Decoupling of Background and Resonance Scatterings in Multichannel Quantum Defect Theory and Extraction of Dynamic Parameters from Lu-Fano Plot

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Giusti-Suzor and Fano introduced translations of the scales of Lu-Fano plots by phase renormalization in order to decouple the intra- and inter-channel couplings in multichannel quantum defect theory (MQDT). Their theory was further developed by others to deal with systems involving a larger number of channels. In different directions, MQDT was reformulated into forms with a one-to-one correspondence to those in Fano's configuration mixing theory of resonance for photofragmentation processes involving one closed and many open channels. In this study, the theory was further developed to fully reveal the coupling nature, decoupling of the background and resonance scattering in physical scattering matrices as well as to further extract the dynamic parameters undiscovered by Fano and his colleagues. This theory was applied to the photoabsorption spectrum of H_2 observed by Herzberg's group.

Key Words: MQDT, Resonance, Background scattering, Phase renormalization

Introduction

Although multichannel quantum defect theory (MQDT) is a powerful theory of resonance that can describe complex spectra including both bound and continuum regions with only a few parameters, the resonance structures are not identified transparently in its formulation due to the indirect treatment of resonance.[1] In order to identify the resonance terms, a special treatment is needed, such as that introduced by Giusti-Suzor and Fano for the two channel case.[2,3] They noticed that the usual Lu-Fano plot often obscures the symmetry apparent in its extended version. This symmetry can be brought out in the MQDT formulation by shifting the origin of the plot to the center of symmetry using the phase-shifted base pairs first considered in Ref.[4]. Their theory was further developed by others in an attempt to deal with systems involving a larger number of channels.[5-6] In a different direction, MQDT was reformulated into forms with a one-to-one correspondence to those in Fano's configuration mixing (CM) theory of resonance for photofragmentation processes involving a single closed and many open channels.[7-8] The reformulation relies on an identification of the background scattering matrix σ^{oo} of the MQDT version, which satisfies the unitarity and is simultaneously diagonalizable with the open channel part K^{oo} of the sub-matrices of Seaton's short-range reactance matrix K.[1] However, such identification was motivated simply by mathematics without any physical basis.

Although fundamental in nature, it is very important to have a physical basis for this identification because theories cannot be developed further without a proper understanding. Giusti-Suzor and Fano tackled this problem using Lippmann-Schwinger's theory.[9] In this study, it was tackled by examining the transformation relations to identify the true resonance scattering. The results revealed the coupling nature, decoupling of the background and resonance scatterings, and extracted further dynamic parameters undiscovered by Fano *et al*. The theory was applied to the photoabsorption spectrum of H_2 observed by Herzberg's group.[10]

Brief Introduction of MQDT

In the multichannel quantum defect theory of the photofragmentation process, the coordinate R for the relative motion of colliding partners along which fragmentation occurs is divided into two ranges $R \le R_0$ and $R > R_0$, the inner and outer ones, respectively. In contrast to the inner range, where transfers in energy, momentum, angular momentum, spin, or the formation of a transient complex occur due to the strong interactions there, channels are decoupled in an outer range. Consequently, the motion is governed by ordinary second-order differential equations and can be described by a superposition of the energy-normalized regular and irregular base pair $f_j(R)$ and $g_j(R)$ or the incoming and outgoing base pair $\exp(-ik_jR)$ and $\exp(ik_jR)$. Using these pairs, N independent degenerate solutions of the Schrödinger equation for the decoupled motion in $R \ge R_0$ for an N-channel system can be expressed as a standing- wave type

$$\Psi_i(R,\omega) = \sum_{j=1}^{N} \Phi_j(\omega)\left[f_j(R)\delta_{ji} - g_j(R)K_{ji} \right] \tag{1}$$

or an incoming-wave type

$$\Psi_i^{(-)}(R,\omega) = \sum_{j=1}^{N} \Phi_j(\omega)\left[\phi_j^{+}(R)\delta_{ji} - \phi_j^{-}(R)S_{ji} \right] \tag{2}$$

where $\Phi_j(\omega)$ are the channel basis functions for the coordinate space excluding R, and $\phi_j^{\pm}$ are the modified outgoing and incoming base pair defined as $(\pm f_j + ig_j)/2$. Using the quantum defect theory parameters η_j, β_j and D_j in Ref. [11] for an arbitrary field, $\phi_j^{\pm}$ are given in the outer range $R \ge R_0$ by $-i(m_j/2\pi k_j)^{1/2}\exp(\pm i\eta_j)\ f_j^{\pm}$ for the open channels and $\pm(m_j/\pi\kappa_j)^{1/2}\exp(\pm i\beta_j)(D_j f_j^{+} \pm iD_j^{-1} f_j^{-})/2$ for the closed channels, where $f_j^{\pm}$ denotes $\exp(\pm ik_jR)$. K_{ji} and S_{ji} are the (j, i) -elements of the short-range reactance and scattering matrices, respectively, and are related to each other in matrix notation by $S =$

$(1-iK)(1+iK)^{-1}$ (S is taken as a complex conjugate of the usual definition, for convenience).

