Electromagnetic theory of double Fano resonances in plasmonic nanostructures and metamaterials

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The *ab initio* electromagnetic theory of Fano resonances in resonant plasmonic nanostructures and metamaterials, developed by Gallinet and Martin [Phys. Rev. B 83 (2011) 235427], is generalized to the case of double Fano resonances. The system is considered in which two uncoupled non-radiative modes interfere with a broad radiative mode driven by incident electromagnetic radiation. Feshbach–Fano partitioning formalism is employed to recover formula for the double Fano resonance spectral line shape suggested by Fano phenomenologically in his original work, and derive the exact microscopic expressions for the parameters governing optical response of the system.

I. INTRODUCTION

Interference of a narrow discrete state with a broad continuum band of states produces a narrow asymmetric spectral line shape in the adsorption spectrum. This effect, explained by Ugo Fano [1] and now known as Fano resonance, has found numerous applications in photonics and nanotechnology [2–12].

A variety of theoretical and numerical methods are used to analyse Fano resonances in specific systems, including classical coupled oscillators model [13, 14], coupled-mode theory [15–18], Green's function formalism [19], various computational electromagnetics methods [20]. The classical description of the resonance profile $\sigma(\varepsilon)$ is provided by the famous formula derived by Fano [1]:

$$\sigma(\varepsilon) = \frac{(q+\varepsilon)^2}{1+\varepsilon^2}. \tag{1}$$

Here q is the phenomenological parameter (known as asymmetry parameter or Fano parameter) which describes the degree of asymmetry of the line shape, $\varepsilon = (E-E_0)/(\Gamma/2)$ is the normalized energy deviation from the resonance energy E_0, Γ is the resonance width. Fano formula, Eq. (1), can be applied to different types of optical spectra in different systems.

A photonic structure of Fano-resonant metamaterials possesses, in analogy with the original atomic system considered by Fano, a non-radiative (dark) mode with a weak coupling to the environment and a long lifetime, coupled to a broad radiative (bright) mode which is strongly coupled to incident electromagnetic radiation and has short lifetime [21]. Considering Fano resonances in plasmonic systems where a flat continuum of states is replaced with a broad plasmonic resonance, Giannini et al. [22] gained insight into the role of its width and the energy. Gallinet and Martin [23] employed *ab initio* electromagnetic approach to generalize Fano formula to the case of vectorial fields and lossy materials:

$$\sigma(\omega) = a\frac{(q+\kappa)^2+b}{1+\kappa^2}. \tag{2}$$

In this formula, the reduced frequency $\kappa = (\omega^2 - \omega_d^2 - \Delta\omega_d)/\Gamma$ is shifted with respect to the frequency of the non-radiative mode ω_d, and the values of the resonance width and shift, Γ and Δ, asymmetry parameter q, the non-resonance transfer amplitude a, and the screening parameter b, all depend on the degree of intrinsic material losses.

In the cases when more than one discrete state interfere with a broad background, multiple Fano resonances are possible. Such a case was considered, in particular, by Fano [1] to describe excitation spectra of Rydberg atoms. Mies [24] extended Fano theory to the case of many resonances interacting with many continua and inelastic couplings between continuum states. Several methods for realizing and controlling double Fano resonances have been recently reported [25–35].

The resonant frequencies of different discrete states are often well separated from each other. In such cases the spectra can be described using a superposition of individual Fano resonances [25]:

$$\sigma(\omega) \propto \sum_k \frac{(q_k+\varepsilon_k)^2}{1+\varepsilon_k^2} \tag{3}$$

with several asymmetry parameters q_k and reduced frequencies $\varepsilon_k = 2(\omega-\omega_k)/\Gamma_k$, where ω_k and Γ_k are the frequency and width of the kth resonance.

It is, however, possible that the distance between resonant frequencies of different discrete states is not large compared to their widths. Such cases can be realized and controlled by careful design of the geometry of the plasmonic structure [29, 36, 37] or by utilizing plasmon hybridization between sub-radiant modes [27, 38, 39]. In nearly-degenerate cases the spectra can no longer be accurately described using a superposition of individual Fano resonances [29, 37].

