations in the MQDT formulation are revealed and classified by combining Lecomte and Ueda's theory with the geometrical method devised to study the coupling between background and resonance scatterings.

Key Words : MQDT, Photofragmentation cross-section, Resonance, Phase renormalization

Introduction

Though multichannel quantum defect theory (MQDT) is one of the powerful theories for resonances in that it allows us to describe complex spectra including both bound and continuum regions with only a few parameters, resonance structures are not transparently identified in its formulation as resonances are treated indirectly.[1,2] In order to identify resonance terms, special treatment is needed as Giusti-Suzor and Fano did for the two channel system by the phase renormalization.[3] They noticed that the usual Lu-Fano plot often obscures the symmetry of the curve in it which is apparent when the plot is extended to infinity. The symmetry can be brought into the MQDT formulation by using the techniques first considered in Ref. [4] which move the origin of the plot to the center of symmetry by the use of base pair whose phase is shifted from that of the base pair (f, g) by μ:

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

By this phase renormalization, the diagonal elements of short-range reactance matrices K become zero and the resonance structures are separated from the background in two channel systems (Dubau and Seaton also obtained the same results as Giusti-Suzor and Fano's ones from a different approach[5]).

The generalizations of their method to systems 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] Cooke and Cromer,[12] Lecomte, and Ueda showed that, for such general systems, making the diagonal elements of reactance matrices K zero can only be achieved with the modification to the transformation so that it performs an orthogonal transformation of basis functions besides a phase renormalization. We will call this transformation the Lecomte-Ueda transformation hereinafter. Using this transformation, Lecomte found the best parameters to describe total cross sections shorn of the background part for autoionization spectra for general systems. Ueda derived total cross section formulas analogous to Fano's resonance formula for some cases including one closed and an arbitrary number of open channels. Giusti-suzor and Lefebvre-Brion,[9] and Wintgen and Fridrich[10] did the detailed study for the system involving two closed and one open channels and Cohen[11] for the system involving two closed and two open channels. The present paper deals with the system involving two open and one closed channels and is thus more restrictive than the previous work in this sense. But the present work obtained several results which are absent or not dealt in the other people's work. It obtained the partial cross section formulas for photofragmentation processes analogous to Fano's resonance one, which is not trivial since it is generally believed that final state distributions described by partial cross section formulas contain detailed pieces of information sensitive to some features of dynamical couplings. The present paper also succeeded in obtaining the complete relations between MQDT and configuration mixing (CM)[13-16] formulas for this concrete examples, the general features of which were studied before by Fano and Mies.[17-19] We achieved this by reformulating MQDT into the form of the CM theory using Giusti-Suzor and Fano's method so that the Lu-Fano plot becomes symmetrical. But the short-range reactance matrix K obtained in this way in Ref. [20] was not the kind of form considered by Giusti-Suzor and Fano in that its diagonal elements are not zero. It means that intra- and inter-channel-block couplings are not fully separated yet. Making diagonal elements of K zero can be done by the method prescribed by Lecomte.[7] In the present paper, his method is coupled with the geometrical method developed in Ref. [21] for studying the coupling between the background and resonance scatterings so that the hierarchical resonance structures are fully investigated and the MQDT reformulation is made to

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match fully with the CM theory.

In the following section, we will summarize the transformation intro- duced by Lecomte and Ueda with some additions needed for the present work. In the next section, we consider the short-range reactance matrices in various channel basis wavefunctions and investigates the resonance structures using the Lecomte-Ueda transformation. After that, the photofragmentation cross sections and relations between those and the CM ones is derived. Finally, the summary and discussion is given in Section 5.

The Lecomte-Ueda Transformation

We may describe the Lecomte-Ueda transformation using either standing-wave channel basis functions or incoming-wave channel basis functions. Both descriptions have their own advantages. The former is suitable for the study of the reactance matrix K which provides much simpler description than the scattering matrix. The latter, on the other hand, is suitable for the description of the photofragmentation cross sections. We will give both descriptions.

A. The Lecomte-Ueda Transformation in Terms of Standing Waves. Lecomte and Ueda considered the transformation in which the basis sets are not only phase renormalized but also transformed by an orthogonal matrix W. Let us denote the regular and irregular pair ($\Phi_i f_i$, $\Phi_i g_i$) at $R \geq R_0$ as $(\theta_i, \bar{\theta}_i)$. The Lecomte-Ueda transformation changes this pair to $(\theta_i', \bar{\theta}_i')$ defined as

$$\theta_i' = \sum_j (\theta_j W_{ji} \cos\pi\mu_i - \bar{\theta}_j W_{ji} \sin\pi\mu_i),$$
$$\bar{\theta}_i' = \sum_j (\theta_j W_{ji} \sin\pi\mu_i + \bar{\theta}_j W_{ji} \cos\pi\mu_i) \tag{2}$$

so that the standing-wave channel basis functions

$$\Psi_k = \sum_i (\theta_i \delta_{ik} - \bar{\theta}_i K_{ik}),\ R \geq R_0 \tag{3}$$

are transformed to the new ones

$$\Psi_k' = \sum_i (\theta_i' \delta_{ik} - \bar{\theta}_i' K'_{ik}),\ R \geq R_0 . \tag{4}$$

Φ_i in Eqs. (2) and (3) is the wavefunction describing all the motions in the i-th channel except for the one along the coordinate R in which fragmentation takes place and R_0 is the value of R beyond which channels are decoupled. The transformation relation for the reactance matrix K is given in matrix form by

$$K' = (W^{(T)} K W \sin\pi\mu + \cos\pi\mu)^{-1} (W^{(T)} K W \cos\pi\mu - \sin\pi\mu) \tag{5}$$

and the one for the wavefunctions by

$$\Psi_k' = \sum_j \Psi_j [W(\cos\pi\mu - \sin\pi\mu K')]_{jk}. \tag{6}$$

If W is the unit matrix, the transformation is reduced to the one by Giusti-suzor and Fano. On the other hand, if the phase renormalization is not done, i.e., $\mu_i = 0$ the reactance matrix and wavefunctions transform in matrix form as

$$K' = W^{(T)} K W,$$
$$\Psi' = \Psi W. \tag{7}$$

Besides the reactance matrix K, another type of reactance matrix κ is considered by Lecomte. If we consider the short-range scattering matrix S corresponding to K, it is related to K as

$$S = (1 - iK)(1 + iK)^{-1}, \tag{8}$$

where $\exp(-2i\delta)$ instead of $\exp(2i\delta)$ is used for S with the consequence of i's being replaced by $-i$ from the usual formula of S in Eq. (8) as our interests are in photofragmentation. Let us consider the partitioning of S:

$$S = \begin{pmatrix} S^{oo} & S^{oc} \\ S^{co} & S^{cc} \end{pmatrix}, \tag{9}$$

with indices c for closed channels and o for open channels. The κ^{cc} matrix is defined using the submatrix S^{cc} as

$$S^{cc} = (1 - i\kappa^{cc})(1 + i\kappa^{cc})^{-1}. \tag{10}$$

From the definition, we can express κ^{cc} in terms of the submatrices of K as

$$\kappa^{cc} = K^{cc} - K^{co}(-i + K^{oo})^{-1} K^{oc}. \tag{11}$$

The κ^{cc} matrix is an effective K matrix when open channels are not observed in photofragmentation and can alternatively be obtained by setting the coefficients of outgoing waves in open channels to zero following the prescription described in Fano's book[22] where the coefficients of incoming waves are set to zero as scattering is considered. Lecomte noticed that this κ^{cc} matrix transforms under the restriction of $W^{co} = W^{oc} = 0$ as

$$\kappa'^{cc} = (W^{cc(T)} \kappa^{cc} W^{cc} \sin\pi\mu^c + \cos\pi\mu^c)^{-1}$$
$$\times (W^{cc(T)} \kappa^{cc} W^{cc} \cos\pi\mu^c - \sin\pi\mu^c). \tag{12}$$

Now consider the eigenchannel wavefunction $\boldsymbol{\Psi}_\rho'$ of the physical reactance matrix $\boldsymbol{K}'$ which can be obtained as a superposition of Ψ_k' of Eq. (4) as

$$\boldsymbol{\Psi}_\rho' = \sum_{k \in P} \Psi_k' Z_{k\rho}' \cos\delta_\rho' + \sum_{k \in Q} \Psi_k' Z_{k\rho}' \cos\beta_k' \tag{13}$$

and satisfies the boundary condition at $R \to \infty$ as

$$\boldsymbol{\Psi}_\rho' \to \sum_{j,k \in P} (\theta_j' \delta_{jk} - \bar{\theta}_j' \boldsymbol{K}_{jk}') T_{k\rho}' \cos\delta_\rho'. \tag{14}$$

where P and Q denote the sets of open and closed channels, respectively, δ_ρ' the eigenphase shift for $\boldsymbol{K}'$ and β_k' the accumulated phase shift in the k-th closed channel.[23] Now we want to make Eq. (13) satisfy the boundary condition (14). For that purpose, let us first consider the form of Eq. (13) in $R \geq R_0$:

$$\begin{aligned}\boldsymbol{\Psi}_\rho' = \sum_{j \in P} [\,&\theta_j' Z_{j\rho}'^{o} \cos\delta_\rho' \\ &- \bar{\theta}_j' (K'^{oo} Z'^{o} \cos\delta' + K'^{oc} \cos\beta' Z'^{c})_{j\rho}] \\ &+ \sum_{j \in Q} [\theta_j' Z'^{c}_{j\rho} \cos\beta_j' \\ &- \bar{\theta}_j' (K'^{cc} \cos\beta' Z'^{c} + K'^{co} Z'^{o} \cos\delta')_{j\rho}].\end{aligned} \tag{15}$$

The coefficient of the exponentially rising term of the second sum on the right-hand side of Eq. (15) should be zero. The closed-channel forms of θ_j' and $\bar{\theta}_j'$ obtained from those of f_i and g_i in Ref. [23] are given by

$$\theta_j' = \sum_{i \in Q} \sqrt{\frac{m_i}{\pi \kappa_i}} \Phi_i [-D_i f_i^+ W_{ij}^{cc} \cos(\beta_i + \pi\mu_j) + D_i^{-1} f_i^- W_{ij}^{cc} \sin(\beta_i + \pi\mu_j)], \quad (R \geq R_0)$$

$$\bar{\theta}_j' = -\sum_{i \in Q} \sqrt{\frac{m_i}{\pi \kappa_i}} \Phi_i [D_i f_i^+ W_{ij}^{cc} \sin(\beta_i + \pi\mu_j) + D_i^{-1} f_i^- W_{ij}^{cc} \cos(\beta_i + \pi\mu_j)], \quad (16)$$

with $f_i^{\pm}$ which are introduced to denote $\exp(\pm ik_iR)$, respectively, for the open channels but become exponentially decreasing and rising terms $\exp(\mp\kappa_i R)$, respectively, for the closed channels $[k_i = i\kappa_i = \sqrt{2m_i(E - E_i)}]$. Substituting Eq. (16) into Eq. (15) and setting the coefficients of the exponentially rising term to zero, we obtain

$$(K'^{cc} + \tan\beta_W')\cos\beta' Z'^c = -K'^{co} Z'^o \cos\delta', \quad (17)$$

where $\tan\beta_W'$ is defined as

$$\tan\beta_W' = (\cos\beta W^{cc}\cos\pi\mu^c - \sin\beta W^{cc}\sin\pi\mu^c)^{-1} \times (\sin\beta W^{cc}\cos\pi\mu^c + \cos\beta W^{cc}\sin\pi\mu^c). \quad (18)$$

The mass m_i in Eq. (16) denotes the reduced mass for the motion along the coordinate R in the channel i and κ_i is defined as $\sqrt{2m_i(E_i - E)}$ with the energy E of the system and the core energy E_i in the i-th channel. Comparison of the asymptotic form of Ψ_ρ' given in Eq. (14) with the open channel part of Eq. (15) yields

$$Z'^o_{j\rho} = T'_{j\rho},$$
$$K'^{oo} Z'^o \cos\delta' + K'^{oc}\cos\beta' Z'^c = \boldsymbol{K}' T' \cos\delta'. \quad (19)$$

Inserting Eq. (17) into Eq. (19), we obtain

$$\boldsymbol{K}' = K'^{oo} - K'^{oc}(K'^{cc} + \tan\beta_W')^{-1} K'^{co}, \quad (20)$$

which is different from the well-known relation

$$\boldsymbol{K}' = K'^{oo} - K'^{oc}(K'^{cc} + \tan\beta')^{-1} K'^{co}, \quad (21)$$

in that $\tan\beta'$ is replaced by $\tan\beta_W'$ of Eq. (18). Two relations become identical when W^{cc} is the unit matrix. Notice that, in order for $\boldsymbol{\Psi}'_\rho$ to be eigenchannels, the following relation holds from Eq. (14):

$$T'^{(T)} \boldsymbol{K}' T' = \tan\delta'. \quad (22)$$

Therefore the meanings of $\tan\delta'$ and T' as eigenvalues and the collection of eigenvectors of $\boldsymbol{K}'$ still remain the same. The eigenvalues and eigenvectors of $\boldsymbol{K}'$ may be obtained alternatively by solving the so-called compatibility equations given in matrix form as

$$(K'^{oo} - \tan\delta')Z'^o\cos\delta' + K'^{oc}\cos\beta' Z'^c = 0,$$
$$K'^{co} Z'^o \cos\delta' + (K'^{cc} + \tan\beta_W')\cos\beta' Z'^c = 0, \quad (23)$$

which are obtained from Eqs. (17), (19), and (22).

B. The Lecomte-Ueda Transformation in Terms of Incoming Waves. When we consider the photofragmentation cross section formulas, it is much more convenient to use incoming-wave channel basis functions instead of standing-wave ones. To handle incoming-wave channel basis functions, usually the basis pair $\{f_i^-, f_i^+\}$ is used instead of $\{f_i, g_i\}$. But, $f_i^{\pm}$ are just exponential functions defined as $\exp(\pm ik_iR)$ with $k_i = \sqrt{2m_i(E - E_i)}$ and do not directly correspond to the pair $\{f_i, g_i\}$. (When the i-th channel becomes closed, k_i becomes $i\kappa_i$.) It may therefore be a good idea to introduce the basis pair which directly corresponds to it. Let us define this basis pair as $\phi_i^{\pm}$ which is related to $f_i^{\pm}$ as

$$\phi_i^+ = \frac{1}{2i}\sqrt{\frac{2m_i}{\pi k_i}} e^{i\eta_i} f_i^+,$$
$$\phi_i^- = \frac{1}{2i}\sqrt{\frac{2m_i}{\pi k_i}} e^{-i\eta_i} f_i^-, \quad (R \geq R_0) \quad (24)$$

for open channels and

$$\phi_i^+ = -\frac{1}{2}\sqrt{\frac{m_i}{\pi \kappa_i}} e^{i\beta_i}(D_i f_i^+ + iD_i^{-1} f_i^-),$$
$$\phi_i^- = \frac{1}{2}\sqrt{\frac{m_i}{\pi \kappa_i}} e^{-i\beta_i}(D_i f_i^- - iD_i^{-1} f_i^+), \quad (R \geq R_0) \quad (25)$$

for closed channels. The relation between them is given by $\phi_i^{+*} = -\phi_i^-$. They are related to the basis pair $\{f_i, g_i\}$ as

$$\phi_i^+ = \frac{1}{2}(f_i + ig_i),$$
$$\phi_i^- = \frac{1}{2}(-f_i + ig_i), \quad (26)$$

regardless of open- or closed-ness of channels. The phase shift η_i in Eq. (24) is the one for the base pair f_i and g_i for an open channel.