Although all the N solutions are needed to describe the motion in the intermediate range, some become closed and no longer exist in the limit of $R\to\infty$. Therefore, classification of these channels as open or closed is meaningful only at a large R. Nonetheless, it may still be convenient to keep this classification in the intermediate range. The notations P and Q were used for the sets of open and closed channels, respectively, and the super-indices o and c were used for the dynamic quantities belonging to the open and closed channels, respectively. The wave function, $\Psi_i^{(-)}$ for the photofragmentation process into the i-th fragmentation channel should satisfy the incoming-wave boundary condition, $\Psi_i^{(-)}\to\Sigma_{j\in P}\,(\phi_j^{+}\,\delta_{ji}-\phi_j^{-}\boldsymbol{S}_{ji})$ at a large R, which can be obtained by making a linear combination of the incoming channel basis functions $\Psi_i^{(-)}$ of Eq. (2). The physical scattering matrix $\boldsymbol{S}$ can be obtained by substituting the explicit forms for $\phi_j^{\pm}$ given above and then setting the coefficients of the exponentially increasing terms to zero as follows:

$$\boldsymbol{S}=S^{oo}-S^{oc}(S^{cc}-e^{2i\beta})^{-1}S^{co}\,. \tag{3}$$

Whilst the above equation shows how the resonance arises by the channels being closed at a large R, the background and resonance contributions are intertwined in a subtle way to prevent efforts to determine the dynamic interactions between them.

Separation of Background and Resonance Terms in the Physical Scattering Matrix

Experience in the configuration interaction resonance theory[11] suggests that it is imperative to use some 'effective' S^{oo} that is simultaneously diagonalizable with K^{oo} imbedded in S^{oc}. This logical train of thought leads us to introduce σ^{oo}, which is defined as $(1-iK^{oo})(1+iK^{oo})^{-1}$, to supersede S^{oo}. Note that σ^{oo} can be expressed as $S^{oo}-S^{oc}(S^{cc}+1)^{-1}S^{co}$, whose form is quite similar to that of the physical scattering matrix $\boldsymbol{S}$, except that $-\exp(2i\beta)$ is replaced by 1. Hence, the physical scattering matrix (3) can be formulated in terms of σ^{oo} by expressing $[\,S^{cc}-\exp(2i\beta)\,]^{-1}$ into $(S^{cc}+1)^{-1}$ using the matrix identity of $A^{-1}=B^{-1}+B^{-1}U(C-\tilde{U}B^{-1}U)^{-1}UB^{-1}$, where $A=B-UC^{-1}\tilde{U}$. The relation,

$$\left(S^{cc}-e^{2i\beta}\right)^{-1}=(S^{cc}+1)^{-1}+\tfrac{i}{2}(1+i\kappa^{cc})\times\left(\tan\beta+\kappa^{cc}\right)^{-1}(1+i\kappa^{cc})\;, \tag{4}$$

one obtains using $(S^{cc}+1)^{-1}=\tfrac{1}{2}(1+i\kappa^{cc})$ allows us to rewrite Eq. (3) into

$$\boldsymbol{S}=\sigma^{oo}-2i(1+iK^{oo})^{-1}K^{oc}(\tan\beta+\kappa^{cc})^{-1}K^{co}(1+iK^{oo})^{-1}\cdot \tag{5}$$

Since $\sigma^{oo}=(1-iK^{oo})(1+iK^{oo})^{-1}$, σ^{oo} and K^{oo} commute with each other and can be diagonalized simultaneously as $\sigma^{oo}=Ue^{-2i\delta^{o}}U^{T}$ and $K^{oo}=U\tan\delta^{o}U^{T}$. Substitution of these into (5) yields

$$\begin{aligned}\boldsymbol{S}&=Ue^{-i\delta^0}\left[1+2i\xi\left(\tan\beta+\kappa^{cc}\right)^{-1}\xi^{T}\right]e^{-i\delta^0}U^{T}\\&\equiv Ue^{-i\delta^0}\boldsymbol{S}_r e^{-i\delta^0}U^{T}\end{aligned} \tag{6}$$

where ξ denotes $\cos\delta^{o}U^{T}K^{oc}$ and the part inside the bracket is denoted as $\boldsymbol{S}_r$. The form of the above physical scattering matrix suggests that $\boldsymbol{S}_r$ is related to the resonance. The resonance structure in the physical scattering matrix can best be seen in the behavior of its eigenphase shift. The orthogonal matrix that diagonalizes it is related to the geometrical factor and represents the frame transformation between the resonance and fragmentation eigenchannels. The dynamic behavior of the resonance pertaining to potential scattering can be seen in its eigenphase shifts. However, each eigenphase shift is not only affected by the resonance but also by the avoided interactions between the different eigenphases. Hence, the pure resonance behavior is only observed in the eigenphase sum, which can be obtained by calculating the determinant of the physical scattering matrix. The calculation of its determinant can be accomplished using the matrix identity $\det(1-UV)=\det(1-VU)$ as follows