The way to describe multiple resonances was outlined by Fano in his original work [1]. In the case of two discrete states interfering with one continuum the spectrum can be represented in form [29, 40, 41]

$$\sigma(\omega) \propto \frac{\left(1+\frac{q_1}{\kappa_1}+\frac{q_2}{\kappa_2}\right)^2 + \left(\frac{b_1}{\kappa_1}+\frac{b_2}{\kappa_2}\right)^2}{1+\left(\frac{1}{\kappa_1}+\frac{1}{\kappa_2}\right)^2} \tag{4}$$

with two reduced shifted resonance frequencies, κ_1 and κ_2, and two asymmetry parameters, q_1 and q_2, each corresponding to one of the two discrete states, and two screening parameters, b_1 and b_2.

Dana and Bahabad [29] reported the results of numerical simulations which confirm validity of Eq. (4). Furthermore, the authors explore the differences between a single and a double Fano resonance. At that, they obtain the values of the parameters in Eq. (2) by least-squares optimization fitting to the data of the numerical simulations.

Although most studies on double Fano resonances in photonics have employed empirical interpretations using the approximated fitting formula (4) or numerical analysis, there are certain advantages in rigorous theoretical analysis compared to simplified analytical tools widely used in photonics, such as coupled mode theory [17, 18]. In the case of single Fano resonance, such analysis can reveal the role played by the electromagnetic modes and material losses in the system, provide physical insight into the parameters describing the spectra [23], enable description of the spectra without using any fitting parameters [22], and engineering of nanostructures and metamaterials in which Fano resonances play an important role [42].

The aim of this paper is to generalize the electromagnetic theory for Fano resonances in plasmonic nanostructures and metamaterials by Gallinet and Martin [23] to the case of double Fano resonances. We use Fano–Feshbach partitioning formalism to obtain the analog of formula (4) and derive expressions for the parameters it contains.

II. THEORY

In this section we derive the formula for the spectral line shape of double Fano resonance, Eq. (4), from the first principles. We consider scattering of electromagnetic radiation, described by frequency-dependent electric field $\mathbf{E} \equiv \mathbf{E}(\omega) = \mathbf{E}_0 e^{-i\omega t}$, on a dielectric or metallic object in a dispersive dielectric medium with relative dielectric permittivity $\epsilon(\mathbf{r}, \omega)$. Our derivation follows work by Gallinet and Martin [23] very closely. The main difference with Ref. [23] is that we assume there is not one but two non-radiative (dark) modes interacting with a radiative (bright) mode.

A. Wave equation

Maxwell's equations allow us to represent the wave equation for the vectorial wave function $|\mathbf{E}\rangle$ in form

$$\left(\mathbb{M}_\omega - \omega^2 \mathbb{I}\right) |\mathbf{E}\rangle = 0 \tag{5}$$

with the frequency-dependent differential operator

$$\mathbb{M}_\omega \equiv \frac{c^2}{\epsilon(\mathbf{r}, \omega)} \nabla \times \nabla \times \tag{6}$$

and the identity operator $\mathbb{I}$.

B. Solution of wave equation

In order to facilitate solution of the wave equation, we employ Feshbach–Fano partitioning formalism [43–45] and introduce two complementary projection operators, P and Q, which divide the wave function $|\mathbf{E}\rangle$ into a bright and a dark parts:

$$|\mathbf{E}\rangle = P\,|\mathbf{E}\rangle + Q\,|\mathbf{E}\rangle\,. \tag{7}$$

The projection operators are idempotent, i.e. they satisfy $P^2 = P$ and $Q^2 = Q$. Substituting decomposition (7) in the wave equation (5), and applying the projection operators, we obtain two coupled equations for $P\,|\mathbf{E}\rangle$ and $Q\,|\mathbf{E}\rangle$:

$$\left(P\mathbb{M}_\omega P - \omega^2 \mathbb{I}\right) P\,|\mathbf{E}\rangle = -P\mathbb{M}_\omega Q\,|\mathbf{E}\rangle\,, \tag{8}$$

$$\left(Q\mathbb{M}_\omega Q - \omega^2 \mathbb{I}\right) Q\,|\mathbf{E}\rangle = -Q\mathbb{M}_\omega P\,|\mathbf{E}\rangle\,. \tag{9}$$