The Lecomte-Ueda transformation changes this pair $\{\Phi_i\phi_i^-, \Phi_i\phi_i^+\}$ into a new one. Let us denote the old pair as $\{\theta_i^+, \theta_i^-\}$ and the new one as $\{\theta_j'^+, \theta_j'^-\}$. Then the relation between two pairs is given by

$$\theta_j'^+ = \sum_i \theta_i^+ W_{ij} e^{i\pi\mu_j},$$
$$\theta_j'^- = \sum_i \theta_i^- W_{ij} e^{-i\pi\mu_j}. \quad (27)$$

As W is real, we have the relation $\theta_j'^{+*} = -\theta_j'^-$. With this transformation, the incoming-wave channel basis function

$$\Psi_k^{(-)} = \sum_i \Phi_i(\phi_i^+ \delta_{ik} - \phi_i^- S_{ik}), \ R \geq R_0 \quad (28)$$

transforms into

$$\Psi'^{(-)}_k = \sum_i (\theta'^+_i \delta_{ik} - \phi'^-_i S_{ik}'), \ R \geq R_0. \quad (29)$$

By inserting Eq. (27) into (29), we find the transformation relation between two wavefunctions as

$$\Psi'^{(-)} = \Psi^{(-)} W e^{i\pi\mu} \quad (30)$$

and the one for the short-range scattering matrices as

$$S' = e^{i\pi\mu} W^{(T)} S W e^{i\pi\mu}. \tag{31}$$

It may be easily checked that the relation between the incoming-wave and standing-wave channel basis functions is invariant under the Lecomte-Ueda transformation, *i.e.*,

$$\Psi_k' = \sum_j \Psi'^{(-)}_j (1 + iK')_{jk}. \tag{32}$$

Notice that the summations in Eqs. (28) and (29) include closed-channel contributions which can grow exponentially. The physical solutions satisfying the boundary conditions at the asymptotic region can be obtained by the superposition of $\Psi'^{(-)}_k$ as

$$\boldsymbol{\Psi}'^{(-)}_j = \sum_k \Psi'^{(-)}_k A_{kj}' = \sum_{k\in P} \Psi'^{(-)}_k A'^{o}_{kj} + \sum_{k\in Q} \Psi'^{(-)}_k A'^{c}_{kj} \tag{33}$$

so that they take the following form in the asymptotic region

$$\boldsymbol{\Psi}'^{(-)}_j \to \sum_i (\theta'^{+}_i \delta_{ij} - \theta'^{-}_i \boldsymbol{S}_{ij}') \tag{34}$$

and the coefficients of the exponentially rising terms become zero. The incoming-wave boundary condition is satisfied when

$$A'^{o} = 1,$$
$$S'^{oo} A'^{o} + S'^{oc} A'^{c} = \boldsymbol{S}', \tag{35}$$

which yield the solutions

$$A'^{c} = -(S'^{cc} - e^{2i\beta_W'})^{-1} S'^{co}, \tag{36}$$

where $\exp(2i\beta_W')$ denotes

$$e^{2i\beta_W'} = e^{i\pi\mu^c} (W^{cc})^{(T)} e^{2i\beta} W^{cc} e^{i\pi\mu^c}. \tag{37}$$

From the solutions (36), the physical scattering matrix is expressed in terms of the submatrices of the short-range scattering matrix as

$$\boldsymbol{S}' = S'^{oo} - S'^{oc} (S'^{cc} - e^{2i\beta_W'})^{-1} S'^{co}. \tag{38}$$

In Appendix A, it is shown that $\boldsymbol{K}'$ of Eq. (20) can be derived from $\boldsymbol{S}'$ of Eq. (38).

With the expansion coefficients obtained in Eqs. (35) and (36), Eq. (33) can be written as

$$\boldsymbol{\Psi}'^{(-)}_j = \Psi'^{(-)}_j - \sum_{k\in Q} \Psi'^{(-)}_k [(S'^{cc} - e^{2i\beta_W'})^{-1} S'^{co}]_{kj}. \tag{39}$$

Inserting Eqs. (A1) and (A3) in Appendix A, A'^{c} of Eq. (36) may be expressed in terms of the submatrices of the short-range reactance matrix K as

$$A'^{c} = (1 + iK'^{cc})(\tan\beta_W' + K'^{cc})^{-1}(i + \tan\beta_W')$$
$$\times (1 + iK'^{cc})^{-1} K'^{co} (-1 + K'^{oo})^{-1}, \tag{40}$$

which is rather complicated. When W^{cc} is the unit matrix, Eq. (40) becomes simplified as

$$A'^{c} = (\tan\beta' + i)(\tan\beta' + K'^{cc})^{-1} K'^{co} (-i + K'^{oo})^{-1} \tag{41}$$

and Eq. (39) becomes

$$\boldsymbol{\Psi}'^{(-)}_j = \Psi'^{(-)}_j + \sum_{k\in Q} \Psi'^{(-)}_k [(\tan\beta' + i)$$
$$\times (\tan\beta' + K'^{cc})^{-1} K'^{co} (-i + K'^{oo})^{-1}]_{kj}. \tag{42}$$

It can easily be shown that similar equations to Eqs. (30) and (31) hold for the physical incoming wavefunctions $\boldsymbol{\Psi}'^{(-)}_j$ and physical scattering matrix $\boldsymbol{S}$ in matrix form as

$$\boldsymbol{\Psi}'^{(-)} = \boldsymbol{\Psi}^{(-)} W^{oo} e^{i\pi\mu^o}, \tag{43}$$

$$\boldsymbol{S}' = e^{i\pi\mu^o} W^{oo(T)} \boldsymbol{S} W^{oo} e^{i\pi\mu^o}. \tag{44}$$

If the original matrix $\boldsymbol{S}$ is symmetric, its transform given by Eq. (44) is also symmetric when W is real and orthogonal. The reality of W also ensures that the transform of the reactance matrix given by Eq. (5) is real. $\boldsymbol{S}^{T} = \boldsymbol{S}$ implies that the related processes are invariant under time reversal. Thus, with W real, the Lecomte-Ueda transformation conserves the time reversal invariance. Notice that channel basis functions cannot be used to describe a fragmentation process $\boldsymbol{\Psi}^{(-)}_j$ when a particular channel is observed at the asymptotic region as they are given by superpositions of fragmentation processes. Thus channel basis functions $\Psi'^{(-)}_k$ which are obtained from the Lecomte-Ueda transformation cannot in general be used to calculate partial photofragmentation cross sections. In this regard, wavefunctions obtained from the fragmentation channel basis functions by the phase renormalization alone are different and can still be used for the calculation of the partial cross sections. Wavefunctions produced by the Lecomte-Ueda transformation including an orthogonal one, however, can still be useful for other purposes. They can be used to find eigenchannel basis functions for the scattering matrix containing only a resonance contribution. They can also be used for the calculation of the total cross sections as Lecomte and Ueda did as channels are not detected separately in the measurement of total cross sections.

Before ending this section, let us briefly comment on the matrix β_W'. The right-hand side of Eq. (37) is a product of unitary transformations and is itself a unitary transformation and thus can be expressed as the form given on the left-hand side, where β_W' is the Hermitian matrix and no longer diagonal. Though it is difficult to show that the right-hand side of Eq. (18) is equal to the tangent function of this matrix β_W', it should be so as we can derive one from another as shown in Appendix A.

C. The Restricted and Successive Lecomte-Ueda Teransformation. Lecomte and Ueda's transformation is too general for most purposes. Many useful conclusions can be drawn with more restricted transformations. Throughout the paper, orthogonal transformations will not be allowed between closed and open channel basis functions, *i.e.*, $W^{co} = W^{oc} = 0$. With this restriction, Lecomte-Ueda transformation is described by μ^o, μ^c, W^{oo}, W^{cc} and will be denoted by $T(\pi\mu^o, \pi\mu^c, W^{oo}, W^{cc})$. Let us first consider the orthogonal trans- formation which is allowed only among open channel basis functions, *i.e.*, let us consider the transformation $T(\pi\mu^o, \pi\mu^c, W^{oo}, I^{cc})$ and the problem of separating out the intra-channel-block couplings from the inter-channel-block ones in the reactance matrices. The way to separate those couplings out in the reactance matrices is to let basis functions have intra-channel-block couplings as far as possible so that they are removed in the reactance matrices as far as possible. Or, adjust the parameters in the Lecomte-Ueda transformation so that intra-channel-blocks of reactance matrices become zero as far as possible. Lecomte showed that this can be achieved up to the level that $K'^{oo} = 0$ and $K'^{cc}_{ii} = 0$ [$i = 1, \ldots, N_c$ (the number of closed channels)] with the transformation $T(\pi\mu^o, \pi\mu^c, W^{oo}, I^{cc})$ when there are no degenerate levels in closed channels. Let us briefly describe this.

The submatrix K'^{oo} of K' can be related to the unprimed quantities in the same way as the whole K' matrix is related to the whole K:

$$K'^{oo} = (W^{(T)oo}K''^{oo}W^{oo}\sin\pi\mu^o + \cos\pi\mu^o)^{-1} \times (W^{(T)oo}K''^{oo}W^{oo}\cos\pi\mu^o - \sin\pi\mu^o) \tag{45}$$

if we introduce the K''^{oo} matrix defined as

$$K''^{oo} = K^{oo} - K^{oc}\sin\pi\mu^c(K^{cc}\sin\pi\mu^c + \cos\pi\mu^c)^{-1}K^{co}. \tag{46}$$

The right-hand side of Eq. (45) may be made zero by simply choosing the transformation parameters W^{oo} and μ^o so that $W^{oo(T)}K''^{oo}W^{oo}$ equals $\tan\pi\mu^o$. But notice that the definition of the K''^{oo} matrix requires the values of μ^c in advance. Of course, $K'^{oo} = 0$ regardless of the values of μ^c as far as $W^{oo(T)}K''^{oo}W^{oo}$ equals $\tan\pi\mu^o$. In other words, we have freedom in choosing the values of μ^c. The best way of choosing their values is, of course, to make the elements of K'^{cc} zero as far as possible. If $K'^{oo} = 0$, the corresponding κ'^{cc} in Eq. (11) becomes

$$\kappa'^{cc} = K'^{cc} - iK'^{co}K'^{oc} \tag{47}$$

and we have $K'^{cc} = \Re(\kappa'^{cc})$. If we apply the N_c conditions of $\Re(\kappa'^{cc}_{ii}) = 0$ ($i = 1, \ldots, N_c$) to Eq. (12), we have N_c equations for μ^c which completely determine μ^c. That is, with the conditions of zero diagonal elements of $\Re(\kappa'^{cc})$ all the transformation parameters of $T(\pi\mu^o, \pi\mu^c, W^{oo}, I^{cc})$ are determined and no freedom is left in the transformation. If we consider the system involving only one closed channel, the complete separation of the intra- and inter-channel-block couplings expressed as $K'^{oo} = K'^{cc} = 0$ is achieved with this transformation $T(\pi\mu^o, \pi\mu^c, W^{oo}, I^{cc})$.

Let us limit the discussion to the system involving only one closed channel for the time being. In this case, the contribution of the closed channels to the physical wave-functions (42) becomes extremum at $\tan\beta' + \Re(\kappa'^{cc}) = 0$ at which resonance takes place.[24] (We will follow other people's convention of calling this extremum point the 'pole'. It is different from the mathematical term 'pole' which includes an imaginary part as well.) Thus the condition $\Re(\kappa'^{cc}) = 0$ is equal to $\tan\beta' = 0$ indicating that it is also the condition for positioning the resonance center to the origin in the Lu-Fano plot. But, here, it should be noticed that $\Re(\kappa'^{cc}) = 0$ does not mean $K'^{cc} = 0$. They are identical only when $K'^{oo} = 0$. As we shall see, the case that K'^{oo} is not a zero matrix but $\Re(\kappa'^{cc})$ still remains zero plays an important role in studying the resonance structures. Since the pole position is moved to the origin in the Lu-Fano plot when $\Re(\kappa'^{cc}) = 0$, let us call this kind of representation the "resonance-centered representation". As stated above, not only K'^{oo} but also K'^{cc} can be made zero with the transformation $T(\pi\mu^o, \pi\mu^c, W^{oo}, I^{cc})$ when there is only one closed channel. In this case, both $\Re(\kappa'^{cc})$ and $\Re(\kappa'^{oo})$ become zero and, as will be discussed more in detail later, the rank of the physical reactance matrix is one, which indicates that only one channel basis function shows a resonance behavior while others do not. In other words, the resonance and background contributions are completely separated. We will call this kind of representation the "pure-resonance representation". If there are more than one closed channel involved, the pole position is approximately obtained at $\det[\tan\beta' + \Re(\kappa'^{cc})] = 0$.[7] In this case, $\Re(\kappa'^{cc}) = 0$ means $\Pi_{i\in Q}\tan\beta_i' = 0$ and resonances are centered. Further discussion on this problem is beyond the scope of the present paper.

Let us next consider the successive Lecomte-Ueda transformations. At first, the Lecomte-Ueda transformation starts from the base pair for a single fragmentation channel. Generally, the base pair after the transformation does not belong to a single fragmentation channel and becomes unsuitable for the description of partial cross sections. But, if Lecomte-Ueda transformations involve only phase renormalization, the base pair after the transformation still remains in the same single fragmentation channel and can thus be used for the description of partial cross sections.

It is sometimes useful to consider the single Lecomte-Ueda transformation as composed of two successive Lecomte-Ueda transformations. Successive Lecomte-Ueda transformations considered by Lecomte are the ones that the first transformation only changes the base pairs for open channels followed by the change of the base pairs for closed channels. We can easily show that these successive Lecomte-Ueda transformations are equivalent to a single Lecomte-Ueda transformation. For example, if the first and second Lecomte-Ueda transformations are $T_1(\pi\mu^o, 0, W^{oo}, I^{cc})$ and $T_2(0, \pi\mu^c, I^{oo}, W^{cc})$, respectively, then T_2T_1 is equal to the single one given by $T(\pi\mu^o, \pi\mu^c, W^{oo}, W^{cc})$. In this case, the order of transformation is commutable, that is, $T_2T_1 = T_1T_2$. There is another case where a single transformation can be easily decomposed into two successive transformations. Actually, all the Lecomte-Ueda transformations can be considered as composed of two successive transformations, first by an orthogonal transformation and then by a phase renormalization by $\pi\mu$.

Applying the Lecomte-Ueda Transformation to the K Matrix for the Two Open and One Closed Channel System

Recently, for the system involving two open and one closed channels, we reformulated MQDT into the forms of the CM one, where we find that the resultant reactance matrix still keeps non-zero diagonal elements even when the axes of the Lu-Fano plot are translated so that the plot becomes symmetrical.[20] This contrasts with the system involving two channels studied by Giusti-Suzor and Fano, where the symmetrical Lu-Fano plot is obtained for the reactance matrix whose diagonal elements are zero. This contrast can be studied by using the Lecomte-Ueda transformation. Before doing this, let us briefly describe how such a strange reactance matrix is obtained. The physical scattering matrix $\boldsymbol{S}$ can be written as a product of background and resonance terms, *i.e.*, $\boldsymbol{S} = \boldsymbol{S}^0\boldsymbol{S}_r$. The background scattering matrix $\boldsymbol{S}^0$ may be expressed in matrix form as $\boldsymbol{S}^0 = U^0\exp(-2i\delta^0)U^{0(T)}$ with the background eigenphase shifts δ_i^0 (i = 1, 2, ...) and the orthogonal matrix U^0. The resonance scattering matrix likewise may be written into the form exp $(-2i\delta_r\boldsymbol{P}_r)$ for an isolated resonance where δ_r is the phase shift due to the resonance and is defined by $-\cot\delta_r = 2(E-E_0)/\Gamma$ with the resonance energy E_0 and the half-width Γ. $\boldsymbol{P}_r$ is the projection matrix into the resonance eigenchanenls.[21] Let us consider the transforms $U^{0(T)}\boldsymbol{S}U^0$, $U^{0(T)}\boldsymbol{S}^0U^0$, and $U^{0(T)}\boldsymbol{S}_rU^0$ and denotes them as $\mathcal{S}$, $\mathcal{S}^0$, and $\mathcal{S}_r$, respectively. If we restrict the number of open channels to two, the orthogonal matrix U^0 is expressed with one parameter, say θ_0, as $\exp(-i\theta_0\sigma_y/2)$ and the transforms $\mathcal{S}^0$ and $\mathcal{S}_r$ may be expressed in terms of Pauli matrices as[21,25]

$$\mathcal{S}^0 = e^{-i(\delta_\Sigma^0\mathbf{1} + \Delta_{12}^0\boldsymbol{\sigma}_z)},$$
$$\mathcal{S}_r = e^{i(\delta_r\mathbf{1} - \delta_r\boldsymbol{\sigma}\cdot\boldsymbol{n}_r')}, \tag{48}$$

where $\delta_\Sigma^0 \equiv \delta_1^0 + \delta_2^0$, $\Delta_{12}^0 \equiv \delta_1^0 - \delta_2^0$ and $\boldsymbol{n}_r'$ is defined as

$$\boldsymbol{n}_r' = R_z(-\Delta_{12}^0)R_y(\theta_r)\boldsymbol{z}$$
$$= (\sin\theta_r\cos\Delta_{12}^0, -\sin\theta_r\sin\Delta_{12}^0, \cos\theta_r) \tag{49}$$

with θ_r defined in terms of half-widths Γ_1 and Γ_2 as

$$\cos\theta_r \equiv \frac{\Gamma_1 - \Gamma_2}{\Gamma_1 + \Gamma_2},$$
$$\sin\theta_r \equiv \frac{2\sqrt{\Gamma_1\Gamma_2}}{\Gamma_1 + \Gamma_2}. \tag{50}$$