$$\begin{aligned}\det(\boldsymbol{S})&=e^{-2i\delta_\Sigma^0}\det\left[1+2i\xi^{T}\xi\left(\tan\beta+\kappa^{cc}\right)^{-1}\right]\\&=e^{-2i\delta_\Sigma^0}\frac{\det\left(\tan\beta+\kappa^{cc}\,*\right)}{\det\left(\tan\beta+\kappa^{cc}\right)}\end{aligned} \tag{7}$$

where δ^0_Σ is the shorthand notation for the sum $\Sigma_i\delta^0_i$ of the eigenphase shifts of σ^{oo}. The last equality was obtained using the equation

$$\xi^{T}\xi\;=\;K^{co}\left[1+(K^{oo})^2\right]^{-1}K^{oc}=-\Im(\kappa^{cc})\,. \tag{8}$$

Note that relation (7) holds for any arbitrary number of closed channels, and is not restricted to a single one. Eq. (8) becomes $\Im(\kappa^{cc})=-\xi^2$ for a system involving 1 closed channel. Eq. (7) can be written in a more suggestive form by identifying $\exp(-2i\delta^0_\Sigma)$ with $\det(\sigma^{oo})$

$$\det(\boldsymbol{S})=\det(\sigma^{oo})\frac{\det\left(\tan\beta+\kappa^{cc}\,*\right)}{\det\left(\tan\beta+\kappa^{cc}\right)}\;\cdot \tag{9}$$

This form suggests that δ^B_Σ is a better notation for δ^0_Σ, which will be clarified later. On the other hand, $\det(\boldsymbol{S})$ can be identified with $\exp(-2i\delta_\Sigma)$. For the system with 1 closed channel, $\tan\beta+\kappa^{cc}$ is just a number, and there is no need to take its determinant. In this case, we obtain

$$\tan(\delta_\Sigma-\delta^0_\Sigma)\left[\tan\beta\,+\,\Re(\kappa^{cc})\right]\;=\;\Im(\kappa^{cc})\;=\;-\xi^2\,. \tag{10}$$

Another way of observing this equation comes from a consideration of the reactance matrix $\boldsymbol{K}_r$, which corresponds to $\boldsymbol{S}_r$ as $-i(1-\boldsymbol{S}_r)(1+\boldsymbol{S}_r)^{-1}$. Using Eq. (9) in Ref. [7] and the projection operator P_r defined there, $\boldsymbol{S}_r$ can be written as $P_b + P_r (\tan\beta + \kappa^{cc}*) / (\tan\beta + \kappa^{cc})$, where use is made of another projection operator, P_b, which is defined as $1 - P_r$ and satisfies $P_b P_r = 0$ and $P_b^2 = 1$. Using the properties of the projection operators, $\boldsymbol{K}_r$ can be calculated as $P_r \Im(\kappa^{cc}) / [\tan\beta + \Re(\kappa^{cc})]$. As $\boldsymbol{K}_r$ can be expressed as $\tan\delta_r P_r$ in terms of the phase shift matrices, we obtain

$$\tan\delta_r = \Im(\kappa^{cc}) / \left[\tan\beta + \Re(\kappa^{cc}) \right]. \qquad (11)$$

This identification allows $\delta_\Sigma - \delta^0_\Sigma = \delta_r$ to be deduced from Eq. (10).

Transformation Relation of Background and Resonance Terms under Phase Renormalization

Now let us apply the phase renormalizations $\eta'_i = \eta_i + \pi\mu_i^o$ and $\beta'_i = \beta_i + \pi\mu_i^c$ for the open and closed channels, respectively. In the new phase renormalized base functions, Eq. (9) becomes

$$\det(\boldsymbol{S}') = \det(\sigma'^{oo}) \frac{\det(\tan\beta' + \kappa'^{cc}*)}{\det(\tan\beta' + \kappa'^{cc})}. \qquad (12)$$

Consider each of the two factors in the right-hand side of Eq. (12) separately. Substituting $\beta'_i - \pi\mu_i^c$ for β_i in $\tan\beta + \kappa^{cc}$, we obtain

$$\begin{aligned} &\tan(\beta' - \pi\mu^c) + \kappa^{cc} \\ &= [\tan\beta'(\kappa^{cc}\sin\pi\mu^c + \cos\pi\mu^c) + \kappa^{cc}\cos\pi\mu^c - \sin\pi\mu^c] \\ &\quad \times (\cos\pi\mu^c + \tan\beta'\sin\pi\mu^c)^{-1} \\ &= [\tan\beta' + \kappa'^{cc}](\kappa^{cc}\sin\pi\mu^c + \cos\pi\mu^c) \\ &\quad \times (\cos\pi\mu^c + \tan\beta'\sin\pi\mu^c)^{-1} \end{aligned} \qquad (13)$$