We study the system in the frequency range which covers resonance frequencies of two dark modes. In this frequency range these two modes form a complete set, hence we can decompose the projection operator Q as

$$Q = \sum_{k=1}^{2} |\mathbf{E}_{d_k}\rangle \langle \mathbf{E}_{d_k}| \equiv Q_1 + Q_2, \tag{10}$$

where $|\mathbf{E}_{d_k}\rangle$ are the eigenfunctions of Q, defined by

$$Q\,|\mathbf{E}_{d_k}\rangle = |\mathbf{E}_{d_k}\rangle\,, \tag{11}$$

satisfying the equations

$$Q\mathbb{M}_{\omega_k} Q\,|\mathbf{E}_{d_k}\rangle = z_k^2\,|\mathbf{E}_{d_k}\rangle\,, \tag{12}$$

and normalised as

$$|\langle \mathbf{E}_{d_k} | \mathbf{E}_{d_k}\rangle| = 1 \tag{13}$$

with the inner product is defined by

$$\langle \mathbf{E}_1 | \mathbf{E}_2 \rangle = \int \mathbf{E}_1^*(\mathbf{r}) \cdot \mathbf{E}_2(\mathbf{r})\, d^3\mathbf{r}. \tag{14}$$

The quantities $z_k = \omega_k + i\gamma_k$ are generally complex, with ω_k and γ_k being the resonance frequency and intrinsic damping of the kth mode, respectively.

We use operators Q_k defined by Eq. (10) to project Eq. (9) in the subspaces corresponding to each dark mode:

$$Q_1\,|\mathbf{E}\rangle = \frac{1}{\omega^2 - z_1^2}\,|\mathbf{E}_{d_1}\rangle \langle \mathbf{E}_{d_1}|\,\mathbb{M}_\omega P\,|\mathbf{E}\rangle\,, \tag{15}$$

$$Q_2\,|\mathbf{E}\rangle = \frac{1}{\omega^2 - z_2^2}\,|\mathbf{E}_{d_2}\rangle \langle \mathbf{E}_{d_2}|\,\mathbb{M}_\omega P\,|\mathbf{E}\rangle\,. \tag{16}$$

Inserting these equations in the decomposition given by Eq. (10), and then in Eq. (8) yields the equation for

$P\left|\mathbf{E}\right\rangle$:

$$\begin{aligned}\left(P\mathbb{M}_\omega P-\omega^2\mathbb{I}\right)P\left|\mathbf{E}\right\rangle &= \\ &= \frac{1}{z_1^2-\omega^2}P\mathbb{M}_\omega\left|\mathbf{E}_{d_1}\right\rangle\left\langle\mathbf{E}_{d_1}\right|\mathbb{M}_\omega P\left|\mathbf{E}\right\rangle \\ &+ \frac{1}{z_2^2-\omega^2}P\mathbb{M}_\omega\left|\mathbf{E}_{d_2}\right\rangle\left\langle\mathbf{E}_{d_2}\right|\mathbb{M}_\omega P\left|\mathbf{E}\right\rangle. \end{aligned} \quad (17)$$

We define the bright wave function $\left|P\mathbf{E}_b\right\rangle$ to satisfy Eq. (17) with both dark modes $\left|\mathbf{E}_{d_k}\right\rangle$ removed:

$$\left(P\mathbb{M}_\omega P-\omega^2\right)\left|P\mathbf{E}_b\right\rangle = 0. \quad (18)$$

Double Fano resonance for the total wave function $\left|\mathbf{E}\right\rangle$ results from interference between the bright mode $\left|P\mathbf{E}_b\right\rangle$ and two dark modes $\left|\mathbf{E}_{d_k}\right\rangle$.

In order to solve equation (17) for $P\left|\mathbf{E}\right\rangle$, we introduce the dyadic Green's function $\mathbb{G}_b$ of Eq. (18), which satisfies the equation

$$\left(P\mathbb{M}_\omega P-\omega^2\right)\mathbb{G}_b = \mathbb{I}. \quad (19)$$