Ref. [21] obtained

$$\mathcal{S} = \mathcal{S}^0\mathcal{S}_r = e^{-i(\delta_\Sigma^0 + \delta_r)}e^{-i\Delta_{12}^0\sigma_z}e^{-i\delta_r\boldsymbol{\sigma}\cdot\boldsymbol{n}_r'}$$
$$= e^{-i(\delta_\Sigma^0 + \delta_r)}e^{-i\delta_a\boldsymbol{\sigma}\cdot\boldsymbol{n}_a}, \tag{51}$$

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

$$\boldsymbol{n}_a = R_y(\theta_a)\mathbf{z}, \tag{52}$$

$$\cot\delta_a = -\cot\Delta_{12}^0\frac{\varepsilon_a - q_a}{\sqrt{\varepsilon_a^2 + 1}} \tag{53}$$

with $q_a \equiv -\cot\theta_r/\cos\Delta_{12}^0$ and ε_a or θ_a are defined as

$$\varepsilon_a \equiv -\cot\theta_a = -\frac{\sin\Delta_{12}^0}{\sin\theta_r}(\cot\delta_r + \cot\Delta_{12}^0\cos\theta_r). \tag{54}$$

The original scattering matrix $\boldsymbol{S}$ differs from $\mathcal{S}$ only in that $\boldsymbol{n}_a$ is replaced by $\boldsymbol{n}_a' \equiv R_y(\theta_0)\boldsymbol{n}_a$ since

$$\boldsymbol{S} = e^{-\frac{i}{2}\theta_0\sigma_y}\mathcal{S}e^{\frac{i}{2}\theta_0\sigma_y} = e^{i(\delta_\Sigma^0 + \delta_r)}e^{i\delta_a\boldsymbol{\sigma}\cdot\boldsymbol{n}_a'}. \tag{55}$$

It is shown in Ref. [21] that of Eq. (51) can be obtained from $\mathcal{S}^0$ and $\mathcal{S}_r$ of Eq. (48) by making use of spherical trigonometry for the spherical triangle shown in Figure 1. In Ref. [20], Giusti-Suzor and Fano's method of phase renormalization is used to transform the physical scattering matrix of MQDT into a form of CM given in Eq. (55). This reformulation is not a simple task if three channels are involved since eigenphase shifts do not transform linearly but in a rather complicated way by phase renormalization, described by the spherical triangle in Figure 1. The summary of the results of Ref. [20] is described in the next subsection.

A. Translation of the Axes in the Lu-Fano Plot. MQDT can be reformulated so that its physical scattering matrix $\boldsymbol{S}$ takes the form (55). This can be achieved when the short-range reactance matrix can be written as[20]

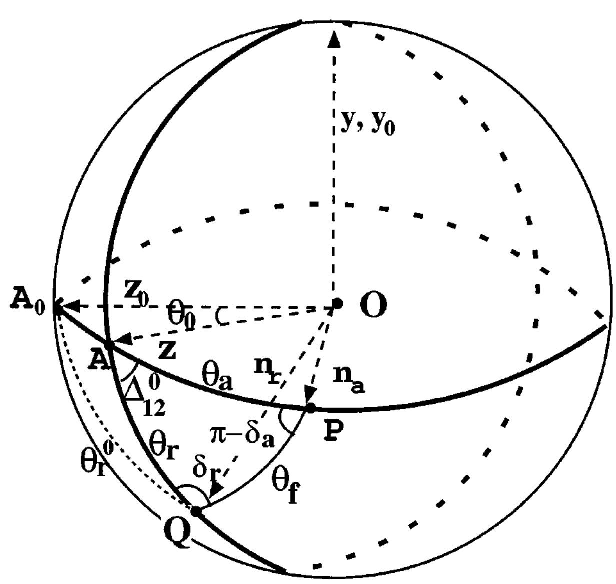

Figure 1. The spherical triangle formed by the three vectors $\mathbf{z}$, $\boldsymbol{n}_r$, and $\boldsymbol{n}_a$ is shown, which is used to show the geometrical relationships among various eigenchannels employed to study resonance structures. Also shown is the spherical triangle formed by the three vectors $\mathbf{z}_0$, $\mathbf{z}$, and $\boldsymbol{n}_r$, which is used for the Gailitis average of the partial cross sections.

$$\tilde{K} = \begin{pmatrix} \tan\frac{\Delta_{12}^0}{2}\cos\theta_0 & \tan\frac{\Delta_{12}^0}{2}\sin\theta_0 & \frac{\xi}{\cos\frac{\Delta_{12}^0}{2}}\cos\frac{1}{2}(\theta_1+\theta_0) \\ \tan\frac{\Delta_{12}^0}{2}\sin\theta_0 & -\tan\frac{\Delta_{12}^0}{2}\cos\theta_0 & \frac{\xi}{\cos\frac{\Delta_{12}^0}{2}}\sin\frac{1}{2}(\theta_1-\theta_0) \\ \frac{\xi}{\cos\frac{\Delta_{12}^0}{2}}\cos\frac{1}{2}(\theta_1+\theta_0) & \frac{\xi}{\cos\frac{\Delta_{12}^0}{2}}\sin\frac{1}{2}(\theta_1-\theta_0) & \xi^2\tan\frac{\Delta_{12}^0}{2}\cos\theta_1 \end{pmatrix}. \tag{56}$$

where ξ is defined by

$$\xi^2 = \frac{\mathrm{tr}(\tilde{K}^{oc}\tilde{K}^{co})}{1-|\tilde{K}^{oo}|}. \tag{57}$$

In this representation, the physical scattering matrix $\tilde{S}$ is shown in Ref. [20] to be related to the scattering matrix S(CM) of the CM theory given in Eq. (55) by

$$\tilde{S} = e^{i\delta_\Sigma^0}S(\mathrm{CM}). \tag{58}$$

$\tilde{S}$ of MQDT can completely be made equal to that of CM by phase renormalization but is left in the present form in order to make the Lu-Fano plot symmetrical. This point will be explained shortly afterwards. Let us denote the solutions of the compatibility equation

$$\begin{vmatrix} \tilde{K}^{oo} - \tan\tilde{\delta} & \tilde{K}^{oc} \\ \tilde{K}^{co} & \tilde{K}^{cc} + \tan\tilde{\beta} \end{vmatrix} = 0 \tag{59}$$

for this system as $\tan\tilde{\delta}_+$ and $\tan\tilde{\delta}_-$. In this formulation, the eigenphase sum $\delta_\Sigma(=\delta_+ + \delta_-)$ is made identical to the phase shift δ_r due to the resonance in conformity with Simonius and Hazi's theorem[26,27] by imposing the condition

$$\tan\tilde{\delta}_\Sigma = -\xi^2/\tan\tilde{\beta}. \tag{60}$$

which holds when $\tilde{K}$ satisfies

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

This $\tilde{K}$ matrix is obtained from the original K matrix by only allowing the phase renormalization. Here, it should be noted that the Lu-Fano plot for the system involving two open and one closed channels is composed of two curves (β, δ_+) and (β, δ_-) However, the graph we want to make symmetric in the new coordinate system is not those two curves. Those two curves are not suitable for that purpose because of the mutual repulsion which makes both graphs complicated. The one we want to make symmetrical is (β, δ_Σ) as the eigenphase sum in CM shows the same behavior as that in a single open channel problem[26,27]:

$$\delta_\Sigma(\mathrm{CM}) = \delta_\Sigma^0 - \cot^{-1}\frac{2(E-E_r)}{\Gamma} = \delta_\Sigma^0 + \delta_r. \tag{62}$$

To make the Lu-Fano plot symmetrical, the term δ_Σ^0 of S(CM) is removed in $\tilde{S}$ as shown in Eq. (58). Let $\pi\mu_3$ and $\pi\mu_\Sigma$ denote the shifts to β and δ_Σ, respectively, so that the new curve $(\tilde{\beta}, \tilde{\delta}_\Sigma)$ is symmetrical. Their values are obtained in Ref. [20] as

$$\tan(2\pi\mu_3) = \frac{2\{\mathrm{tr}K^{oo}[K^{cc}\mathrm{tr}K^{oo} - \mathrm{tr}(K^{oc}K^{co})] + (1-|K^{oo}|)(K^{cc}-|K|)\}}{(\mathrm{tr}K^{oo})^2 - [K^{cc}\mathrm{tr}K^{oo} - \mathrm{tr}(K^{oc}K^{co})]^2 + (1-|K^{oo}|)^2 - (K^{cc}-|K|)^2} \tag{63}$$

and

$$\tan(2\pi\mu_\Sigma) = \frac{2\{(1-|K^{oo}|)\mathrm{tr}K^{oo} + [K^{cc}\mathrm{tr}K^{oo} - \mathrm{tr}(K^{oc}K^{co})](K^{cc}-|K|)\}}{(1-|K^{oo}|)^2 + (K^{cc}-|K|)^2 - (\mathrm{tr}K^{oo})^2 - [K^{cc}\mathrm{tr}K^{oo} - \mathrm{tr}(K^{oc}K^{co})]^2}. \tag{64}$$

Using the relations

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

$$|\kappa^{cc}|^2 = \frac{(|K|-K^{cc})^2 + [K^{cc}\mathrm{tr}K^{oo} - \mathrm{tr}(K^{oc}K^{co})]^2}{(|K^{oo}|-1)^2 + (\mathrm{tr}K^{oo})^2}, \tag{65}$$

Eq. (63) can be rewritten as

$$\tan(2\pi\mu_3) = \frac{2\Re(\kappa^{cc})}{1-|\kappa^{cc}|^2}. \tag{66}$$

If we recall the transformation relation (12) for κ^{cc}, it is easily checked that Eq. (66) is equal to $\Re(\tilde{\kappa}^{cc}) = 0$. The latter is true for the $\tilde{K}$ matrix given by Eq. (56). Actually $\tilde{\kappa}^{cc}$ corresponding to $\tilde{K}$ is obtained as

$$\tilde{\kappa}^{cc} = -i\xi^2 \tag{67}$$

and is purely imaginary.

We earlier started that the representation where $\Re(\tilde{\kappa}^{cc}) = 0$ belongs to the class of the resonance-centered representation. Let us repeat it by restricting the argument to this specific representation. The pole position in Eq. (42) and observables are given by the root of the real part of $\tan\beta + \tilde{\kappa}^{cc}$ for the one closed channel system, *i.e.*,

$$\tan\tilde{\beta} + \Re(\tilde{\kappa}^{cc}) = 0. \tag{68}$$

If we want the pole position becomes the origin of the Lu-Fano plot $(\tilde{\beta}, \tilde{\delta}_\Sigma)$, then $\Re(\tilde{\kappa}^{cc})$ should be zero so that $\tilde{\beta}$ is zero at the origin. Thus the value of μ_3 given by Eq. (63) is the one which moves the origin of the Lu-Fano plot to the pole position.

B. The Matrix in the Background Eigenchannel Basis. The short-range reactance matrix $\tilde{K}$, given in Eq. (56), yields the Lu-Fano plot where the pole position is the origin but the matrix still has non-zero diagonal elements, meaning that intra- and inter-channel-block couplings are not fully separated yet. Notice that, in order to obtain $\tilde{K}$, only phase renormalization is used. But, Lecomte and Ueda previously showed that making the diagonal elements of reactance matrices zero cannot be achieved by phase renormalization alone. We have to include orthogonal transformation as well.

Before considering the Lecomte-Ueda transformation which makes the diagonal submatrices K^{oo} and K^{cc} zero. let us first consider getting rid of θ_0 from the reactance matrix $\tilde{K}$. The way of doing this is to transform the basis functions from the background fragmentation ones to the background eigenchannel ones as we will see below. It corresponds to the transformation $T[0, 0, 0, \exp(-i\theta_0\sigma_y/2), I^{cc}]$. (Previously, the notation $T(\pi\mu^o, \pi\mu^c, W^{oo}, W^{cc})$ is used to denote a Lecomte-Ueda transformation. A little modified notation $T(\pi\mu_1, \pi\mu_2, \pi\mu_3, W^{oo}, W^{cc})$ suitable for the system involving two open and one closed channels may also be used. Since they have a different number of arguments, no confusion may arise in using both of them at the same time.) If we use the double bar for the transformed quantities, the transformation relation between the reactance matrices are given by $\bar{\bar{K}} = W^T\tilde{K}W$ according to Eq. (7), where W is given by

$$W = \begin{pmatrix} W^{oo} & 0 \\ 0 & W^{cc} \end{pmatrix} = \begin{pmatrix} e^{-i\frac{1}{2}\theta_0\sigma_y} & 0 \\ 0 & I^{cc} \end{pmatrix}. \tag{69}$$

It can be calculated as

$$\bar{\bar{K}} = \begin{pmatrix} e^{i\frac{1}{2}\theta_0\sigma_y}\tilde{K}^{oo}e^{i\frac{1}{2}\theta_0\sigma_y} & e^{i\frac{1}{2}\theta_0\sigma_y}\tilde{K}^{oc} \\ \tilde{K}^{co}e^{i\frac{1}{2}\theta_0\sigma_y} & \tilde{K}^{cc} \end{pmatrix}. \tag{70}$$

Using the Pauli matrix form of $\tilde{K}^{oo}$ in Eq. (56) given as

$$\tilde{K}^{oo} = \tan\frac{1}{2}\Delta_{12}^0\boldsymbol{\sigma}\cdot[R_y(\theta_0)z], \tag{71}$$

the $\bar{\bar{K}}$ matrix may be rewritten as

$$\bar{\bar{K}} = \begin{pmatrix} \tan\frac{\Delta_{12}^0}{2} & 0 & \frac{\xi}{\cos\frac{\Delta_{12}^0}{2}}\cos\frac{1}{2}\theta_r \\ 0 & -\tan\frac{\Delta_{12}^0}{2} & \frac{\xi}{\cos\frac{\Delta_{12}^0}{2}}\sin\frac{1}{2}\theta_r \\ \frac{\xi}{\cos\frac{\Delta_{12}^0}{2}}\cos\frac{1}{2}\theta_r & \frac{\xi}{\cos\frac{\Delta_{12}^0}{2}}\sin\frac{1}{2}\theta_r & \xi^2\tan\frac{\Delta_{12}^0}{2}\cos\theta_r \end{pmatrix}. \tag{72}$$

Notice that θ_0 in $\tilde{K}$ is removed in $\bar{\bar{K}}$ and included into the transformation. The transformation $T[0, 0, 0, \exp(-i\theta_0\sigma_y/2), I^{cc}]$ causes a similarity transformation in the reactance matrix as $\bar{\bar{K}} = W^T\tilde{K}W$ and therefore eigenvalues of the reactance matrix and the solutions of the compatibility equation (23) are not changed by it. Accordingly, the Lu-Fano plot remains invariant under the transformation.

According to Eqs. (7) and (30), only open channel basis wavefunctions are transformed by this transformation. Incoming-wave channel basis functions, for example, are transformed as

$$(\bar{\bar{\Psi}}_1^{(-)}, \bar{\bar{\Psi}}_2^{(-)}) = (\tilde{\Psi}_1^{(-)}, \tilde{\Psi}_2^{(-)})e^{-\frac{i}{2}\theta_0\sigma_y},$$
$$\bar{\bar{\Psi}}_3^{(-)} = \tilde{\Psi}_3^{(-)}. \tag{73}$$

From Eqs. (43) and (44), the transformation relations between physical incoming wavefunctions and scattering matrices are given in matrix form as

$$\bar{\bar{\Psi}}^{(-)} = \tilde{\Psi}^{(-)}e^{-\frac{i}{2}\theta_0\sigma_y} = \tilde{\Psi}^{(-)}U^0,$$
$$\bar{\bar{\boldsymbol{S}}} = e^{\frac{i}{2}\theta_0\sigma_y}\tilde{\boldsymbol{S}}e^{-\frac{i}{2}\theta_0\sigma_y} = U^{0(T)}\tilde{\boldsymbol{S}}U^0 = e^{i\delta_s}e^{i\delta_v\boldsymbol{\sigma}\cdot\boldsymbol{n}_a}, \tag{74}$$

where $\exp(-i\theta_0\sigma_y/2)$ is identified with the original matrix U^0 which diagonalizes the background scattering matrix $\boldsymbol{S}^0$ of CM. Since $\tilde{\boldsymbol{S}}$ is identical to $\boldsymbol{S}$ of CM except for a trivial scalar factor, $\bar{\bar{\boldsymbol{S}}}$ is identical to S except for the trivial factor. Since the background scattering matrix in $U^{0(T)}\boldsymbol{S}U^0$ of CM is diagonal, the incoming-wave channel basis functions (73) obtained from the Lecomte-Ueda transformation $T[0, 0, 0, \exp(-i\theta_0\sigma_y/2), I^{cc}]$ are background eigenchannel basis functions.