This means that $\det(\tan\beta + \kappa^{cc}*) / \det(\tan\beta + \kappa^{cc})$ is transformed to

$$\frac{\det(\tan\beta' + \kappa'^{cc}*)}{\det(\tan\beta' + \kappa'^{cc})} = \frac{\det(\tan\beta + \kappa^{cc}*)}{\det(\tan\beta + \kappa^{cc})} \frac{\det(\cot\pi\mu^c + \kappa^{cc})}{\det(\cot\pi\mu^c + \kappa^{cc}*)}. \qquad (14)$$

For systems with 1 closed channel, κ^{cc} can be written as $\tan\Delta^c$, as described in Appendix A, where Δ^c is the complex phase shift considered by Dubau and Seaton[3] and is given by $\delta^c - i\gamma^c$. The first term of the right hand side of Eq. (14) can then be shown to be equal to

$$\frac{\det(\tan\beta + \kappa^c*)}{\det(\tan\beta + \kappa^{cc})} = \frac{\sin(\beta + \Delta^c*)}{\sin(\beta + \Delta^c)} \frac{\cos\Delta^c}{\cos\Delta^c*} = e^{-2i\delta_r}. \qquad (15)$$

The right-hand side of the first equality of Eq. (15) is composed of two ratios. The first is the sole source of long-range dynamics because the complex phase shift Δ^c includes only short-range dynamics and the long-range dynamics are only contained in β. This means that strongest energy dependence arises from the first ratio terms, as energy-sensitive dynamics occur only over the long-range. Similarly, $\det(\cot\pi\mu^c + \kappa^{cc}*) / \det(\cot\pi\mu^c + \kappa^{cc})$ can be shown to be equal to $\cos\Delta'^c*\cos\Delta^c / \cos\Delta'^c\cos\Delta^c*$. The formulation in terms of the complex phase shifts allows use of the laws of trigonometry, and reveals that Eq. (14) is simply an identity in that context.

The numerator in the left-hand side of Eq. (15) is just a complex conjugate of the denominator whereby the modulus of their quotient is unity and thus the quotient can be written as $\exp(-2i\delta_r)$ giving the second equality of Eq. (15). Here δ_r is the phase of the denominator and is equal to the one in Eq. (11). Likewise, the phase μ_r can be introduced to denote the quotient $\det(\cot\pi\mu^c + \kappa^{cc}*)/\det(\cot\pi\mu^c + \kappa^{cc})$ as $\exp(-2i\pi\mu_r)$. Transformation (14) can then be expressed in terms of the phase shifts as

$$\delta_r' = \delta_r - \pi\mu_r, \qquad (16)$$

which takes the form of phase renormalization, and was not introduced on purpose but was induced. Before investigating the properties of this transformation further, consider the transformation relation of σ^{oo}, which is the remaining part of Eq. (9).

To determine the transformation relation between σ^{oo} and σ'^{oo}, first consider the definition of σ'^{oo}:

$$\begin{aligned} \sigma'^{oo} &= S'^{oo} - S'^{oc}(S'^{cc}+1)^{-1}S'^{co} \\ &= e^{i\pi\mu^o}\left[S^{oo} - S^{oc}\left(S^{cc} + e^{-2i\pi\mu^c}\right)^{-1} S^{co}\right] e^{i\pi\mu^o}. \end{aligned} \qquad (17)$$

If $\exp(2i\beta)$ is replaced with $-\exp(-2i\pi\mu)$ in Eq. (4), we obtain

$$\begin{aligned} &\left(S^{cc} + e^{-2i\pi\mu}\right)^{-1} \\ &= (S^{cc} + 1)^{-1} + \tfrac{i}{2}(1 + i\kappa^{cc})\left(\cot\pi\mu^c + \kappa^{cc}\right)^{-1}(1 + i\kappa^{cc}). \end{aligned} \qquad (18)$$

By substituting Eq. (18) and using $-2i(1 + iK^{oo})^{-1} K^{oc}(1 + iK^{cc})^{-1}$ for S^{oc} and its transpose for S^{co}, Eq. (17) yields the transformation relation for σ^{oo} under the phase renormalization as follows:

$$\begin{aligned} \sigma'^{oo} = e^{i\pi\mu^o} \big[&\sigma^{oo} + 2i(1 + K^{oo})^{-1} K^{oc}(\cot\pi\mu^c + \kappa^{cc})^{-1} \\ &K^{co}(1 + K^{oo})^{-1} \big] e^{i\pi\mu^o}. \end{aligned} \qquad (19)$$

As in Eq. (6), the above equation can be simplified using the simultaneous diagonalization of σ^{oo} and K^{oo} as

$$\sigma'^{oo} = e^{i\pi\mu^o} U e^{i\delta^0}\left[1 + 2i\xi(\cot\pi\mu^c + \kappa^{cc})^{-1}\xi^T\right] e^{i\delta^0} U^T e^{i\pi\mu^o}. \qquad (20)$$