For self-adjoint operator $P\mathbb{M}_\omega$, the set of solutions $\left|P\mathbf{E}_b\right\rangle$ of Eq. (18) can be selected which forms an orthogonal basis of modes. Expanding $\mathbb{G}_b$ in this basis as

$$\mathbb{G}_b = \frac{1}{\pi}\mathcal{P}\int\frac{\left|P\mathbf{E}_b(\omega')\right\rangle\left\langle P\mathbf{E}_b(\omega')\right|}{\omega'^2-\omega^2}d\omega', \quad (20)$$

where $\mathcal{P}$ denotes the Cauchy principal value of the integral, we can write the solution to equation (17) as

$$\begin{aligned}P\left|\tilde{\mathbf{E}}\right\rangle = P\left|\mathbf{E}_b\right\rangle &+ \frac{\langle\mathbf{E}_{d_1}|\mathbb{M}_\omega P|\tilde{\mathbf{E}}\rangle}{z_1^2-\omega^2}\mathbb{G}_b P\mathbb{M}_\omega\left|\mathbf{E}_{d_1}\right\rangle \\ &+ \frac{\langle\mathbf{E}_{d_2}|\mathbb{M}_\omega P|\tilde{\mathbf{E}}\rangle}{z_2^2-\omega^2}\mathbb{G}_b P\mathbb{M}_\omega\left|\mathbf{E}_{d_2}\right\rangle. \end{aligned} \quad (21)$$

Multiplication of Eq. (21) on the left by $\left\langle\mathbf{E}_{d_1}\right|\mathbb{M}_\omega$ and $\left\langle\mathbf{E}_{d_2}\right|\mathbb{M}_\omega$ results in the system of two linear equations for $\langle\mathbf{E}_{d_1}|\mathbb{M}_\omega P|\tilde{\mathbf{E}}\rangle$ and $\langle\mathbf{E}_{d_2}|\mathbb{M}_\omega P|\tilde{\mathbf{E}}\rangle$. Substituting the solutions to these equations back in Eq. (21), we obtain

$$P\left|\tilde{\mathbf{E}}\right\rangle = P\left|\mathbf{E}_b\right\rangle + K_1\mathbb{G}_b P\mathbb{M}_\omega\left|\mathbf{E}_{d_1}\right\rangle + K_2\mathbb{G}_b P\mathbb{M}_\omega\left|\mathbf{E}_{d_2}\right\rangle, \quad (22)$$

where

$$\begin{aligned}K_1 = \frac{1}{L}&\left[\langle\mathbf{E}_{d_1}|\mathbb{M}_\omega|P\mathbf{E}_b\rangle\left(z_2^2-\omega^2+\omega_2\Delta_2\right)\right. \\ &\left.+\langle\mathbf{E}_{d_2}|\mathbb{M}_\omega|P\mathbf{E}_b\rangle\langle\mathbf{E}_{d_1}|\mathbb{M}_\omega\mathbb{G}_b P\mathbb{M}_\omega|\mathbf{E}_{d_2}\rangle\right], \end{aligned} \quad (23)$$

$$\begin{aligned}K_2 = \frac{1}{L}&\left[\langle\mathbf{E}_{d_2}|\mathbb{M}_\omega|P\mathbf{E}_b\rangle\left(z_1^2-\omega^2+\omega_1\Delta_1\right)\right. \\ &\left.+\langle\mathbf{E}_{d_1}|\mathbb{M}_\omega|P\mathbf{E}_b\rangle\langle\mathbf{E}_{d_2}|\mathbb{M}_\omega\mathbb{G}_b P\mathbb{M}_\omega|\mathbf{E}_{d_1}\rangle\right], \end{aligned} \quad (24)$$

$$\begin{aligned}L = &\left(z_1^2-\omega^2+\omega_1\Delta_1\right)\left(z_2^2-\omega^2+\omega_2\Delta_2\right) \\ &-\langle\mathbf{E}_{d_1}|\mathbb{M}_\omega\mathbb{G}_b P\mathbb{M}_\omega|\mathbf{E}_{d_2}\rangle\langle\mathbf{E}_{d_2}|\mathbb{M}_\omega\mathbb{G}_b P\mathbb{M}_\omega|\mathbf{E}_{d_1}\rangle, \end{aligned} \quad (25)$$

and the quantities

$$\Delta_k = -\frac{1}{\omega_k}\left\langle\mathbf{E}_{d_k}\right|\mathbb{M}_\omega P\mathbb{G}_b P\mathbb{M}_\omega\left|\mathbf{E}_{d_k}\right\rangle. \quad (26)$$