C. Complete Removal of the Background Part in *K*. Let us now consider obtaining the reactance matrix whose diagonal elements are zero as considered by others. Inspection of Eq. (72) shows that this can be achieved by removing Δ_{12}^0 from $\bar{\bar{K}}$. The removal can be accomplished by two consecutive Lecomte-Ueda transformations $T_1(0, \pi\mu^c, I^{oo}, I^{cc})$ and $T_2(\pi\mu^o, 0, W^{oo}, I^{cc})$ considered by Lecomte and described before. T_1 is built to make $\Re(\kappa''^{cc})$ zero. We first notice that we do not have a use for T_1 as the real part of $\bar{\bar{\kappa}}^{cc}$ is already zero. In other words, T_1 is the identity transformation. The parameters μ^o and W^{oo} for T_2 are defined as eigenvalues and eigenvectors of K''^{oo} of Eq. (46). Since T_1 is the identity transformation, K''^{oo} equals $\bar{\bar{K}}^{oo}$. That is, they are obtained by diagonalizing $\bar{\bar{K}}^{oo}$ but $\bar{\bar{K}}^{oo}$ is already diagonalized. Thus W^{oo} is the unit matrix and μ^o are given by $\Delta_{12}^0/2$ and $-\Delta_{12}^0/2$. Let us denote the reactance matrix obtained by this transformation $T(\Delta_{12}^0/2, -\Delta_{12}^0/2, 0, I^{oo}, I^{cc})$ as $\bar{K}$. The only nonzero submatrices in $\bar{K}$ are $\bar{K}^{oc}$ and $\bar{K}^{co}$ calculated as

$$\bar{K}^{co} = \bar{\bar{K}}^{co}\cos\pi\mu^o = \bar{\bar{K}}^{co}\cos\frac{1}{2}\Delta_{12}^0 = \left(\xi\cos\frac{1}{2}\theta_r, \xi\sin\frac{1}{2}\theta_r\right). \tag{75}$$

$$\bar{K}^{oc} = \cos\frac{1}{2}\Delta_{12}^0\bar{\bar{K}}^{oc} = \begin{pmatrix} \xi\cos\frac{1}{2}\theta_r \\ \xi\sin\frac{1}{2}\theta_r \end{pmatrix}. \tag{76}$$

Overall, the $\bar{K}$ matrix is obtained as

$$\bar{K} = \begin{pmatrix} 0 & 0 & \xi\cos\frac{1}{2}\theta_r \\ 0 & 0 & \xi\sin\frac{1}{2}\theta_r \\ \xi\cos\frac{1}{2}\theta_r & \xi\sin\frac{1}{2}\theta_r & 0 \end{pmatrix}. \tag{77}$$

Note that the parameter β for the $\bar{K}$ matrix is not changed by the transformations and remains the same as the one $\tilde{\beta} = \beta$

$= \beta + \pi\mu_3$ as the transformations do not change the phase shift for the closed channel, *i.e.*, we have

$$\bar{\beta} = \bar{\bar{\beta}} = \tilde{\beta} = \beta + \pi\mu_3. \tag{78}$$

The physical $\bar{\boldsymbol{K}}$ matrix corresponding to $\bar{\boldsymbol{K}}$ is obtained as

$$\begin{aligned}\bar{\boldsymbol{K}} &= \bar{K}^{oo} - \bar{K}^{oc}(\tan\tilde{\beta} + \bar{K}^{cc})^{-1}\bar{K}^{co} \\ &= -\frac{\xi^2}{\tan\tilde{\beta}}\begin{pmatrix} \cos^2\frac{1}{2}\theta_r & \sin\frac{1}{2}\theta_r\cos\frac{1}{2}\theta_r \\ \sin\frac{1}{2}\theta_r\cos\frac{1}{2}\theta_r & \sin^2\frac{1}{2}\theta_r \end{pmatrix} \\ &= -\frac{\xi^2}{\tan\tilde{\beta}}\frac{1}{2}(1 + \boldsymbol{\sigma}\cdot\boldsymbol{n}_r),\end{aligned} \tag{79}$$

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

$$\boldsymbol{n}_r = R_y(\theta_r)\boldsymbol{z} = \boldsymbol{z}\cos\theta_r + \boldsymbol{x}\sin\theta_r. \tag{80}$$

Eq. (79) can be rewritten as

$$\bar{\boldsymbol{K}} = \tan\delta_r\boldsymbol{P}_r, \tag{81}$$

where we have made use of

$$\tan\delta_r = -\frac{\xi^2}{\tan\tilde{\beta}} \tag{82}$$

and

$$\boldsymbol{P}_r = \frac{1}{2}(1 + \boldsymbol{\sigma}\cdot\boldsymbol{n}_r). \tag{83}$$

Now let us consider $\bar{\boldsymbol{S}}$ which is related to $\bar{\boldsymbol{K}}$ of Eq. (81) by

$$\bar{\boldsymbol{S}} = (1 - i\bar{\boldsymbol{K}})(1 + i\bar{\boldsymbol{K}})^{-1}. \tag{84}$$

By inserting Eq. (81) into (84) and making use of

$$(1 + i\bar{\boldsymbol{K}})^{-1} = 1 - \boldsymbol{P}_r + e^{-i\delta_r}\cos\delta_r\boldsymbol{P}_r \tag{85}$$

and the properties of projection operators, we obtain

$$\bar{\boldsymbol{S}} = 1 - \boldsymbol{P}_r + e^{-2i\delta_r}\boldsymbol{P}_r = e^{-2i\delta_r P_r} = e^{-i\delta_r}e^{-i\delta_r\boldsymbol{\sigma}\cdot\boldsymbol{n}_r}. \tag{86}$$

Let us quit at this point the further study of the properties of the present representation as the present one has only a use for providing a means of obtaining more important representation, which will become clear later. In the CM theory for an isolated resonance, the 'a' state considered in Ref. [14] plays an important role. The continua in CM for an isolated resonance are divided into the 'a' state and the remaining ones orthogonal to it. Only the 'a' state can interact with the discrete state to produce resonance phenomena while the remaining continua can contribute to the resonance phenomena only through the interference with the 'a' state. If we can construct the kind of 'a' state in MQDT, the MQDT reformulation can be directly compared with the CM theory and utilize all its advantages. Let us do this in the next subsection.

D. The Matrix in the Resonance Eigenchannel Basis. Let us consider further elimination of the matrix elements of the short-range reactance matrix K so that it contains only the inter-channel coupling parameter ξ by separating out the geometrical parameter θ_r. This can be achieved by the orthogonal transformation W given by

$$W = \begin{pmatrix} e^{-i\frac{1}{2}\theta_r\sigma_y} & 0 \\ 0 & I^{cc} \end{pmatrix} \tag{87}$$

which can also be expressed as $T[0, 0, 0, \exp(-i\theta_r\sigma_y/2), I^{cc}]$. Let us denote the reactance matrix obtained by this transformation as K_r. Then, it is easily obtained as

$$K_r = \begin{pmatrix} 0 & 0 & \xi \\ 0 & 0 & 0 \\ \xi & 0 & 0 \end{pmatrix}. \tag{88}$$

Since the transformation does not include a phase renormalization, we have

$$\beta_r = \bar{\beta} = \tilde{\beta}. \tag{89}$$

Using the relation $S_r = (1 - iK_r)(1 + iK_r)^{-1}$, the short-range scattering matrix S_r is easily calculated from K_r as

$$S_r = \begin{pmatrix} \frac{1-\xi^2}{1+\xi^2} & 0 & \frac{-2i\xi}{1+\xi^2} \\ 0 & 1 & 0 \\ \frac{-2i\xi}{1+\xi^2} & 0 & \frac{1-\xi^2}{1+\xi^2} \end{pmatrix}. \tag{90}$$

Using Eq. (90), the form of incoming-wave channel basis functions useful for the future derivation is obtained as

$$\begin{aligned}(\Psi_r^{(-)})_1 &= (\theta_r^+)_1 - \frac{1-\xi^2}{1+\xi^2}(\theta_r^-)_1 + \frac{2i\xi}{1+\xi^2}(\theta_r^-)_3, \\ (\Psi_r^{(-)})_2 &= (\theta_r^+)_2 - (\theta_r^-)_2, \qquad (R \geq R_0). \\ (\Psi_r^{(-)})_3 &= (\theta_r^+)_3 - \frac{1-\xi^2}{1+\xi^2}(\theta_r^-)_3 + \frac{2i\xi}{1+\xi^2}(\theta_r^-)_1.\end{aligned} \tag{91}$$

By making use of the formula (30), the transformation relations of $(\Psi_r^{(-)})_i$ with other incoming-wave channel basis functions are given in matrix form as

$$\begin{aligned}\Psi_r^{(-)} &= \bar{\Psi}^{(-)}\begin{pmatrix} e^{-\frac{i}{2}\theta_r\sigma_y} & 0 \\ 0 & 1 \end{pmatrix} \\ &= \tilde{\Psi}^{(-)}\begin{pmatrix} e^{-\frac{i}{2}\theta_0\sigma_y} & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} e^{\frac{i}{2}\Delta_{12}\sigma_z} & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} e^{-\frac{i}{2}\theta_r\sigma_y} & 0 \\ 0 & 1 \end{pmatrix} \\ &= \tilde{\Psi}^{(-)}\begin{pmatrix} e^{-\frac{i}{2}\theta_0\sigma_y}e^{\frac{i}{2}\Delta_{12}\sigma_z}e^{-\frac{i}{2}\theta_r\sigma_y} & 0 \\ 0 & 1 \end{pmatrix}.\end{aligned} \tag{92}$$

Or, more specifically, we have

$$((\Psi_r^{(-)})_1, (\Psi_r^{(-)})_2) = (\overline{\Psi}_1^{(-)}, \overline{\Psi}_2^{(-)})e^{\frac{i}{2}\theta_r\sigma_y}$$

$$= (\tilde{\Psi}_r^{(-)}{}_1, \tilde{\Psi}_r^{(-)}{}_2)e^{\frac{i}{2}\theta_0\sigma_y}e^{\frac{i}{2}\Lambda_{12}\sigma_z}e^{\frac{i}{2}\theta_r\sigma_y},$$

$$(\Psi_r^{(-)})_3 = \overline{\Psi}_3^{(-)} = \tilde{\Psi}_3^{(-)}. \tag{93}$$

Likewise, we can obtain the transformation relation between scattering matrices. For example, let us consider the relation between $\tilde{S}$ and S_r. For the later use, if we express sub-matrices of $\tilde{S}$ in terms of those of S_r, they are given by

$$\tilde{S}^{oo} = e^{\frac{i}{2}\Lambda_{12}^0\boldsymbol{\sigma}\cdot\boldsymbol{n}_0}e^{\frac{i}{2}(\theta_r - \theta_0)\sigma_y}S_r^{oo}e^{\frac{i}{2}(\theta_r - \theta_0)\sigma_y}e^{\frac{i}{2}\Lambda_{12}^0\boldsymbol{\sigma}\cdot\boldsymbol{n}_0},$$

$$\tilde{S}^{oc} = e^{\frac{i}{2}\Lambda_{12}^0\boldsymbol{\sigma}\cdot\boldsymbol{n}_0}e^{\frac{i}{2}(\theta_r - \theta_0)\sigma_y}S_r^{oc},$$

$$\tilde{S}^{co} = S_r^{co}e^{\frac{i}{2}(\theta_r + \theta_0)\sigma_y}e^{\frac{i}{2}\Lambda_{12}^0\boldsymbol{\sigma}\cdot\boldsymbol{n}_0},$$

$$\tilde{S}^{cc} = S_r^{cc}, \tag{94}$$

where the following relation is used:

$$e^{-\frac{i}{2}\theta_0\sigma_y}e^{\frac{i}{2}\Lambda_{12}^0\sigma_z}e^{-\frac{i}{2}\theta_r\sigma_y} = e^{-\frac{i}{2}\Delta_{12}^0\boldsymbol{\sigma}\cdot\boldsymbol{n}_0}e^{-\frac{i}{2}(\theta_r - \theta_0)\sigma_y}. \tag{95}$$

Let us now consider the physical incoming wavefunctions whose closed channels decrease exponentially in the asymptotic region and whose general form is given by Eq. (39). From Eq. (90), A_r^c is calculated in matrix form as

$$A_r^c = -(S_r^{cc} - e^{2i\beta_r})^{-1}S_r^{co}$$

$$= \frac{i\xi(\tan\tilde{\beta} + i)}{\tan\beta - i\xi^2}(1, 0) \quad (\text{with } \beta_r = \tilde{\beta})$$

$$= e^{i(\tilde{\beta} - \delta_r)}\left(\frac{d\delta_r}{d\tilde{\beta}}\right)^{1/2}(1, 0) \tag{96}$$

and the physical incoming wavefunctions $\boldsymbol{\Psi}_r^{(-)}$ become

$$(\boldsymbol{\Psi}_r^{(-)})_j = \begin{cases} (\Psi_r^{(-)})_1 + (\Psi_r^{(-)})_3 e^{-i(\tilde{\beta} + \delta_r)}\left(\dfrac{d\delta_r}{d\tilde{\beta}}\right)^{1/2} & \text{for } j = 1, \\ (\Psi_r^{(-)})_2 & \text{for } j = 2. \end{cases} \tag{97}$$

The physical incoming wavefunctions $(\boldsymbol{\Psi}_r^{(-)})_1$ and $(\boldsymbol{\Psi}_r^{(-)})_2$ correspond to the CM wavefunctions as

$$((\boldsymbol{\Psi}_r^{(-)})_1, (\boldsymbol{\Psi}_r^{(-)})_2) = -(e^{i\delta_r}\Psi^{(a)}(\text{CM}), \Psi^{(b)}(\text{CM})), \tag{98}$$

as shown in Appendix B. According to Eq. (43), the physical incoming wavefunctions of the r-representation are related to those of the tilde-representation in matrix form as

$$\boldsymbol{\Psi}_r^{(-)} = \tilde{\boldsymbol{\Psi}}^{(-)}e^{-\frac{i}{2}\theta_0\sigma_y}e^{\frac{i}{2}\Delta_{12}^0\sigma_z}e^{-\frac{i}{2}\theta_r\sigma_y}. \tag{99}$$

Let us denote the (j, i)-element of the transformation matrix between the physical incoming wavefunctions of the r-representation and those of the tilde-representation as $(\tilde{\boldsymbol{\Psi}}_j^{(-)} | (\boldsymbol{\Psi}_r^{(-)})_i)$. We may similarly consider the (j, i)-element of the transformation matrix $(\tilde{\Psi}_j^{(-)} | (\Psi_r^{(-)})_i)$ between corresponding channel basis wavefuncitons. From Eqs. (93) and (99), we have

$$\left(\tilde{\boldsymbol{\Psi}}_j^{(-)}\middle|(\boldsymbol{\Psi}_r^{(-)})_i\right) = \left(\tilde{\Psi}_j^{(-)}\middle|(\Psi_r^{(-)})_i\right) = \left[e^{\frac{i}{2}\theta_0\sigma_y}e^{\frac{i}{2}\Lambda_{12}^0\sigma_z}e^{\frac{i}{2}\theta_r\sigma_y}\right]_{ji}. \tag{100}$$

From Eq. (B9), we also have the relation

$$\left(\tilde{\boldsymbol{\Psi}}_j^{(-)}\middle|(\boldsymbol{\Psi}_r^{(-)})_i\right) = \left(\tilde{\Psi}_j^{(-)}\middle|(\Psi_r^{(-)})_i\right) = e^{\frac{i}{2}\delta_2^0}(\psi_j^{(-)}\middle|\psi^{(i)}). \tag{101}$$

where i = 1, 2 corresponds to a, b, respectively.