Using the same technique for obtaining $\det(\boldsymbol{S})$ in Eq. (7), the determinant of σ'^{oo} can be easily obtained as follows:

$$\det(\sigma'^{oo}) = e^{-2i\delta'^0_\Sigma} = e^{2i(\pi\mu^o_\Sigma - \delta^0_\Sigma)} \frac{\det(\cot\pi\mu^c + \kappa^{cc}*)}{\det(\cot\pi\mu^c + \kappa^{cc})}$$

$$= e^{2i\pi\mu_\Sigma^o} \det(\sigma^{oo}) \frac{\det(\cot\pi\mu^c + \kappa^{cc}*)}{\det(\cot\pi\mu^c + \kappa^{cc})} \quad (21)$$

$\det(\boldsymbol{S}') = \exp(2i\pi\mu^o_\Sigma)\det(\boldsymbol{S})$ was obtained by substituting Eqs. (14) and (21) into Eq. (12) and using Eq. (7), and can be expressed in terms of the phase shifts as $\delta'_\Sigma = \delta_\Sigma - \pi\mu^o_\Sigma$. This suggests that $\eta_\Sigma + \delta_\Sigma$ is an invariant form under phase renormalization.

Extraction of Background and Resonance Dynamic Parameters from Lu-Fano Plot

Henceforth, δ^B will be used for the eigenphase shifts of σ^{oo} instead of δ^o *i.e.*, $\sigma^{oo} = \exp(-2i\delta^B)$ and similarly δ'^B will be used for σ'^{oo}. Using these, Eq. (21) can be expressed in a physically more transparent form $\delta'^B_\Sigma = \delta^B_\Sigma - \pi(\mu^o_\Sigma - \mu_r)$, where δ^B_Σ denotes $\Sigma_i\delta^B_i$. The form suggests the definition of a new quantum defect μ^B_Σ for $\mu^o_\Sigma - \mu_r$, whereupon $\delta'^B_\Sigma = \delta^B_\Sigma - \pi\mu^B_\Sigma$. In contrast to μ^o_Σ, whose value is at our disposal, the value of μ^B_Σ cannot be taken arbitrarily and is fixed by the values of μ^o_Σ and μ^c (or equally μ_r). Overall, $\delta'_\Sigma = \delta_\Sigma - \pi\mu^o_\Sigma$ where each term of δ_Σ, δ'_Σ and μ^o_Σ can be decomposed into $\delta'_\Sigma = \delta'^B_\Sigma + \delta'_r$, $\delta_\Sigma = \delta^B_\Sigma + \delta_r$ and $\mu^o_\Sigma = \mu^B_\Sigma + \mu_r$, respectively. Note that in this decomposition into two parts, the background and resonance parts in the decomposition is phase renormalized in its own way as $\delta'^B_\Sigma = \delta^B_\Sigma - \pi\mu^B_\Sigma$ and $\delta'_r = \delta_r - \pi\mu_r$, respectively. Although phase renormalization is also performed for a closed channel as $\beta' = \beta + \pi\mu^c$, its influence on the physical scattering matrix cannot be observed directly, which is in contrast to the case of $\pi\mu^o_\Sigma$ in the open channels, where δ_Σ is influenced in a linear manner. It influences indirectly through the form of μ_r, which is related to μ^c nonlinearly as $\exp(-2i\pi\mu_r) = (\cot\pi\mu^c + \kappa^{cc}*) / (\cot\pi\mu^c + \kappa^{cc})$. The equation can be written in terms of the complex phase shifts as follows:

$$\frac{\cot\pi\mu^c + \kappa^{cc}*}{\cot\pi\mu^c + \kappa^{cc}} = e^{-2i\pi\mu_r} = \frac{\cos\Delta'^c*}{\cos\Delta'^c}\frac{\cos\Delta^c}{\cos\Delta^c*} \quad (22)$$

where Δ'^c denotes $\Delta^c - \pi\mu^c$. Another relation $\tan\pi\mu_r = \Im(\kappa^{cc}) / [\cot\pi\mu^c + \Re(\kappa^{cc})]$ can be obtained considering the quotient of the real and imaginary parts of $\cot\pi\mu^c + \kappa^{cc}$. Since $\Im(\kappa^{cc}) = -\xi^2$, $\tan\pi\mu_r$ can be equated to $-\xi^2 / [\cot\pi\mu^c + \Re(\kappa^{cc})]$.

Although the strongest energy dependence of $\det(\boldsymbol{S})$ originates from the second term of the right-hand side of Eq. (9), it still contains an energy insensitive short-range dynamic term, as shown in Eq. (15). This energy insensitive term can be removed by the phase renormalization of $\pi\mu^c = \delta^c$. Let us denote the renormalized δ_r as $\tilde{\delta}_r$. The representation obtained by this phase renormalization can be called the tilde representation. Now, $\tilde{\delta}_r$ satisfies

$$e^{-2i\tilde{\delta}_r} = \frac{\sin(\tilde{\beta} + \tilde{\Delta}^c*)}{\sin(\tilde{\beta} + \tilde{\Delta}^c)} = \frac{\sin(\beta + \Delta^c*)}{\sin(\beta + \Delta^c)} . \quad (23)$$

Note that $\tilde{\delta}_r$ is determined only by the energy sensitive terms. This indicates that energy-insensitive background contributions are completely removed in the formula for δ_r and the purely resonance terms for $\tilde{\delta}_r$ remain. Therefore, in the tilde representation, only subindex r, which signifies resonance, is perfectly correct.

