

Machine learning method for predicting line-shapes of Fano resonances induced by bound states in the continuum

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1 S -matrix reduction

We start by rewriting Eq. (3) for the 4×4 S -matrix

$$\hat{S}_4 = \begin{pmatrix} 0 & \hat{S}_2 \\ \hat{S}_2^\dagger & 0 \end{pmatrix} \quad (1)$$

The symmetry operation of the group C_2^z has a matrix representation

$$\hat{P} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \quad (2)$$

in the space of the incident/outgoing amplitude vectors. Now assuming that the channel functions are defined to be symmetric with respect to the mirror operation Eq. (2) one can state

$$\hat{S}_4 = \hat{P}^{-1} \hat{S}_4 \hat{P}. \quad (3)$$

After substituting Eq. (1) to Eq. (3) one finds

$$\hat{S}_2 = \hat{S}_2^\dagger. \quad (4)$$

2 Derivation of Eq. (6)

The first line in Eq. (6) can be proven by the same method as suggested in¹. First of all, we assume that the resonant eigenmode is normalized to carry a unit energy whereas the scattering carry a unit a energy per unit of time across the interface between the far-field and the scattering domain. Thus, the absence of incidence wave the energy conservation leads to

$$\frac{dE}{dt} = \frac{d|a|^2}{dt} = \mathbf{d}^\dagger \mathbf{d} |a|^2 \quad (5)$$

with E being the energy stored in the resonant mode. Given that the solution of the first line in Eq. (5) is

$$a(t) = a_0 e^{-(i\omega_0 + \gamma)t} \quad (6)$$

we immediately have

$$\mathbf{d}^\dagger \mathbf{d} = 2\gamma. \quad (7)$$

The derivation of the other relationships in Eq. (6) is more complicated. We start from the time-harmonic substitution in Eq. (5) which leads to the time-stationary TCMT equations in the following form

$$\begin{aligned} [i(\omega_0 - \omega) + \gamma]a &= \kappa^\top \mathbf{s}^{(+)}, \\ \mathbf{s}^{(-)} &= \hat{C}\mathbf{s}^{(+)} + \mathbf{d}a. \end{aligned} \quad (8)$$

The solution of Eq.(8) can be written in the form of S -matrix

$$\hat{S}_2(\omega) = \hat{C} + \frac{\mathbf{d}\kappa^\top}{i(\omega_0 - \omega) + \gamma}. \quad (9)$$

We notice that since $\hat{S}_2(\infty) = \hat{C}$ the matrix $\hat{C}$ has the same symmetry and unitarity properties as $\hat{S}_2(\omega)$. After applying $\hat{S}_2^{-1} = \hat{S}_2^\dagger$ we find

$$\begin{aligned} \hat{C}^* \mathbf{d}\kappa^\top [-i(\omega_0 - \omega) + \gamma] + \kappa^* \mathbf{d}^\dagger \hat{C} [i(\omega_0 - \omega) + \gamma] \\ + 2\gamma \kappa^* \kappa^\top = 0. \end{aligned} \quad (10)$$

By considering ω -dependent terms one finds that

$$\kappa^* \mathbf{d}^\dagger \hat{C} = \hat{C}^* \mathbf{d}\kappa^\top. \quad (11)$$

Applying the above equation in Eq. (10) and examining the terms independent of ω we write

$$\hat{C}^* \mathbf{d}\kappa^\top = -\kappa^* \kappa^\top \quad (12)$$

Next, assuming that the coupling vector κ has at least one non-zero element we have

$$\hat{C}\mathbf{d}^* = -\kappa. \quad (13)$$

Let us now utilize the symmetry of the scattering matrix. After applying $\hat{S}_2 = \hat{S}_2^\top$ in Eq. (9) we immediately have

$$\mathbf{d}\kappa^\top = \kappa\mathbf{d}^\top. \quad (14)$$

Multiplying the above equation from the left by $\mathbf{d}^\dagger$ one obtains

$$\kappa = \frac{\mathbf{d}^\dagger \kappa}{2\gamma} \mathbf{d}. \quad (15)$$

Alternatively, by multiplying Eq. (14) from the left by $\kappa^\dagger$ one has

$$\mathbf{d} = \frac{\kappa^\dagger \mathbf{d}}{\kappa^\dagger \kappa} \kappa. \quad (16)$$