The physical reactance matrix can easily be calculated from the short-range one given by Eq. (88) as

$$\boldsymbol{K}_r = \tan\delta_r\boldsymbol{p}_r, \tag{102}$$

where the projection operator $\boldsymbol{p}_r$ is defined as

$$\boldsymbol{p}_r = \frac{1}{2}(1 + \sigma_z). \tag{103}$$

By making use of the relation $\boldsymbol{S}_r = (1 - i\boldsymbol{K}_r)(1 + i\boldsymbol{K}_r)^{-1}$, the physical scattering matrix can be calculated from the physical reactance matrix as

$$\boldsymbol{S}_r = e^{-i\delta_r}e^{-i\delta_r\sigma_z}. \tag{104}$$

Notice that this $\boldsymbol{S}_r$ is the diagonal form of the resonance part $\boldsymbol{S}_r$ (CM) in the factorization of the physical scattering matrix into the background and resonance parts as $\boldsymbol{S} = \boldsymbol{S}^0\boldsymbol{S}_r$ (CM) in the CM theory. This indicates that $\boldsymbol{S}_r$ is represented in terms of the resonance eigenchannel basis functions.

Now, let us consider obtaining the solutions of the compatibility equation for this representation. Let us denote the solution of the compatibility equation as Then the compatibility equation (23) for this representation yields the following equation:

$$\tan\delta\,(\tan\delta\,\tan\tilde{\beta} + \xi^2) = 0, \tag{105}$$

which yields two solutions consistent with those of (102) and (104), namely, only one of them has a nonzero value whose phase is equal to δ_r, just the phase shift due to the resonance. Expansion coefficients $(Z_r)_{i\rho}$ are equal to $(T_r)_{i\rho} = \delta_{i\rho}$ for $i \in P$ and become for $i \in Q$ as follows[28]

$$(Z_r)_{3\rho} = \begin{cases} -\dfrac{\xi\cos\delta_r}{\sin\tilde{\beta}} = \left(\dfrac{d\delta_r}{d\tilde{\beta}}\right)^{1/2} & \text{for } \rho = 1, \\ 0 & \text{for } \rho = 2. \end{cases} \tag{106}$$

This may be compared with the $\tilde{Z}$ coefficient for the $\tilde{K}$ matrix obtained in Ref. [20] as

$$\tilde{Z}_{3\rho} = \left(\frac{d\delta_r}{d\tilde{\beta}}\right)^{1/2}\begin{cases} \cos\frac{1}{2}\theta_f \text{ for } \rho = 1, \\ \sin\frac{1}{2}\theta_f \text{ for } \rho = 2. \end{cases} \tag{107}$$

E. Transformation Diagram and Hierarchical Structure of Resonances. The transformations and resultant reactance matrices considered so far can be summarized with the following diagram:

$$
\left\{\begin{array}{l} K \\ \Re(\kappa^{cc}) \neq 0 \\ \Re(\kappa^{oo}) \neq 0 \end{array}\right.
\xrightarrow{T(\pi\mu_1,\ \pi\mu_2,\ \pi\mu_3,\ I^{oo},\ I^{cc})}
$$

$$
\left\{\begin{array}{l} \tilde{K} \\ \Re(\tilde{\kappa}^{cc}) = 0 \\ \Im(\tilde{\kappa}^{cc}) = -\xi^2 \\ \Re(\tilde{\kappa}^{oo}) \neq 0 \end{array}\right.
\xrightarrow{T\left(0,\ 0,\ 0,\ e^{i\frac{1}{2}\theta_0\sigma_y},\ I^{cc}\right)}
$$

$$
\left\{\begin{array}{l} \bar{\bar{K}} \\ \Re(\bar{\bar{\kappa}}^{cc}) = 0 \\ \Im(\bar{\bar{\kappa}}^{cc}) = -\xi^2 \\ \Re(\bar{\bar{\kappa}}^{oo}) \neq 0 \end{array}\right.
\xrightarrow{T\left(\frac{1}{2}\Delta_{12}^0,\ -\frac{1}{2}\Delta_{12}^0,\ 0,\ I^{oo},\ I^{cc}\right)}
$$

$$
\left\{\begin{array}{l} \bar{K} \\ \Re(\bar{\kappa}^{cc}) = 0 \\ \Im(\bar{\kappa}^{cc}) = -\xi^2 \\ \Re(\bar{\kappa}^{oo}) = 0 \end{array}\right.
\xrightarrow{T\left(0,\ 0,\ 0,\ e^{i\frac{1}{2}\theta_r\sigma_y},\ I^{cc}\right)}
\left\{\begin{array}{l} K_r \\ \Re(\kappa_r^{cc}) = 0 \\ \Im(\kappa_r^{cc}) = -\xi^2 \\ \Re(\kappa_r^{oo}) = 0 \end{array}\right. . \tag{108}
$$

In the above diagram, the last four representations belong to the group of the resonance-centered representation as the values of $\Re(\kappa^{cc})$ are zero in all of them. Actually the values of κ^{cc} themselves are the same in all four representations as $\kappa^{cc} = -i\xi^2$. This derives from that the four representations are connected by the transformations with no phase renormalization and no orthogonal transformations in closed channel base pairs so that κ^{cc} remains unchanged as evident in Eq. (12). Generally, $\Re(\kappa_{ii}^{cc}) = 0$ does not imply $\mu_i^c = 0$ and $W^{cc} = I^{cc}$ as can be easily seen from the counts of the number of conditions. But if it is assumed to be so as in the present system involving only one closed channel, all resonance-centered representations have the identical energy dependence in wavefunctions (42) and subsequently in the cross section formulas. The important thing worth of notice related to the resonance-centered representation is that the present system has a resonance-centered representation, the tilde-representation, which is suitable for the description of the fragmentation processes and obtainable from the starting representation by the phase renormalization alone.

The last two representations enjoy further zero given by $\Re(\bar{\kappa}^{oo}) = \Re(\kappa_r^{oo}) = 0$. If $K'^{co}K'^{oc} < 1$, the solution for both's being zero is obtained only when both K'^{cc} and K'^{oo} are zero as shown in Appendix C. For this solution, the physical reactance matrix K' has rank one and thus has only one nonzero eigenvalue given by the tangent of the phase shift δ_r due to the resonance. The representation where a reactance matrix has nonzero elements only for K^{oc} and K^{co} submatrices so that the physical reactance matrix has rank one was already considered and used by Ueda for obtaining a Beutler-Fano total cross section formula in MQDT for the systems involving one closed and an arbitrary number of open channels.[8] Representations showing this behavior were called the "pure-resonance representations" earlier in this paper. In the two channel system, the translation of the origin of the Lu-Fano plot to the inflection point is equivalent to finding the phase renormalization so that $\Re(\tilde{\kappa}^{cc}) = 0$ and $\Re(\tilde{\kappa}^{oo}) = 0$. For the system involving two open and one closed channels, $\Re(\tilde{\kappa}^{cc}) = 0$ is still the condition for the location of the origin to the inflection point of the Lu-Fano plot, but $\Re(\tilde{\kappa}^{oo}) = 0$ is no longer obtained by making the Lu-Fano plot symmetrical through phase renormalization.

It may be convenient if each representation has its own name. Let us call the last four representations in the diagram as the tilde-, double-bar-, bar-, and r-representations, respectively. The diagram shows that the Lecomte-Ueda transformations among these representations are expressed in terms of parameters θ_0, Δ_{12}^0, and θ_r which are used before to construct the spherical triangle in Figure 1 for geometrically representing the coupling between background and resonance scatterings in the scattering matrix. Therefore, it may be natural to examine the correspondence between the diagram and the spherical triangle. Though in MQDT all the open and closed channels should be included while only open channels are involved in constructing the spherical triangle, this is no problem in the current study of correspondence as the four representations of our interests differ only in open channel parts. The space spanned by open channel basis functions for each representation appears as a coordinate system in Figure 1. This coordinate system undergoes a rotation about the y axis to a new one by an orthogonal transformation in a Lecomte-Ueda transformation. It undergoes a much more complicated transformation by phase renormalization as we will see in a particular example shortly afterwards. A physical scattering matrix is represented as a vector in the space (called the Liouville space by Fano[29]) where the spherical triangle is drawn. In Figure 1, the coordinate system corresponding to the tilde-representation is given by $x_0y_0z_0$ (the x_0 axis is not drawn in the figure). From Eq. (74), we see that $\boldsymbol{n}_a'$ is transformed to $\boldsymbol{n}_a$ by T[0, 0, 0, $\exp(-i\theta_0\sigma_y/2)$, I^{cc}], *i.e.*, $\boldsymbol{n}_a = R_y(-\theta_0)\boldsymbol{n}_a'$ in the transformation from the tilde- to the double-bar-representation. This means that the coordinate system is rotated about the y_0 axis by θ_0. Therefore the z axis of the double-bar-representation is equal to the vector z in the figure. Let us next consider the transformation from the double-bar-representation to the bar-representation. The coordinate system corresponding to the double-bar-representation undergoes a rather complicated transformation. In order to see what is happening, let us consider the formula of $\bar{\boldsymbol{S}}$ from $\bar{\bar{\boldsymbol{S}}}$ and then rewrite it as follows:

$$\bar{S} = e^{-i\delta_r} e^{\frac{i}{2}\Delta_{12}^0\sigma_z} e^{-i\delta_a \boldsymbol{\sigma}\cdot\boldsymbol{n}_a} e^{\frac{i}{2}\Delta_{12}^0\sigma_z}$$
$$= e^{-i\delta_r} e^{\frac{i}{2}\Delta_{12}^0\sigma_z} e^{-i\delta_r \boldsymbol{\sigma}\cdot\boldsymbol{n}_r'} e^{\frac{i}{2}\Delta_{12}^0\sigma_z}$$
$$= e^{i\delta_r} e^{i\delta_r \boldsymbol{\sigma}\cdot\boldsymbol{n}_r}. \tag{109}$$

The second equality of Eq. (109) follows from the reverse coupling of Eq. (51), that is,

$$e^{i\Delta_{12}^0\sigma_z} e^{-i\delta_a \boldsymbol{\sigma}\cdot\boldsymbol{n}_a} = e^{-i\delta_r \boldsymbol{\sigma}\cdot\boldsymbol{n}_r'} \tag{110}$$

which shows that the phases are not simply renormalized. Actually, eigenchannels which are the very nature of dynamic coupling are also changed. Such a change appears as a change from $\boldsymbol{n}_a$ to $\boldsymbol{n}_r$. The phase is renormalized from δ_a to δ_r. The third equality of Eq. (109) indicates that the phase renormalization also causes the rotation of the coordinate system about the z axis by $-\Delta_{12}^0$, that is, $\boldsymbol{n}_r = R_z(\Delta_{12}^0)\boldsymbol{n}_r'$. The Lecomte-Ueda transformation from the bar-representation to the r-representation corresponds to the rotation of the coordinate system about the y axis by $-\theta_r$ so that $\boldsymbol{n}_r$ is now the z axis in the r-representation.

Let us end this section with some comments on the above resonance structure diagram. The representations in the diagram are classified with respect to the structures of the short-range reactance matrices K. Short-range scattering matrices S cannot be used for this purpose of classification as they still keep nonzero diagonal terms even in S_r. It may derive from the restrictions scattering matrices should satisfy such as the unitarity and the existence of the pole due to the resonance. The latter pole structure, visible in Eq. (90), is absent in the reactance matrix.[18,30] In order to obtain the bar-representation, we do not have to consider the double-bar-representation. It can be obtained from the tilde-one by the transformation $T[\Delta_{12}^0/2, -\Delta_{12}^0/2, \exp(-i\theta_0\sigma_y/2), I^{cc}]$. Also the r-representation can directly be obtained from the tilde-one by the successive transformations $T[\Delta_{12}^0/2, -\Delta_{12}^0/2, 0, \exp(-i\theta_0\sigma_y/2), I^{cc}]\ T[0, 0, 0, \exp(-i\theta_r\sigma_y/2), I^{cc}]$.

Photofragmentation Cross Section Formulas

Though it is customary in MQDT to use the asymptotic eigenchannels $\tilde{\Psi}_\rho$ to expand $\tilde{\Psi}_j^{(-)}$

$$\tilde{\Psi}_j^{(-)} = \sum_\rho \tilde{\Psi}_\rho \zeta_{\rho j}^{(-)}, \tag{111}$$

it may be more natural to use the incoming waves as expansion channel basis functions as in Eq. (42) which is reproduced below:

$$\Psi_j'^{(-)} = \Psi_j'^{(-)} + \sum_{k\in Q} \Psi_k'^{(-)}[(\tan\beta' + i)(\tan\beta' + \kappa'^{cc})^{-1} K'^{co}(-i + K'^{oo})^{-1}]_{kj}. \tag{112}$$

Strong energy dependence enters Eq. (112) only as a term $(\tan\beta' + i)(\tan\beta' + \kappa'^{cc})^{-1}$ and becomes simpler in the resonance-centered representation as $(\tan\beta' + i)[\tan\beta' + i\Im(\kappa'^{cc})]^{-1}$. As stated before, the term is invariant under the transformation $T(\pi\mu^c, 0, U^{oo}, I^{cc})$.

Let us first consider the tilde representation. From Eq. (56), the submatrix $\tilde{K}^{oo}$ of $\tilde{K}$ can be expressed as

$$\tilde{K}^{oo} = \tan\frac{1}{2}\Delta_{12}^0 \boldsymbol{\sigma}\cdot\boldsymbol{n}_0, \tag{113}$$

where the vector $\boldsymbol{n}_0$ is defined as

$$\boldsymbol{n}_0 = R_y(\theta_0)\boldsymbol{z} = \boldsymbol{z}\cos\theta_0 + \boldsymbol{x}\sin\theta_0. \tag{114}$$

With this $\tilde{K}^{oo}$, $(-i + \tilde{K}^{oo})^{-1}$ can be written as $i\cos(\Delta_{12}^0/2)\exp(-i\Delta_{12}^0\boldsymbol{\sigma}\cdot\boldsymbol{n}_0/2)$. Multiplying this into the submatrix $\tilde{K}^{co}$ of $\tilde{K}$ in Eq. (56), the physical incoming wavefunction decomposing into the j-th channel becomes

$$\tilde{\Psi}_j^{(-)} = \tilde{\Psi}_j^{(-)} + i\xi\tilde{\Psi}_3^{(-)} \frac{\tan\tilde{\beta} + i}{\tan\tilde{\beta} - i\xi^2}\left(e^{\frac{i}{2}(\theta_r + \theta_0)\sigma_y} e^{-\frac{i}{2}\Delta_{12}^0\boldsymbol{\sigma}\cdot\boldsymbol{n}_0}\right)_{1j}. \tag{115}$$

Using the relation

$$e^{i(\tilde{\beta}+\delta_r)}\left(\frac{d\delta_r}{d\tilde{\beta}}\right)^{1/2} = i\xi\frac{\tan\tilde{\beta} + i}{\tan\tilde{\beta} - i\xi^2}, \tag{116}$$

it can be put into

$$\tilde{\Psi}_j^{(-)} = \tilde{\Psi}_j^{(-)} + \tilde{\Psi}_3^{(-)} e^{i(\tilde{\beta}+\delta_r)}\left(\frac{d\delta_r}{d\tilde{\beta}}\right)^{1/2}\left(e^{\frac{i}{2}(\theta_r + \theta_0)\sigma_y} e^{-\frac{i}{2}\Delta_{12}^0\boldsymbol{\sigma}\cdot\boldsymbol{n}_0}\right)_{1j}, \tag{117}$$

similar to the form derived in Ref. [31] for the two channel system. The explicit expression of the last term of Eq. (115) is given by

$$\left(e^{\frac{i}{2}(\theta_r + \theta_0)\sigma_y} e^{-\frac{i}{2}\Delta_{12}^0\boldsymbol{\sigma}\cdot\boldsymbol{n}_0}\right)_{1j}$$
$$= \begin{pmatrix} \cos\frac{1}{2}(\theta_0+\theta_r)\cos\frac{1}{2}\Delta_{12}^0 & \sin\frac{1}{2}(\theta_0+\theta_r)\cos\frac{1}{2}\Delta_{12}^0 \\ -i\cos\frac{1}{2}(\theta_0-\theta_r)\sin\frac{1}{2}\Delta_{12}^0 & -i\sin\frac{1}{2}(\theta_0-\theta_r)\sin\frac{1}{2}\Delta_{12}^0 \end{pmatrix}$$
$$= \begin{pmatrix} \cos\frac{1}{2}\theta_0\cos\frac{1}{2}\theta_r e^{-\frac{i}{2}\Delta_{12}^0} & \sin\frac{1}{2}\theta_0\cos\frac{1}{2}\theta_r e^{-\frac{i}{2}\Delta_{12}^0} \\ -\sin\frac{1}{2}\theta_0\sin\frac{1}{2}\theta_r e^{\frac{i}{2}\Delta_{12}^0} & \cos\frac{1}{2}\theta_0\sin\frac{1}{2}\theta_r e^{\frac{i}{2}\Delta_{12}^0} \end{pmatrix}. \tag{118}$$