Table 1. Dynamic parameters extracted from the Lu-Fano plot of H_2.

δ^c	γ^c	δ^B_Σ
0.40	0.23	0.04
μ^c	μ_r	μ^o_Σ
0.13	-0.031	-0.018
$\Re(\kappa^{cc})$	$\Im(\kappa^{cc})$	ξ^2
0.40	-0.27	0.27
$\Re(\tilde{\kappa}^{cc})$	$\Im(\tilde{\kappa}^{cc})$	$\tilde{\xi}^2$
0	-0.23	0.23

The situation so far can be interpreted as follows. Phase renormalization is performed for the base pair defined in the long-range while the background and resonance scattering do not entirely come from the long-range dynamics. This suggests that the separation of background and resonance scatterings cannot be achieved directly by phase renormalization. The present derivation confirms that their nature is not precisely compatible with the closed and open nature of the channels. Besides the presence of closed-channels, additional requirements are needed to be in the correct resonance eigenchannels. Eq. (15) shows that $\cos\Delta^c / \cos\Delta^c*$ needs to be removed in order to have a pure resonance nature. This is achieved using the phase renormalization by $\pi\mu_r$ which cannot be controlled directly by the phase renormalization accessible through the fragmentation channels but can be performed indirectly.

With $\pi\mu^c = \delta^c$ satisfied, the tilde representation is not completely specified and there is still freedom in choosing the value of μ^o_Σ. The logical choice will be that the sum of the background eigenphase shifts become zero, *i.e.* $\tilde{\delta}^B_\Sigma = 0$. Since $\tilde{\delta}^B_\Sigma = \delta^B_\Sigma - \pi\mu^B_\Sigma$ and $\mu^B_\Sigma = \mu^o_\Sigma - \mu_r$, this can be obtained with $\mu^o_\Sigma = \mu_r + \delta^B_\Sigma / \pi$. A complete definition of the tilde representation demands this condition in addition to $\pi\mu^c = \delta^c$. As both phase renormalizations are accounted, Eq. (10) becomes

$$\tan\tilde{\delta}_\Sigma \tan\tilde{\beta} = \Im(\tilde{\kappa}^{cc}) = -\tilde{\xi}^2 . \quad (24)$$

Since $\pi\mu^c = \delta^c$ holds in this representation, the renormalized complex phase shift $\tilde{\Delta}^c$ becomes a purely imaginary number, and $\tilde{\kappa}^{cc}$ becomes $\tan\tilde{\Delta}^c = \tan(-i\gamma^c) = -i\tanh\gamma^c$ and $\tilde{\xi}^2 = \tanh\gamma^c$. It should be noted that the tilde representation satisfying $\tilde{\delta}^B_\Sigma = 0$ and $\tilde{\Delta}^c = -i\gamma^c$ is still not unique, even though the remaining indeterminacy is not related to the resonance and is thus trivial. Refer to Ref. [7] for various representations satisfying them. Interestingly, the symmetric Lu-Fano plot was obtained not only from the graph of (β, δ_Σ) by simply translating the origin of the coordinate system by the respective $-\pi\mu^c$ and $\pi\mu^o_\Sigma$ but also from that of $(\beta, \delta_\Sigma - \delta^B_\Sigma)$ given by Eq. (10) by the respective $-\pi\mu^c$ and $\pi\mu_r$. Since the Lu-Fano plot of (β, δ_Σ) can be obtained easily from the spectrum, μ^c and $\tilde{\xi}^2$ can be derived easily by symmetrizing it into the graph given by Eq. (24). Recall that δ^c was obtained from μ^c. Eq. (A2) of $\tan\pi\mu_r = -\tilde{\xi}^2 \tan\delta^c$ can be used to obtain

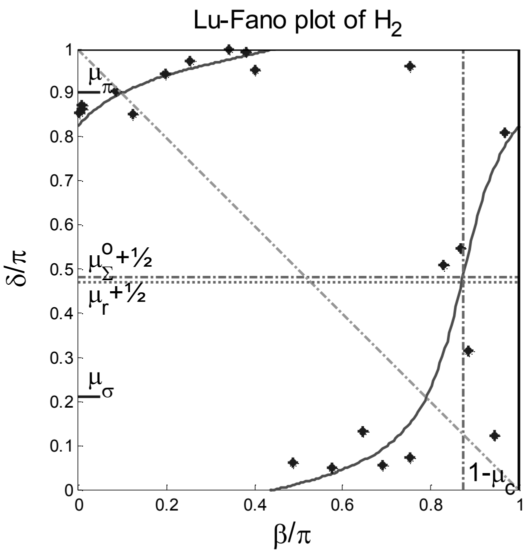

Figure 1. Lu-Fano plot of H_2 drawn using data from Table 1 with the experimental spectroscopic data indicated by * for comparison.