The latter two equations combined result in

$$2\gamma \kappa^\dagger \kappa = |\mathbf{d}^\dagger \kappa|^2 \quad (17)$$

Next, by multiplying Eq. (13) from the left by its Hermitian adjoint one obtains

$$2\gamma = \kappa^\dagger \kappa \quad (18)$$

After analysing Eq. (15), Eq. (17), and Eq. (18) one can write

$$\mathbf{d} = e^{i\eta} \kappa, \quad \eta \in [0, 2\pi). \quad (19)$$

Let us now give interpretation to the phase η . By recollecting that the resonant mode is normalized to carry a unit energy we immediately see that its normalization constant is defined up to an arbitrary phase factor. Thus, all the TCMT equations have to be invariant under the $U(1)$ transformation

$$a = e^{i\alpha} a' \quad (20)$$

By plugging the above into Eq. (8) we find that it remains invariant, i.e. the same for the primed quantities, if the coupling and decoupling vectors are transformed as follows

$$\begin{aligned}\mathbf{d} &= e^{-i\alpha} \mathbf{d}', \\ \kappa &= e^{+i\alpha} \kappa'.\end{aligned}\tag{21}$$

By choosing $\alpha = \eta/2$ one derives from Eq. (13) and Eq. (19)

$$\begin{aligned}\widehat{C}(\mathbf{d}')^* + \mathbf{d}' &= 0, \\ \kappa' &= \mathbf{d}'.\end{aligned}\tag{22}$$

This equations are identical to the last two lines in Eq. (6).

3 Decoupling vector

We start with the third line in Eq. (6) that reads

$$\widehat{C}\mathbf{d}^* = -\mathbf{d}.\tag{23}$$

Vector $\mathbf{d}$ is in general parameterized by four independent real numbers

$$\mathbf{d} = \begin{pmatrix} a_{(r)} + ia_{(i)} \\ b_{(r)} + ib_{(i)} \end{pmatrix}.\tag{24}$$

Substituting the above into Eq. (23) one obtains a set of linear homogeneous equations of rank two

$$\begin{pmatrix} 1+\rho & 0 & 0 & \tau \\ 0 & 1-\rho & \tau & 0 \\ 0 & \tau & 1+\rho & 0 \\ \tau & 0 & 0 & 1-\rho \end{pmatrix} \begin{pmatrix} a_{(r)} \\ a_{(i)} \\ b_{(r)} \\ b_{(i)} \end{pmatrix} = 0,\tag{25}$$

which has the general two-parametric solution

$$\mathbf{d} = \begin{pmatrix} \tau b_{(i)} - i(1+\rho)a_{(i)} \\ \tau a_{(i)} - i(1+\rho)b_{(i)} \end{pmatrix}.\tag{26}$$

By recollecting that according to Eq. (6) $2\gamma = \mathbf{d}^\dagger \mathbf{d}$ one can find

$$\gamma = (1+\rho)(a_{(i)}^2 + b_{(i)}^2).\tag{27}$$

After combining Eq. (26) with Eq. (27) one arrives at the general solution of the form

$$\mathbf{d} = \sqrt{\frac{\gamma}{(1+\rho)}} \begin{pmatrix} \tau \cos \alpha - i(1+\rho) \sin \alpha \\ \tau \sin \alpha - i(1+\rho) \cos \alpha \end{pmatrix}, \quad \alpha \in [-\pi/2, \pi/2],\tag{28}$$

where the range $[-\pi/2, \pi/2]$ is chosen since $\kappa = \mathbf{d}$ and, therefore, the sign of $\mathbf{d}$ is not important for the S -matrix Eq. (9).

References

1. Fan, S., Suh, W. & Joannopoulos, J. D. Temporal coupled-mode theory for the fano resonance in optical resonators. *J. Opt. Soc. Am. A* **20**, 569, DOI: [10.1364/josaa.20.000569](https://doi.org/10.1364/josaa.20.000569) (2003).