Now let us introduce the new short-range wavefunctions $\tilde{M}_j^{(-)}$ and $\tilde{N}_j^{(-)}$ defined by

$$\tilde{M}_j^{(-)} = \tilde{\Psi}_j^{(-)} + \tilde{\Psi}_3^{(-)}[\tilde{K}^{co}(-i + \tilde{K}^{oo})^{-1}]_{3j},$$
$$\tilde{N}_j^{(-)} = \tilde{\Psi}_j^{(-)} - \frac{1}{\xi^2}\tilde{\Psi}_3^{(-)}[\tilde{K}^{co}(-i + \tilde{K}^{oo})^{-1}]_{3j} \tag{119}$$

so that the square of the modulus of the transition dipole moment is expressed into the Beulter-Fano formula:

$$\left|\tilde{D}_j^{(-)}\right|^2 = \left|(\tilde{\Psi}_j^{(-)}|T|i)\right|^2 = \left|(\tilde{M}_j^{(-)}|T|i)\right|^2 \frac{\left|\tan\tilde{\beta}/\xi^2 + \tilde{q}_j\right|^2}{\tan^2\tilde{\beta}/\xi^4 + 1}, \tag{120}$$

where T is the dipole moment operator. i stands for the initial bound state, and the complex $\tilde{q}_j$ gives the line-profile for spectra and is defined by

$$\tilde{q}_j = i\frac{(\tilde{N}_j^{(-)}|T|i)}{(\tilde{M}_j^{(-)}|T|i)}. \tag{121}$$

The forms of $M^{(-)}$ and $N^{(-)}$ functions which yield the Beutler-Fano formula are the same if the representation belongs to the resonance-centered one. In that representation, the physical incoming wavefunctions are expressed in terms of them as

$$\begin{aligned}\Psi_j^{(-)} &= M_j^{(-)}\frac{\tan\tilde{\beta}/\xi^2}{\tan\tilde{\beta}/\xi^2 - 1} - N_j^{(-)}\frac{i}{\tan\tilde{\beta}/\xi^2 - 1}\\ &= e^{-i\delta_r}(M_j^{(-)}\cos\delta_r + iN_j^{(-)}\sin\delta_r).\end{aligned} \tag{122}$$

Here $M_j^{(-)}$ plays the role of the background wavefunction in the CM theory and dominate the physical incoming-waves at the region of no resonance effect where the phase shift δ_r due to the resonance is zero. Especially, $M^{(-)}$ is related in matrix form to the standing-wave channel basis functions belonging to open channels as

$$\Psi^o = M^{(-)}(1 + iK^{oo}). \tag{123}$$

Eq. (123) is the contracted form of $\Psi_i = \Sigma_j \Psi_j^{(-)}(1 + iK)_{ji}$ with $M_j^{(-)}$ corresponding to $\Psi_j^{(-)}$. In this case, the contractions is made so that $M_j^{(-)}$ alone measures the partial cross section in the region of no resonance, which is attained by making the contribution of regular part of closed channels zero:

$$M_j^{(-)} = \theta_j - \sum_{i\in P}\theta_i^-\sigma_{ij}^{oo} - \sum_{i\in Q}(\theta_i^1 + \theta_i^-)[(1 + S^{cc})^{-1}S^{co}]_{ij}. \tag{124}$$

where $(\theta_i^1 + \theta_i^-)$ is eventually a unitary transform of only irregular functions $i\Phi_k g_k$. Eq. (120) may be used to obtain partial cross sections σ_j (for $\left|(\tilde{M}_j^{(-)}|T|i)\right|^2$), $\Re(\tilde{q}_j)$, $\Im(\tilde{q}_j)$, and the functional form of $\tan\tilde{\beta}$ as a function of energy from the experimental data using the method developed in the field of modeling of data.[32] For sharp resonances, we may use the well-known first-order expansion

$$\varepsilon = \frac{\tan\tilde{\beta}}{\xi^2} \simeq \frac{E - E_n}{\Gamma_n/2} \tag{125}$$

near the n-th resonance to extract E_n and Γ_n instead of the functional form of $\tan\tilde{\beta}$ as a function of energy from the experimental data.

In some experimental situations, cross sections averaged over resonances are only observable. For this, let us first write the square of the modulus of transition dipole moments using Eq. (117) with Eqs. (100) and (101) as

$$\left|\tilde{D}_j^{(-)}\right|^2 = \left|\tilde{D}_j^{(-)} + \tilde{D}_3^{(-)}(\psi^{(a)}|\psi_j^{(-)})e^{i(\tilde{\beta} - \delta_r - \delta_r^0/2)}\left(\frac{d\delta_r}{d\tilde{\beta}}\right)^{1/2}\right|^2. \tag{126}$$

where $\tilde{D}_j^{(-)}$ denotes $(\tilde{\Psi}_j^{(-)}|T|i)$. Let us next take an average of Eq. (126) over one resonance interval with respect to $\tilde{\beta}$. The energy dependence of an interference term is given by either $(\tan\tilde{\beta} + i)/(\tan\tilde{\beta} - i\xi^2)$ or its complex conjugate and its integral over one resonance interval can easily be shown to be zero. Getting rid of the interference terms and utilizing the integral $\int_{-\pi/2}^{\pi/2}(d\delta_r/d\tilde{\beta})d\tilde{\beta}/\pi = \int_0^{\pi}d\delta_r/\pi = 1$, the energy average of Eq. (126) over one resonance cycle is obtained as

$$\langle\left|\tilde{D}_j^{(-)}\right|^2\rangle = \left|\tilde{D}_j^{(-)}\right|^2 + \left|\tilde{D}_3^{(-)}\right|^2\left|(\psi^{(a)}|\psi_j^{(-)})\right|^2. \tag{127}$$

Eq. (127) is identical with the result of Gailitis's formula given by[1]

$$\langle\left|\tilde{D}_j^{(-)}\right|^2\rangle = \left|\tilde{D}_j^{(-)}\right|^2 + \frac{\left|\tilde{S}_{3j}\right|^2}{1 - \left|\tilde{S}_{33}\right|^2}\left|\tilde{D}_3^{(-)}\right|^2 \tag{128}$$

as can be easily seen from Eq. (94). $\left|\tilde{S}_{3j}\right|^2/(1 - \left|\tilde{S}_{33}\right|^2)$ is the probability that break-up of the resonance gives j and in the present form is given by

$$\frac{\left|\tilde{S}_{3j}\right|^2}{1 - \left|\tilde{S}_{33}\right|^2} = \left|(\psi^{(a)}|\psi_j^{(-)})\right|^2 = \begin{cases}\cos^2\dfrac{\theta_r^0}{2} & \text{for } j=1,\\[2ex] \sin^2\dfrac{\theta_r^0}{2} & \text{for } j=2.\end{cases} \tag{129}$$

where θ_r^0 is defined as the side angle for A_0Q of the spherical triangle ΔAA_0Q in Fig. 1. Notice that the fragmentation branching ratio averaged one resonance interval is determined by $\cos^2\theta_r^0/2 : \sin^2\theta_r^0/2$ where is constant of energy and the same for all resonance levels belonging to the same threshold. The unaveraged branching ratio varies as a function of energy as far as the line profile $\tilde{q}_1$ and $\tilde{q}_2$ are different.

A. Total Cross Section Formulas and the r-Representation. As is well-known, the photofragmentation cross section formulas take the simplest form in the r-representation which is corresponding to Fano's 'abc..' representation (the 'a' state is also called the 'effective continuum'). In the r-representation, only the process to $(\Psi_r^{(-)})_1$ shows the resonance behavior while the remaining processes, the one to $(\Psi_r^{(-)})_2$ here, are energy-insensitive. The transition dipole moment formula to $(\Psi_r^{(-)})_1$ can be expressed into the Beutler-Fano form with introduction of $(M_r^{(-)})_j$ and $(N_r^{(-)})_j$ defined with the same formula as the one (119) for $\tilde{M}_j^{(-)}$ and $\tilde{N}_j^{(-)}$, *i.e.*,

$$\begin{aligned}(M_r^{(-)})_1 &= (\Psi_r^{(-)})_1 + i\xi(\Psi_r^{(-)})_3,\\ (N_r^{(-)})_1 &= (\Psi_r^{(-)})_1 - \frac{i}{\xi}(\Psi_r^{(-)})_3,\\ (M_r^{(-)})_2 &= (N_r^{(-)})_2 = (\Psi_r^{(-)})_2.\end{aligned} \tag{130}$$

With these, the elements of the transition dipole moment vector to $(\Psi_r^{(-)})_j$ can be written as

$$(\boldsymbol{D}_r^{(-)})_1 = ((M_r^{(-)})_1|T|i)\frac{\tan\tilde{\beta}/\xi^2+q_r}{\tan\tilde{\beta}/\xi^2+i},$$

$$(\boldsymbol{D}_r^{(-)})_2 = ((M_r^{(-)})_2|T|i) = ((\Psi_r^{(-)})_2|T|i), \tag{131}$$

with the line profile index q_r defined as

$$q_r = i\frac{((N_r^{(-)})_1|T|i)}{((M_r^{(-)})_1|T|i)}. \tag{132}$$

In the r-representation, $(M_r^{(-)})_j$ and $(N_r^{(-)})_j$ become standing waves. From Eqs. (32) and (88), the relation between standing-wave and incoming-wave channel basis functions is obtained as

$$(\Psi_r)_1 = (\Psi_r^{(-)})_1+i\xi(\Psi_r^{(-)})_3,$$
$$(\Psi_r)_2 = (\Psi_r^{(-)})_2,$$
$$(\Psi_r)_3 = i\xi(\Psi_r^{(-)})_1+(\Psi_r^{(-)})_3. \tag{133}$$

Comparison of Eqs. (130) and (133) yields

$$(M_r^{(-)})_1 = (\Psi_r)_1,$$
$$(N_r^{(-)})_1 = -\frac{i}{\xi}(\Psi_r)_3,$$
$$(M_r^{(-)})_2 = (N_r^{(-)})_2 = (\Psi_r)_2. \tag{134}$$

Inserting Eq. (134) into (131), we obtain

$$(\boldsymbol{D}_r^{(-)})_1 = ((\Psi_r)_1|T|i)\frac{\tan\tilde{\beta}/\xi^2+q_r}{\tan\tilde{\beta}/\xi^2+i},$$
$$(\boldsymbol{D}_r^{(-)})_2 = ((\Psi_r)_2|T|i) \tag{135}$$

with the new formula for the line profile index q_r:

$$q_r = -\frac{((\Psi_r^{(-)})_3|T|i)}{\xi((\Psi_r^{(-)})_1|T|i)}. \tag{136}$$

The new formula for q_r clearly shows that q_r is real.

From Eq. (99), the transition dipole moment vector $\boldsymbol{D}_r^{(-)}$ is $\tilde{\boldsymbol{D}}^{(-)}$ related by the unitary transformation as

$$\boldsymbol{D}_r^{(-)} = \tilde{\boldsymbol{D}}^{(-)}e^{\frac{i}{2}\theta_0\sigma_z}e^{\frac{i}{2}\Lambda_{12}^0\sigma_y}e^{\frac{i}{2}\theta_r\sigma_z}, \tag{137}$$

implying that

$$\sum_{j\in P}\left|\tilde{D}_j^{(-)}\right|^2 = \sum_{j\in P}\left|(\boldsymbol{D}_r^{(-)})_j\right|^2$$
$$= \left|((\Psi_r)_1|T|i)\right|^2\frac{(\tan\tilde{\beta}/\xi^2+q_r)^2}{\tan^2\tilde{\beta}/\xi^4+1} + \left|((\Psi_r)_2|T|i)\right|^2. \tag{138}$$

With the substitution $-\cot\delta_r$ for $\tan\tilde{\beta}/\xi^2$ and the introduction of the angle θ_q defined by

$$\cos\theta_q = \frac{q_r}{\sqrt{1+q_r^2}}, \qquad \sin\theta_q = \frac{-1}{\sqrt{1+q_r^2}}, \tag{139}$$

Eq. (138) becomes

$$\sum_{j\in P}\left|\tilde{D}_j^{(-)}\right|^2 = \left|((\Psi_r)_1|T|i)\right|^2(1+q_r^2)\sin^2(\delta_r+\theta_q)$$
$$+ \left|((\Psi_r)_2|T|i)\right|^2, \tag{140}$$

if we take an average of Eq. (140) over one resonance interval with respect to $\tilde{\beta}$ and use the formula $\int_{-\pi/2}^{\pi/2}\sin^2(\delta_r+\theta_q)\,d\tilde{\beta}/\pi = (\xi^2q_r^2+1)/[(1+\xi^2)(1+q_r^2)]$, we obtain

$$\left\langle\sum_{j\in P}\left|\tilde{D}_j^{(-)}\right|^2\right\rangle = \frac{1}{1+\xi^2}\left(\left|((\Psi_r)_1|T|i)\right|^2+\left|((\Psi_r)_3|T|i)\right|^2\right)$$
$$+\left|((\Psi_r)_2|T|i)\right|^2$$
$$= \left|((\Psi_r^{(-)})_1|T|i)\right|^2+\left|((\Psi_r^{(-)})_2|T|i)\right|^2+\left|((\Psi_r^{(-)})_3|T|i)\right|^2$$
$$= \left|(\tilde{\Psi}_1^{(-)}|T|i)\right|^2+\left|(\tilde{\Psi}_2^{(-)}|T|i)\right|^2+\left|(\tilde{\Psi}_3^{(-)}|T|i)\right|^2, \tag{141}$$

which is the expected result from the theorem due to Gailitis[33] and ensures that total cross sections are continuous across the thresholds.

Eq. (138) resembles the well-known total cross section formula for photofragmentation in the neighborhood of an isolated resonance given by[14]

$$\sigma_{\text{tot}} = \sigma_a\frac{(\varepsilon+q)^2}{\varepsilon^2+1}+\sigma_b \quad (\text{CM}) \tag{142}$$

if we substitute ε for $\tan\tilde{\beta}/\xi^2$. In Eq. (142), σ_a and σ_b denote the cross sections to $\psi^{(a)}$ and $\psi^{(b)}$, respectively. For the comparison, let us first relate $(\Psi_r)_1$, $(\Psi_r)_2$, and $(\Psi_r)_3$ with $\psi^{(a)}$, $\psi^{(b)}$, and Φ_{E_n}, respectively. From Eqs. (91), (133), and (B2), we have in $R\geq R_0$

$$(\Psi_r)_1 = (\theta_r^+)_1-(\theta_r^-)_1+i\xi[(\theta_r^-)_3+(\theta_r^-)_3]$$
$$= \psi^{(a)}+i\xi[(\theta_r^-)_3+(\theta_r^-)_3],$$
$$(\Psi_r)_2 = \psi^{(b)},$$
$$(\Psi_r)_3 = (\theta_r^+)_3-(\theta_r^-)_3+i\xi[(\theta_r^-)_1+(\theta_r^-)_1]. \tag{143}$$

From Eq. (B15), we have

$$\frac{\phi_{E_n}}{\pi(\Sigma_k|\Gamma_{kE}|^2)^{1/2}} \simeq -\left\{\frac{1}{\xi\cos^2\tilde{\beta}}[(\theta_r^-)_3-(\theta_r^-)_3]\right\}\Bigg|_{\tilde{\beta}=n\pi}, \quad R\geq R_0. \tag{144}$$

Then

$$\frac{\Phi_{E_n}}{\pi(\Sigma_k|\Gamma_{kE}|^2)^{1/2}} \equiv \frac{\phi_{E_n}}{\pi(\Sigma_k|\Gamma_{kE}|^2)^{1/2}}+\bar{\psi}^{(a)}$$
$$\simeq -i[(\theta_r^-)_1+(\theta_r^-)_1]-\frac{1}{\xi\cos^2\tilde{\beta}}[(\theta_r^-)_3-(\theta_r^-)_3]\Bigg|_{\tilde{\beta}=n\pi}, \quad R\geq R_0 \tag{145}$$

and we obtain

$$\frac{\Phi_{E_a}}{\pi(\Sigma_k|V_{kE}|^2)^{1/2}} \simeq -\frac{1}{\xi}(\Psi_r)_3 \tag{146}$$

Eqs. (143) and (146) tell us that the background parts of MQDT and CM are identical but the resonance parts which are described by closed channels in MQDT and by a discrete state in CM become equal when ξ become zero. As a result, we obtain the approximate equalities between MQDT and CM formulas for small ξ:

$$((\Psi_r)_1|T|i) \simeq (\psi^{(a)}|T|i), \tag{147}$$

$$q_r = -\frac{((\Psi_r)_3|T|i)}{\xi((\Psi_r)_1|T|i)} \simeq \frac{(\Phi_{E_a}|T|i)}{(\psi^{(a)}|T|i)\pi(\Sigma_k|V_{kE}|^2)^{1/2}} = q(\text{CM}). \tag{148}$$

Notice that the difference between $(\Psi_r)_1$ and $\psi^{(a)}$ is an exponentially rising term in $i\xi[(\theta_r^+)_3 + (\theta_r^-)_3]$ from Eq. (143) but its contribution to the transition dipole moment vector becomes finite as it is multiplied by the initial bound state i. Then in the narrow resonance limit, Eq. (147) is expected to hold.