μ_r. A subsequent translation of the Lu-Fano plot yields $\Re(\kappa^{cc})$ and ξ^2. With these, the selfconsistency of the experimental data can be examined by checking the relationship between the two coupling strengths ξ^2 and $\tilde{\xi}^2$ given by $\xi^2 = -\sinh 2\gamma^c / (\cos 2\delta^c + \cosh 2\gamma^c) = \tilde{\xi}^2 / (\tilde{\xi}^4 \sin^2 \delta^c + \cos^2 \delta^c)$. This relation can be simplified to $\xi \cos \pi\mu^c = \tilde{\xi} \cos \pi\mu_r$ which is confirmed numerically using the values in Table 1. It becomes the physically evident $\xi = \tilde{\xi}$ when $\mu^c = \mu_r$ or when $\mu_\Sigma^B = 0$. Similarly, the formula for $\Re(\kappa^{cc})$ can be written as $(\tan^2 \pi\mu^c - \tan^2 \pi\mu_r)\cos^2 \pi\mu_r \cot \pi\mu^c$, which becomes zero when $\mu^c = \mu_r$.

Extraction of Dynamic Parameters from the Lu-Fano Plot of H_2

Now, let us apply the theory to the extraction of dynamical parameters from the Lu-Fano plot of H_2 which is simplest case of one open and one closed channels. In this case, all sub-matrices become scalars and the sums of the phases become simple phases so that the sub-index Σ signifying the summation is no longer needed. The values of $\tilde{K}^{oo}$ and $\tilde{K}^{cc}$ of $\tilde{K}$ are obtained explicitly as zero and $\tilde{K}^{oc} = \tilde{K}^{co} = \tilde{\xi}$ as described by Suzor and Fano.[2] $\tilde{S}^{oo} = \tilde{S}^{cc} = (1-\tilde{\xi}^2)/(1+\tilde{\xi}^2)$ and $\tilde{S}^{oc} = \tilde{S}^{co} = -2i\tilde{\xi}/(1+\tilde{\xi}^2)$ can be obtained using these values.

The basic parameters are the phases δ^c and γ^c of S^{cc}, which are represented in the form of the complex phase $\Delta^c = \delta^c - i\gamma^c$, where S^{cc} is given by $\exp(-2i\Delta^c)$. The coupling parameter $\tilde{\xi}$ between the open and closed channels can then be obtained as $\tilde{\xi}^2 = \tanh \gamma^c$. Another basic parameter is the background eigenphase δ^B obtained from either $K^{oo} = \tan \delta^B$ or $\sigma^{oo} = \exp(-2i\delta^B)$. The tilde representation can be derived using the phase renormalization, $\mu^c = \delta^c / \pi$ and $\mu^o = \mu_r + \delta^B / \pi$, where μ_r was obtained from $\tan \pi\mu_r = -\tilde{\xi}^2 \tan \delta^c$ of Eq. (A2) in Appendix A. When the short-range K matrix is obtained from Lu-Fano plots, S^{cc} can be calculated from $[1+|K|+i(K^{oo}-K^{cc})]/[1-|K|+i(K^{oo}+K^{cc})]$. δ^c and γ^c (or $\tilde{\xi}^2$) can be calculated from the phase and absolute value of S^{cc}. The remaining parameters can be calculated using the method described above. The values of the dynamic parameters extracted from the Lu-Fano plot of H_2 following the procedure described above are shown in Table 1. The Lu-Fano plot of H_2 is shown in Fig. 1 along with the experimental spectroscopic data taken from Ref. [10] for comparison.

Results and Discussion

This study obtained the physical basis for the unitary factorizations of the physical scattering matrix $\boldsymbol{S}$ into σ^{oo} and $(\tan\beta + \kappa^{cc}*)(\tan\beta + \kappa^{cc})^{-1}$, which are not themselves pure background and resonance terms but can be transformed to them under the phase renormalization. The essential step was in the recognition that the nature of background and resonance scatterings is not compatible with the closed and open nature of the channels. Thus physically meaningful procedure should be involved in finding phase renormalizations in the background and resonance channels, not in the open and closed channels. In contrast to the phase renormalizations in the open and closed channels which can be directly controllable by means of the adjustments in the 'reference potentials' in the core region, phase renormalizations in the background and resonance channels can only be determined indirectly. Such renormalizations were obtained by examining the transformation relations for both terms of the unitary factorizations of $\boldsymbol{S}$. The extent of the phase renormalization in the resonance channel was identified as being determined by the coupling strength $\tilde{\xi}^2$ between the open and closed channels in the form of $\tan \pi\mu_r = -\tilde{\xi}^2 \tan \delta^c$ with a phase shift δ^c due to the background scattering. By removing the phase renormalization in the resonance channel from the phase renormalization in open channels, the phase renormalization in the background channels was identified. With these phase renormalizations, decoupling of the background and resonance scatterings from their entanglement in the scattering matrix was accomplished and the fundamental dynamic parameters pertaining to them were identified.