would in absence of cross-terms (see Eq. (34)) be the shifts in the resonance positions ω_k due to the field overlap between the continuum $\left|P\mathbf{E}_b\right\rangle$ and $\left|\mathbf{E}_{d_k}\right\rangle$. With help of formulas for the projection operators, Eqs (10), (15), (16) and (22), we obtain the expression for $|\tilde{\mathbf{E}}\rangle$:

$$\begin{aligned}|\tilde{\mathbf{E}}\rangle = \left|P\mathbf{E}_b\right\rangle &+ K_1\left(\mathbb{G}_b P\mathbb{M}_\omega\left|\mathbf{E}_{d_1}\right\rangle - \left|\mathbf{E}_{d_1}\right\rangle\right) \\ &+ K_2\left(\mathbb{G}_b P\mathbb{M}_\omega\left|\mathbf{E}_{d_2}\right\rangle - \left|\mathbf{E}_{d_2}\right\rangle\right). \end{aligned} \quad (27)$$

The wave function $\left|\mathbf{E}\right\rangle$ can be related to $|\tilde{\mathbf{E}}\rangle$ by requiring correct asymptotic behavior in far field. This relation is given in the following section by Eq. (38).

C. Optical response

The optical response of the system to an external excitation is described by the transition operator T between an initial excited state $|g\rangle$ and a final state $|\tilde{\mathbf{E}}\rangle$. It can be represented as a ratio of the transition probability $\left|\langle g|T|\mathbf{E}\rangle\right|^2$ to the probability $\left|\langle g|T|P\mathbf{E}_b\rangle\right|^2$ of transition to the continuum state:

$$\sigma = \frac{\left|\langle g|T|\mathbf{E}\rangle\right|^2}{\left|\langle g|T|P\mathbf{E}_b\rangle\right|^2}. \quad (28)$$

In order to derive the explicit formula for σ, we start with writing the ratio of the matrix elements corresponding to the field $|\tilde{\mathbf{E}}\rangle$, given by Eq. (27), and to the continuum, $\left|P\mathbf{E}_b\right\rangle$, as

$$\begin{aligned}\frac{\langle g|T|\tilde{\mathbf{E}}\rangle}{\langle g|T|P\mathbf{E}_b\rangle} = 1 &- K_1\frac{\langle g|T|\mathbf{E}_{d_1}\rangle - \langle g|T\mathbb{G}_b P\mathbb{M}_\omega|\mathbf{E}_{d_1}\rangle}{\langle g|T|P\mathbf{E}_b\rangle} \\ &- K_2\frac{\langle g|T|\mathbf{E}_{d_2}\rangle - \langle g|T\mathbb{G}_b P\mathbb{M}_\omega|\mathbf{E}_{d_2}\rangle}{\langle g|T|P\mathbf{E}_b\rangle}, \end{aligned} \quad (29)$$

or, equivalently,

$$\begin{aligned}\frac{\langle g|T|\tilde{\mathbf{E}}\rangle}{\langle g|T|P\mathbf{E}_b\rangle} = 1 &- \frac{\left|\langle\mathbf{E}_{d_1}|\mathbb{M}_\omega|P\mathbf{E}_b\rangle\right|^2}{2\omega\left(z_1^2-\omega^2+\omega_1\Delta_1\right)}q_1 \\ &- \frac{\left|\langle\mathbf{E}_{d_2}|\mathbb{M}_\omega|P\mathbf{E}_b\rangle\right|^2}{2\omega\left(z_2^2-\omega^2+\omega_2\Delta_2\right)}q_2 \\ &- \frac{\langle\mathbf{E}_{d_2}|\mathbb{M}_\omega|P\mathbf{E}_b\rangle\langle\mathbf{E}_{d_1}|\mathbb{M}_\omega\mathbb{G}_b P\mathbb{M}_\omega|\mathbf{E}_{d_2}\rangle}{L} \\ &\times\frac{\langle g|T|\mathbf{E}_{d_1}\rangle - \langle g|T\mathbb{G}_b P\mathbb{M}_\omega|\mathbf{E}_{d_1}\rangle}{\langle g|T|P\mathbf{E}_b\rangle} \\ &- \frac{\langle\mathbf{E}_{d_1}|\mathbb{M}_\omega|P\mathbf{E}_b\rangle\langle\mathbf{E}_{d_2}|\mathbb{M}_\omega\mathbb{G}_b P\mathbb{M}_\omega|\mathbf{E}_{d_1}\rangle}{L} \\ &\times\frac{\langle g|T|\mathbf{E}_{d_2}\rangle - \langle g|T\mathbb{G}_b P\mathbb{M}_\omega|\mathbf{E}_{d_2}\rangle}{\langle g|T|P\mathbf{E}_b\rangle} \end{aligned} \quad (30)$$