B. Partial Cross Sections and the r-Representation. In order to understand partial photofragmentation processes, it may be better to express them in terms of the elements of the transition dipole moment vector of the r-representation. This can be achieved with the transformation relation (137) between transition dipole moment vectors. Using the transformation matrices (100), we have

$$\begin{aligned}\tilde{\boldsymbol{D}}_j^{(-)} &= \sum_{i \in P} (\boldsymbol{D}_r^{(-)})_i (\tilde{\Psi}_j^{(-)}|(\boldsymbol{\Psi}_r^{(-)})_i) \\ &= \sum_{i \in P} (\boldsymbol{D}_r^{(-)})_i (\tilde{\Psi}_j^{(-)}|(\Psi_r^{(-)})_i) \\ &= (\tilde{\Psi}_j^{(-)}|T|i)\left[\frac{\tan\tilde{\beta}/\xi^2 + q_r}{\tan\tilde{\beta}/\xi^2 + i}\,\frac{(\tilde{\Psi}_j^{(-)}|(\Psi_r^{(-)})_1)((\Psi_r)_1|T|i)}{(\tilde{\Psi}_j^{(-)}|T|i)}\right. \\ &\quad \left. + \frac{(\tilde{\Psi}_j^{(-)}|(\Psi_r^{(-)})_2)((\Psi_r^{(-)})_2|T|i)}{(\tilde{\Psi}_j^{(-)}|T|i)}\right].\end{aligned} \tag{149}$$

Let us define ρ_j as

$$\rho_j = \frac{(\tilde{\Psi}_j^{(-)}|(\Psi_r^{(-)})_1)((\Psi_r^{(-)})_1|T|i)}{(\tilde{\Psi}_j^{(-)}|T|i)} \tag{150}$$

in analogous to ρ_j (identical to Starace's $\alpha^*(jE)$ [15]) of CM defined as[16]

$$\rho_j(\text{CM}) = \frac{(\psi_j^{(-)}|\psi^{(a)})(\psi^{(a)}|T|i)}{(\psi_j^{(-)}|T|i)} = \frac{(P_a\psi_j^{(-)}|T|i)}{(\psi_j^{(-)}|T|i)}, \tag{151}$$

where P_a is the projection operator to $\psi^{(a)}$. Then, we have

$$1 - \rho_j = \frac{(\tilde{\Psi}_j^{(-)}|(\Psi_r^{(-)})_2)((\Psi_r^{(-)})_2|T|i)}{(\tilde{\Psi}_j^{(-)}|T|i)}, \tag{152}$$

from the identity

$$(|(\Psi_r^{(-)})_1)((\Psi_r^{(-)})_1| + |(\Psi_r^{(-)})_2)((\Psi_r^{(-)})_2|)\tilde{\Psi}_j^{(-)} = \tilde{\Psi}_j^{(-)}. \tag{153}$$

The identity (153) derives from that the transformation matrix $(\tilde{\Psi}_j^{(-)}|(\Psi_r^{(-)})_i)$ is a unitary matrix. From it and Eq. (133), we obtain

$$\begin{aligned}&(|(\Psi_r)_1)((\Psi_r^{(-)})_1| + |(\Psi_r^{(-)})_2)((\Psi_r^{(-)})_2|)\tilde{\Psi}_j^{(-)} \\ &= \tilde{\Psi}_j^{(-)} + i\xi(\Psi_r^{(-)})_3((\Psi_r^{(-)})_1|\Psi_j^{(-)}).\end{aligned} \tag{154}$$

Then

$$\frac{(\tilde{\Psi}_j^{(-)}|(\Psi_r^{(-)})_1)((\Psi_r)_1|T|i)}{(\tilde{\Psi}_j^{(-)}|T|i)} = \rho_j - i\xi\sigma_j. \tag{155}$$

where σ_j is defined as

$$\sigma_j = \frac{(\tilde{\Psi}_j^{(-)}|(\Psi_r^{(-)})_1)((\Psi_r^{(-)})_3|T|i)}{(\tilde{\Psi}_j^{(-)}|T|i)}. \tag{156}$$

We finally obtain

$$\tilde{\boldsymbol{D}}_j^{(-)} = (\tilde{\Psi}_j^{(-)}|T|i)(1 - i\xi\sigma_j)\frac{\tan\tilde{\beta}/\xi^2 + \tilde{q}_j}{\tan\tilde{\beta}/\xi^2 + i}. \tag{157}$$

where $\tilde{q}_j$ is related to $q_j = i + \rho_j(q_r - i)$ as

$$\tilde{q}_j = \frac{q_j - i\xi q_r\sigma_j}{1 - i\xi\sigma_j} \tag{158}$$

and it can easily be shown that

$$(\tilde{\Psi}_j^{(-)}|T|i)(1 - i\xi\sigma_j) = (\tilde{M}_j^{(-)}|T|i) \tag{159}$$

whereby Eq. (157) gives the formula identical to the one in Eq. (120) as it should be. The parameter ρ_j is the analogous form to the line profile index ρ_j (CM) for the partial cross section in the CM theory defined as $q_j(\text{CM}) = i + \rho_j(\text{CM})[q(\text{CM}) - i]$. The parameter $\tilde{q}_j$ may also be written as

$$\tilde{q}_j = i + \tilde{\rho}_j(q_r - i). \tag{160}$$

with $\tilde{\rho}_j$ defined as $(\rho_j - i\xi\sigma_j)/(1 - i\xi\sigma_j)$. Notice that q_r and $\tilde{q}_j$ are obtainable from the total and partial cross section measurements, respectively. Then, Eq. (160) tells us that we can obtain $\tilde{\rho}_j$ not ρ_j from those two measurements. If ξ is negligible, the line profile indices $\tilde{q}_j$ and q_j become equal to the CM line profile q_j(CM) index as shown in Appendix D:

$$\begin{aligned}\tilde{q}_j &\simeq q_j \simeq q_j(\text{CM}), \\ \tilde{\rho}_j &\simeq \rho_j \simeq \rho_j(\text{CM}).\end{aligned} \tag{161}$$

Here, as shown in Appendix D, the above MQDT parameters differ from the corresponding ones in CM not only in the resonance parts but also in the background parts though the difference in the latter is the second order in ξ, in contrast to the case of total cross sections.

Summary and Discussion

The dynamics in the reaction zone are studied in the usual MQDT by the distortion of a fixed regular solution along a fragmentation channel in the outer region. The extent of the distortion is given by the short-range reactance matrices K which multiplies an irregular solution. Giusti-Suzor and Fano modified the usual theory so that the part of the core dynamics incorporated into the base pair for a motion along a fragmentation channel is no longer fixed. The freedom in the allocation of the short-range dynamics between the motion along the fragmentation coordinate and the short-range reaction matrix K is combined with the orthogonal transformation considered by Lecomte. Ueda and others to reformulate the MQDT theory into the form of the CM theory and thus to make MQDT have the full power of the CM one, still keeping its power of being able to describe the photofragmentation processes with only a few parameters. These parameters allow clear physical interpretation in terms of geometrical transformations and interchannel coupling strengths as in the work of Giusti-Suzor and Fano for systems involving only two channels. In the present work, the geometrical transformations have more diverse origins because of the additional open channel and are studied by the geometrical method devised to study the coupling between background and resonance scatterings. The dynamic parameters with simpler and more transparent physical origins or meanings responsible for the experimental data of total and partial photofragmentation cross sections are subsequently identified.

Notice that some short-range reactance matrices are expressed with parameters specific to the open- and closed-ness of channels even though they are defined in the region where open- and closed-ness of channels cannot be defined. This peculiar aspect of the present theory remains to be investigated in the future, besides the extension of the current work to the systems involving more channels. Actually, full investigation of this point is very important if we remember that the unified treatment of discrete and continuum spectra hinges on it.

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Appendix A: The Derivation of Eq. (20) from Eq. (38)

We first notice the relations:

$$S'^{oo} = (1 - i\kappa'^{oo})(1 + i\kappa'^{oo})^{-1},$$

$$S'^{oc} = 2i(1 - iK'^{cc})^{-1}K'^{co}(1 + i\kappa'^{oo})^{-1},$$

$$S'^{co} = -2i(1 - i\kappa'^{oo})^{-1}K'^{oc}(1 + iK'^{cc})^{-1},$$

$$S'^{cc} = (1 + i\kappa'^{cc})(1 - i\kappa'^{cc})^{-1}, \tag{A1}$$

where κ' is defined as

$$\kappa'^{oo} = K'^{oo} - K'^{oc}(-i + K'^{cc})^{-1}K'^{co}. \tag{A2}$$

Let us first rewrite $S'^{cc} - \exp(2i\beta_{\pi}')$ as

$$S'^{cc} - e^{2i\beta_{\pi}'} = (1 - i\kappa'^{cc})(1 + i\kappa'^{cc})^{-1} - e^{i\pi\mu'}U^{c\alpha(T)}e^{2i\beta}U^{c\alpha}e^{i\pi\mu'}$$
$$= -2ie^{i\pi\mu'}U^{c\alpha(T)}e^{i\beta}(\cos\beta U^{c\alpha}\cos\pi\mu' - \sin\beta U^{c\alpha}\sin\pi\mu')$$
$$\times(\tan\beta_{\pi}' + \kappa'^{cc})(1 - i\kappa'^{cc})^{-1} \tag{A3}$$

We will need the following formula for the subsequent derivation:

$$(S'^{cc} - e^{2i\beta_{\pi}'})^{-1} - (S'^{cc} - 1)^{-1} = \frac{i}{2}(1 - i\kappa'^{cc})(\tan\beta_{\pi}' + \kappa'^{cc})^{-1}(1 - i\kappa'^{cc}). \tag{A4}$$

which can be easily derived from Eq. (A3) and $(S'^{cc} - 1)^{-1} = (1 - i\kappa'^{cc})/2$. Substituting Eq. (A1) into Eq. (A4), we obtain

$$S'^{oc}[(S'^{cc} - e^{2i\beta_{\pi}'})^{-1} - (S'^{cc} - 1)^{-1}]S'^{co}$$
$$= -2i(1 - iK'^{oo})^{-1}K'^{oc}(\tan\beta_{\pi}' + \kappa'^{cc})^{-1}K'^{co}(1 - iK'^{oo})^{-1}. \tag{A5}$$

With Eq. (A5), S' of Eq. (38) can be rewritten as

$$S' = \sigma'^{oo} - S'^{oc}[(S'^{cc} - e^{2i\beta_{\pi}'})^{-1} - (S'^{cc} - 1)^{-1}]S'^{co}$$
$$= \sigma'^{oo} + 2i(1 + iK'^{oo})^{-1}K'^{oc}(\tan\beta_{\pi}' + \kappa'^{cc})^{-1}K'^{co}(1 - iK'^{oo})^{-1}. \tag{A6}$$

where the effective σ'^{oo} matrix analogous to K'^{oo} is defined by

$$K'^{oo} = -i(1 + \sigma'^{oo})^{-1}(1 - \sigma'^{oo}) \tag{A7}$$

and obtained as

$$\sigma'^{oo} = S'^{oo} - S'^{oc}(S'^{cc} - 1)^{-1}S'^{co}. \tag{A8}$$

With Eq. (A6), we obtain

$$(1 + S')^{-1} = (1 - \sigma'^{oo})^{-1} - \frac{i}{2}K'^{oc}(\tan\beta_{\pi}' - K'^{cc})^{-1}K'^{co}. \tag{A9}$$

From Eq. (A9) and the following identity

$$(\tan\beta_{\pi}' + K'^{cc})^{-1}K'^{co}(-i + K')^{-1} = (\tan\beta_{\pi}' + \kappa'^{cc})^{-1}K'^{co}(-i + K'^{oo})^{-1}, \tag{A10}$$

Eq. (20) is easily obtained.

Appendix B: The Correspondence between $\Psi_{r}^{(-)}$ and $\Psi^{(\lambda)}$

Inserting Eq. (91), $\Psi_r^{(-)}$ of Eq. (97) can be rewritten in as $R \geq R_0$

$$(\Psi_r^{(-)})_1 = e^{-i\delta}\left[(e^{i\delta_r}(\theta_r^-)_1 - e^{-i\delta_r}(\theta_r^+)_1) + \left(\frac{d\delta_r}{d\bar{\beta}}\right)^{1/2}(e^{-i\beta}(\theta_r^-)_3 - e^{i\beta}(\theta_r^+)_3)\right],$$

$$(\Psi_r^{(-)})_2 = (\Psi_r^{(-)})_2 = (\theta_r^+)_2 - (\theta_r^-)_2. \tag{B1}$$

In order to show that the above physical incoming wavefunctions $(\Psi_r^{(-)})_1$ and $(\Psi_r^{(-)})_2$ correspond to the CM wavefunctions $\Psi^{(-)}\exp(-i\delta_r)$ and $-\Psi^{(-)}$, respectively, we first need the following relations:

$$(\theta_r^+)_1 - (\theta_r^-)_1 = \psi^{(-)},$$

$$(\theta_r^+)_2 - (\theta_r^-)_2 = \psi^{(-)} \tag{B2}$$

which will be derived below, where $\psi^{(-)}$ is the 'a' state introduced by Fano and defined by

$$\psi^{(a)} = \frac{\Sigma_k V_{kE}\psi_k^{(-)}}{(\Sigma_k|V_{kE}|^2)^{1/2}}, \tag{B3}$$

with $\psi_k^{(-)}$ denoting the incoming wavefunction for the continuum which breaks up into the channel k. If we denote the discrete state by ϕ_{E_n} with energy E_n, V_{kE} in Eq. (B3) is defined by $(\psi_k^{(-)}|H|\phi_{E_n})$. Fano's 'a' state can alternatively be given in terms of the background eigenchannel wavefunctions ψ_α for S^0 as

$$\psi^{(a)} = \frac{\Sigma_\alpha \psi_\alpha(\psi_\alpha|H|\phi_{E_n})}{(\Sigma_k|V_{kE}|^2)^{1/2}} = \sum_\alpha \psi_\alpha\left(\frac{\Gamma_\alpha}{\Gamma}\right)^{1/2}, \tag{B4}$$

where the last equality follows from the definition of Γ_α as $(\psi_\alpha|H|\phi_{E_n}) \equiv \sqrt{\Gamma_\alpha/2\pi}$ and $2\pi\Sigma_k|V_{kE}|^2 = 2\pi\Sigma_\alpha|(\psi_\alpha|H|\phi_{E_n})|^2 = \Gamma$ (see Ref. [21]). Note also from Eq. (50) that

$$(\psi^{(a)}|\psi_1) = \sqrt{\frac{\Gamma_1}{\Gamma}} = \cos\frac{\theta_r}{2},$$

$$(\psi^{(a)}|\psi_2) = \sqrt{\frac{\Gamma_2}{\Gamma}} = \cos\frac{\theta_r}{2}. \tag{B5}$$

From Eqs. (B4) and (B5), we have

$$\psi^{(a)} = \psi_1\cos\frac{\theta_r}{2} + \psi_2\cos\frac{\theta_r}{2}. \tag{B6}$$

If we denote the continuum orthogonal to $\psi^{(a)}$ as $\psi^{(b)}$, $\psi^{(b)}$ may be given by

$$\psi^{(b)} = -\psi_1\sin\frac{\theta_r}{2} + \psi_2\cos\frac{\theta_r}{2}. \tag{B7}$$

From the above two equations, the relation between Fano's 'ab' states and the background eigenchannel wavefuncitons can be written in matrix form as

$$(\psi^{(a)}, \psi^{(b)}) = (\psi_1, \psi_2)e^{-\frac{i}{2}\theta_r\sigma_y} = (\psi_1^{(-)}, \psi_2^{(-)})e^{-\frac{i}{2}\theta_0\sigma_y}e^{\frac{i}{2}(\delta_\Sigma^0 + \Delta_{12}^0\sigma_z)}e^{-\frac{i}{2}\theta_r\sigma_y}. \tag{B8}$$