This theory was applied to the photoabsorption spectrum of H_2 observed by Herzberg's group, and additional dynamic parameters were extracted. Future studies will apply the theory to photoabsorption spectra of rare gases where more channels are involved. In addition, the present theory will be extended to systems involving more than one closed channel. In this case, phase renormalization for the imaginary phase shifts may play an important role when more than one imaginary phase shift is present.

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Appendix A: Complex Phase Shifts

S^{oo} or S^{cc} do not satisfy the unitary condition when both open and closed channels exist. If a system of one closed channel is considered for simplicity, the modulus of S^{cc} is smaller than unity and cannot be expressed as $\exp(-2i\delta^c)$. To account for the leakage into open channels, let us use a complex phase shift $\Delta^c = \delta^c - i\gamma^c$ to represent S^{cc} as $S^{cc} = e^{-2i\Delta^c} = e^{-2i\delta^c} e^{-2\gamma^c}$ where $|S^{cc}| = \exp(-2\gamma^c)$. One of the merits of using complex phase shifts can be seen in the transformation of κ^{cc} under phase renormalization. Note that with a complex phase shift, κ^{cc} can be represented as $\kappa^{cc} = \tan\Delta^c = \tan(\delta^c - i\gamma^c)$ Its transformation under phase renormalization of $\beta' = \beta + \pi\mu^c$ is simply a linear transformation of the phase shifts given by $\kappa'^{cc} = \tan\Delta'^c = \tan(\Delta^c - \pi\mu^c)$. Using the angle sum and difference relationships of trigonometry, $\tan(\Delta^c - \pi\mu^c)$ can be expressed in terms of $\tan\Delta^c$ and the relationship between $\kappa^{cc\prime}$ and κ^{cc},

$$\kappa'^{cc} = (\kappa^{cc}\cos\pi\mu^c - \sin\pi\mu^c)\,(\kappa^{cc}\sin\pi\mu^c + \cos\pi\mu^c)^{-1}, \tag{A1}$$

can be obtained easily. Note that the usual phase renormalizations were performed only for real phase shifts without touching the imaginary ones.

As another application, consider Eq. (22) with the tilde representation as the primed one. Since $\tilde{\Delta}^c = -i\gamma^c$, $\tilde{\kappa}^{cc} = \tan\tilde{\Delta}^c$ equals $-i$ than γ^c. For $\cos\tilde{\Delta}^c$, $\cos\tilde{\Delta}^c = \cosh\gamma^c$ so that $\cos\tilde{\Delta}^c = \cos\tilde{\Delta}^{c\,*}$. From this, $\exp(i\pi\mu_r)$ is simply proportional to $\cos\tilde{\Delta}^{c\,*}$. Then, $\tan\pi\mu_r = -\tan\delta^c$ than γ^c or

$$\tan\pi\mu_r = -\tilde{\xi}^2\tan\delta^c \tag{A2}$$

can be obtained easily using the angle sum and difference relationships of trigonometry for $\cos(\delta^c - i\gamma^c)$.

References

1. Seaton, M. J. *Rep. Prog. Phys.* **1983**, *46*, 167; Fano, U.; Rau, A. R. P. *Atomic Collisions and Spectra*; Academic: Orlando, U.S.A., 1986; Baig, M. A. *Phys. Rev.* **2009**, *A79*, 012509.
2. Giusti-Suzor, A.; Fano, U. *J. Phys.* **1984**, *B17*, 215.
3. Dubau, J.; Seaton, M. J. J. Phys. 1984, *B17*, 381.
4. Eissner, W.; Seaton, M. J. *J. Phys.* **1969**, *B2*, 341.
5. Lecomte, J. M. *J. Phys.* **1987**, *B20*, 3645.
6. Cooke, W. E.; Cromer, C. L. *Phys. Rev.* **1985**, *A32*, 2725; Ueda, K. *Phys. Rev.* **1987**, A35, 2484; Giusti-Suzor, A.; Lefebvre-Brion, H. *Phys. Rev.* **1984**, *A30*, 3057; Wintgen, D.; Friedrich, H. *Phys. Rev.* **1987**, *A35*, 1628; Cohen, S. *Eur. Phys. J.* **1998**, *D4*, 31.
7. Lee, C.-W. *Phys. Rev.* **2002**, *A66*, 052704.
8. Lee, C.-W. *Bull. Korean Chem. Soc.* **2002**, *23*, 971; Lee, C.-W.; Kim, J.-H. *Bull. Korean Chem. Soc.* **2002**, *23*, 1560 ; Lee, C.-W. *Physics Essays* **2000**, *13*, 206.
9. Giusti-Suzor, A.; Fano, U. *J. Phys.* **1984**, *B17*, 215.
10. Herzberg, G.; Jungen, Ch. *J. Molec. Spectrosc.* **1972**, *41*, 425.
11. Greene, C. H.; Rau, A. R. P.; Fano, U. *Phys. Rev.* **1982**, *A26*, 2441.
12. Taylor, J. R. *Scattering Theory*; John Wiley and Sons: New York, U.S.A., 1972; p 411.