From this relation, we obtain the transformation relation

$$(\psi^{(-)}, \psi^{(\lambda)}) = e^{\frac{i}{2}\delta_\Sigma^0}\left(e^{-\frac{i}{2}\theta_0\sigma_y}e^{\frac{i}{2}\Delta_{12}^0\sigma_z}e^{-\frac{i}{2}\theta_r\sigma_y}\right)_{j\lambda}, \tag{B9}$$

where λ is used to represent 'ab'. In the CM theory, we use another type of continuum function which lags $\psi^{(a)}$ in phase by 90°. If we denote it as $\overline{\psi}^{(a)}$, it can be expressed as

$$\overline{\psi}^{(a)} = -i[(\theta_r^+)_1 + (\theta_r^-)_1], \quad R \geq R_0. \tag{B10}$$

From the relation $\eta_\Sigma/2 = \delta_\Sigma^0/2$, we have

$$\frac{1}{2i}\Phi_j\sqrt{\frac{2m_j}{\pi k_j}}e^{-ik_jR}e^{\pm\frac{i}{2}\delta_\Sigma^0} = \frac{1}{2i}\Phi_j\sqrt{\frac{2m_j}{\pi k_j}}e^{-ik_jR}e^{\pm i\eta_\Sigma} = \tilde{\theta}_j^{\pm} \tag{B11}$$

Using this relation, the background incoming wave $\psi_j^{(-)}$ can be rewritten as

$$\psi_j^{(-)} \to \frac{1}{2i}\sum_{j'} \Phi_{j'}\sqrt{\frac{2m_{j'}}{\pi k_{j'}}}(e^{ik_{j'}R}\delta_{jj'} - e^{-ik_{j'}R}S_{j'j}^0)$$

$$= e^{-\frac{i}{2}\delta_\Sigma^0}\sum_{j'\in P}\left(\tilde{\theta}_{j'}^+\delta_{jj'} - \tilde{\theta}_{j'}^-\left[e^{-\frac{i}{2}\theta_0\sigma_y}e^{-i\Delta_{12}^0\sigma_z}e^{\frac{i}{2}\theta_0\sigma_y}\right]_{j'j}\right), \quad R \geq R_0. \tag{B12}$$

Multiplying Eq. (B12) by $\exp(i\delta_\Sigma^0/2)\exp(i\theta_0\sigma_y/2)\exp(i\Delta_{12}^0\sigma_z/2)\exp(-i\theta_r\sigma_y/2)$ and using

$$\sum_{j\in P}\tilde{\theta}_j^+\left[e^{-\frac{i}{2}\theta_0\sigma_y}e^{-\frac{i}{2}\Delta_{12}^0\sigma_z}e^{-\frac{i}{2}\theta_r\sigma_y}\right]_{j\alpha} = (\theta_r^+)_\alpha, \tag{B13}$$

and Eq. (B8), we obtain Eq. (B2).

Let us next consider obtaining the CM term corresponding to the second term on the right-hand side of Eq. (B1). Using the formula (25), we can easily check that it is an exponentially decreasing function as

$$e^{i\bar{\beta}}(\theta_r^+)_3 - e^{i\beta}(\theta_r^-)_3 \to \Phi_3\sqrt{\frac{m_3}{\pi\kappa_3}}D_3e^{-\kappa_3R} \tag{B14}$$

as it is constructed so. If only closed channels exist, the above function would be a true bound state. Since open channels also exist, it is not a true bound state. As a good approximation, we may regard it as a discrete state in CM. We can normalize it by the well-known procedure[2] and thus can be related to the space-normalized ϕ_{E_n} in CM as

$$\left(\frac{d\delta_r}{d\bar{\beta}}\right)^{1/2}(e^{i\beta}(\theta_r^+)_3 - e^{i\beta}(\theta_r^-)_3)\Big|_{\beta=\nu\pi} = -\frac{\phi_{E_n}}{\pi(\Sigma_k|V_{kE}|^2)^{1/2}}\sin\delta_r, \quad R \geq R_0. \tag{B15}$$

From Eqs. (B2), (B10), and (B1), we obtain

$$(e^{i\delta_r}(\theta_r^+)_1 - e^{-i\delta_r}(\theta_r^-)_1) + \left(\frac{d\delta_r}{d\bar{\beta}}\right)^{1/2}[e^{i\beta}(\theta_r^+)_3 - e^{i\beta}(\theta_r^-)_3]$$

$$= \psi^{(a)}\cos\delta_r - \overline{\psi}^{(a)}\sin\delta_r - \frac{\phi_{E_n}}{\pi(\Sigma_k|V_{kE}|^2)^{1/2}}\sin\delta_r$$

$$= -\left[\Phi_{E_n}\frac{\sin\delta_r}{\pi(\Sigma_k|V_{kE}|^2)^{1/2}} - \psi^{(a)}\cos\delta_r\right], \tag{B16}$$

where Φ_{E_n} is the modified discrete state with energy E_n introduced by Fano.[13] If we define $\Psi^{(b)}$ as $-\psi^{(b)}$, then we have

$$((\Psi_r^{(-)})_1, (\Psi_r^{(-)})_2) = -(e^{-i\delta_r}\Psi^{(a)}, \Psi^{(b)}), \tag{B17}$$

where $\Psi^{(a)}$ is defined as

$$\Psi^{(a)} = \Phi_{E_n}\frac{\sin\delta_r}{\pi(\Sigma_k|V_{kE}|^2)^{1/2}} - \psi^{(a)}\cos\delta_r \tag{B18}$$

and extensively used in the CM theory.[15,16]

Appemdix C: The Solution of $\Re(\kappa^{OO})=0$ and $\Re(\kappa^{CC})=0$

From both $\Re(\kappa^{OO})$ and $\Re(\kappa^{CC})$ being zero, we have

$$K^{OO} = K^{OC}K^{CO}(1 + K^{CC2})^{-1}K^{CC} \tag{C1}$$

$$K^{CC} = K^{CO}K^{OC}(1 - K^{OO2})^{-1}K^{OO}. \tag{C2}$$

Let us limit the discussion to the system involving only one closed channel. Then insertion of the formula (C1) for K^{OO} into Eq. (C2) and then rearrangement of terms yield

$$K^{CC}\left[1 - \frac{K^{CO}K^{OC}}{1 - K^{OO2}}K^{OC}(1 + K^{CC2})^{-1}K^{CO}\right] = 0. \tag{C3}$$

Eq. (C3) has two solutions, one is $K^{CC} = 0$ and the other is

$$\Im(\kappa^{CC}) = -\frac{1 + K^{CC2}}{K^{CO}K^{OC}}. \tag{C4}$$

$K^{OO} = 0$ follows from Eq. (C1) if $K^{CC} = 0$. This is the desired solution. Let us next consider the other solution. In this case, let us restrict the number of open channels to two as in the present system. In this case, the condition imposed on K^{OO} for all the resonance-centered representations is tr(K^{OO}) = 0 from Eq. (61). From tr(**1**) = 2 and tr(σ_i) = 0, the condition tr(K^{OO}) = 0 for the resonance-centered representation means that K^{OO} is a linear combination of only Pauli matrices. From $(\sigma_i)^2 = 1$, K^{OO2} is easily seen to be a unit matrix multiplied by a positive constant, say a^2. Then,

$$= \Im(\kappa^{cc}) = K^{cc}(1+K^{cc2})^{-1}K^{cc} = K^{cc}K^{cc}(1+a^2)^{-1}. \tag{C5}$$

From Eqs. (C4) and (C5), we have

$$(K^{cc}K^{cc})^2 = (1+K^{cc2})(1+a^2) \geq 1. \tag{C6}$$

From the above equation and the positiveness of $K^{cc}K^{cc}$, we obtain the condition the second solution satisfies.

Appendix D: Relations between Parameters for Partial Cross Sections in MQDT and CM

The ρ_j parameter of Eq. (150) can be rewritten using Eq. (101) as

$$\rho_j = e^{-\frac{i}{2}\delta_j'}\frac{(\psi_j^{(-)}|\psi^{(-)})((\Psi_j^{(-)})_1|T|i)}{(\tilde{\Psi}_j^{(-)}|T|i)}. \tag{D1}$$

In order to give a relation to ρ_j(CM) of Eq. (151), we need relations of $(\Psi_j^{(-)})_1$ and $\tilde{\Psi}_j^{(-)}$ with $\psi^{(-)}$ and $\psi_j^{(-)}$ respectively. From the relation $(\Psi_j^{(-)})_1=[(\Psi_j)_1-i\xi(\Psi_j)_3]/(1+\xi^2)$ inverse to Eq. (133) and Eq. (143), we have

$$(\Psi_j^{(-)})_1 = \frac{1}{1-\xi^2}\{\psi^{(-)}+2i\xi(\theta_-)_3+\xi^2[(\theta_-^+)_1+(\theta_-)_1]\},\ R \geq R_0. \tag{D2}$$

Next, let us consider $\tilde{\Psi}_j^{(-)}$. Its form in $R \geq R_0$ is given by

$$\tilde{\Psi}_j^{(-)} = \tilde{\theta}_j^- - \sum_{i \in P}\tilde{\theta}_i^-\tilde{S}_{ij}^{cc} - \tilde{\theta}_3^-\tilde{S}_{3j}^{cc}. \tag{D3}$$

After some manipulations, $\tilde{S}^{cc}$ and $\tilde{S}^{cc}$ can be calculated from Eq. (94) with $S^{cc}=(1-\xi^2\sigma_z)/(1+\xi^2)$ and $S_j^{cc}=-2i\xi(1,0)/(1-\xi^2)$

$$\tilde{S}^{cc} = \frac{1}{1+\xi^2}e^{-i\Delta_{12}^{\prime}\boldsymbol{\sigma}\cdot\boldsymbol{n}_0}(1-\xi^2\boldsymbol{\sigma}\cdot\boldsymbol{n}_r''),$$

$$\tilde{S}_{3i}^{cc} = \frac{2i\xi}{1+\xi^2}\Big[e^{\frac{i}{2}(\theta_r+\theta_0)\sigma_z}e^{-\frac{i}{2}\Delta_{12}^{\prime}\boldsymbol{\sigma}\cdot\boldsymbol{n}_0}\Big]_{1i}, \tag{D4}$$

where $\boldsymbol{n}_r''=R_{n_0}(-\Delta_{12}^0)R_z(\theta_r-\theta_0)\boldsymbol{z}$. With these, $\tilde{\Psi}_j^{(-)}$ becomes

$$\tilde{\Psi}_j^{(-)} = \tilde{\theta}_j^- - \sum_{i \in P}\tilde{\theta}_i^-\frac{1}{1+\xi^2}[e^{-i\Delta_{12}^{\prime}\boldsymbol{\sigma}\cdot\boldsymbol{n}_0}(1-\xi^2\boldsymbol{\sigma}\cdot\boldsymbol{n}_r'')]_{ij}$$

$$+\frac{2i\xi}{1-\xi^2}\tilde{\theta}_3\Big[e^{\frac{i}{2}(\theta_r+\theta_0)\sigma_z}e^{-\frac{i}{2}\Delta_{12}^{\prime}\boldsymbol{\sigma}\cdot\boldsymbol{n}_0}\Big]_{1j} \tag{D5}$$

in $R \geq R_0$. Expressing $\tilde{\theta}_j^+$ in terms of the background incoming wave $\psi_j^{(-)}$ using

$$\psi_j^{(-)}e^{\frac{i}{2}\delta_j'} = \tilde{\theta}_j^- - \sum_{i \in P}\tilde{\theta}_i^-(e^{-\Delta_{12}^{\prime}\boldsymbol{\sigma}\cdot\boldsymbol{n}_0})_{ij},\ R \geq R_0 \tag{D6}$$

obtainable from Eq. (B12), Eq. (D5) becomes

$$\tilde{\Psi}_j^{(-)} = \psi_j^{(-)}e^{\frac{i}{2}\delta_j'} + \frac{\xi^2}{1+\xi^2}\sum_{i \in P}\tilde{\theta}_i^-[e^{-i\Delta_{12}^{\prime}\boldsymbol{\sigma}\cdot\boldsymbol{n}_0}(1+\boldsymbol{\sigma}\cdot\boldsymbol{n}_r'')]_{ij}$$

$$+\frac{2i\xi}{1-\xi^2}\tilde{\theta}_3\Big[e^{\frac{i}{2}(\theta_r+\theta_0)\sigma_z}e^{-\frac{i}{2}\Delta_{12}^{\prime}\boldsymbol{\sigma}\cdot\boldsymbol{n}_0}\Big]_{1j} \tag{D7}$$

in $R \geq R_0$.

Eqs. (D2), (D7), and (D1) tell us that as ξ goes to zero, we have

$$(\Psi_j^{(-)})_1 \simeq \psi^{(-)},$$

$$\tilde{\Psi}_j^{(-)} \simeq \psi_j^{(-)}e^{\frac{i}{2}\delta_j'},$$

$$\rho_j \simeq \rho_j(\mathrm{CM}). \tag{D8}$$

Here notice that, in contrast to the case of total cross sections, $(\Psi_j^{(-)})_1$ and $\tilde{\Psi}_j^{(-)}$ now differ from the corresponding ones in CM not only in the resonance parts but also in the background parts though the difference in the latter is the second order in ξ. In contrast to this, the difference between two theories in the formulas of partial cross sections does not appear in the background parts. Since partial cross sections are expressed in terms of $(\tilde{M}_j^{(-)}|T|i)$ in MQDT, let us consider the relation between $\tilde{M}_j^{(-)}$ and $\psi_j^{(-)}$. Eq. (119) can be rewritten in $R \geq R_0$ as

$$\tilde{M}_j^{(-)} = \tilde{\theta}_j^- - \sum_{i \in P}\tilde{\theta}_i(\tilde{\sigma}^{cc})_{ij} - \sum_{i \in Q}(\tilde{\theta}_i^- - \tilde{\theta}_i)[(1-\tilde{S}^{cc})^{-1}\tilde{S}^{cc}]_{ij},$$

$$\tilde{N}_j^{(-)} = \tilde{\theta}_j^- - \sum_{i \in P}\tilde{\theta}_i[\tilde{S}^{cc}+\tilde{S}^{cc}(1-\tilde{S}^{cc})^{-1}\tilde{S}^{cc}]_{ij}$$

$$-\sum_{i \in Q}(\tilde{\theta}_i - \tilde{\theta}_i^-)[(1-\tilde{S}^{cc})^{-1}\tilde{S}^{cc}]_{ij}, \tag{D9}$$

where $\tilde{\sigma}^{cc}$ is defined in Eq. (A8). Using Eq. (D4) and after some manipulations, we obtain

$$\tilde{\sigma}^{cc} = e^{-i\Delta_{12}^{\prime}\boldsymbol{\sigma}\cdot\boldsymbol{n}_0},$$

$$[(1-\tilde{S}^{cc})^{-1}\tilde{S}^{cc}]_{3i} = -i\xi\Big[e^{\frac{i}{2}(\theta_r+\theta_0)\sigma_z}e^{-\frac{i}{2}\Delta_{12}^{\prime}\boldsymbol{\sigma}\cdot\boldsymbol{n}_0}\Big]_{1i}. \tag{D10}$$

Then $\tilde{M}_j^{(-)}$ and $\tilde{N}_j^{(-)}$ become

$$\tilde{M}_j^{(-)} = \psi_j^{(-)}e^{\frac{i}{2}\delta_j'} + i\xi(\tilde{\theta}_3^- + \tilde{\theta}_3^-)\Big[e^{\frac{i}{2}(\theta_r-\theta_0)\sigma_z}e^{-\frac{i}{2}\Delta_{12}^{\prime}\boldsymbol{\sigma}\cdot\boldsymbol{n}_0}\Big]_{1j}, \tag{D11}$$

$$\tilde{N}_j^{(-)} = \tilde{\theta}_j + \sum_{i \in P}\tilde{\theta}_i^-[e^{-i\Delta_{12}^{\prime}\boldsymbol{\sigma}\cdot\boldsymbol{n}_0}\boldsymbol{\sigma}\cdot\boldsymbol{n}_r'']_{ij}$$

$$-\frac{i}{\xi}(\tilde{\theta}_3^+ - \tilde{\theta}_3^-)\Big[e^{\frac{i}{2}(\theta_r+\theta_0)\sigma_z}e^{-\frac{i}{2}\Delta_{12}^{\prime}\boldsymbol{\sigma}\cdot\boldsymbol{n}_0}\Big]_{1j} \tag{D12}$$

in $R \geq R_0$. Eq. (D11) shows that $\psi_j^{(-)}$ and $\tilde{M}_j^{(-)}$ differ only in the resonant part.

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