with the dimensionless intrinsic damping parameters

$$\Lambda_k = \frac{|\langle \mathbf{E}_{d_k}|\mathbb{M}_\omega|P\mathbf{E}_b\rangle|^2 \lambda_k}{2\omega_k(\omega_k^2 - \omega^2 + \omega_k\Delta_k)^2}, \tag{31}$$

where

$$\lambda_k = 2\omega_k\gamma_k. \tag{32}$$

The quantities q_k, given by the ratios between the matrix elements corresponding to the respective perturbed dark modes and the continuum, have form

$$q_k = \frac{2\omega}{(\langle \mathbf{E}_{d_k}|\mathbb{M}_\omega|P\mathbf{E}_b\rangle)^*}\times \tag{33}$$
$$\times \frac{\langle g|T|\mathbf{E}_{d_k}\rangle - \langle g|T\mathbb{G}_b P\mathbb{M}_\omega|\mathbf{E}_{d_k}\rangle}{\langle g|T|P\mathbf{E}_b\rangle + \frac{\langle \mathbf{E}_{d_1}|\mathbb{M}_\omega\mathbb{G}_b P\mathbb{M}_\omega|\mathbf{E}_{d_2}\rangle\langle \mathbf{E}_{d_2}|\mathbb{M}_\omega\mathbb{G}_b P\mathbb{M}_\omega|\mathbf{E}_{d_1}\rangle}{(z_1^2-\omega^2+\omega_1\Delta_1)(z_2^2-\omega^2+\omega_2\Delta_2)}}.$$

Since plasmon interactions between dark modes are seldom [27], we henceforth assume the dark modes to be uncoupled from each other in the sense that

$$\langle \mathbf{E}_{d_k}|\mathbb{M}_\omega\mathbb{G}_b P\mathbb{M}_\omega|\mathbf{E}_{d_l}\rangle = 0 \quad \text{for } k \neq l. \tag{34}$$

This reduces Eq. (30) to

$$\frac{\langle g|T|\tilde{\mathbf{E}}\rangle}{\langle g|T|P\mathbf{E}_b\rangle} = 1 - \frac{|\langle \mathbf{E}_{d_1}|\mathbb{M}_\omega|P\mathbf{E}_b\rangle|^2}{2\omega(z_1^2 - \omega^2 + \omega_1\Delta_1)} q_1 - \frac{|\langle \mathbf{E}_{d_2}|\mathbb{M}_\omega|P\mathbf{E}_b\rangle|^2}{2\omega(z_2^2 - \omega^2 + \omega_2\Delta_2)} q_2 \tag{35}$$

with

$$q_k = \frac{2\omega\left(\langle g|T|\mathbf{E}_{d_k}\rangle - \langle g|T\mathbb{G}_b P\mathbb{M}_\omega|\mathbf{E}_{d_k}\rangle\right)}{(\langle \mathbf{E}_{d_k}|\mathbb{M}_\omega|P\mathbf{E}_b\rangle)^* \langle g|T|P\mathbf{E}_b\rangle}. \tag{36}$$

Requirement for the wave function $|\mathbf{E}\rangle$ to have the same asymptotic behavior as $|\mathbf{E}_b\rangle$,

$$\lim_{r\to\infty} |P\,|\mathbf{E}\rangle|^2 = \lim_{r\to\infty} |P\,|\mathbf{E}_b\rangle|^2, \tag{37}$$

leads to the following relation between $|\mathbf{E}\rangle$ and the wave function $|\tilde{\mathbf{E}}\rangle$, given by equation (27):

$$|\mathbf{E}\rangle = \frac{1}{\sqrt{\alpha^2 + \beta^2}}\,|\tilde{\mathbf{E}}\rangle \tag{38}$$

with

$$\alpha = 1 + \frac{\Gamma_1\lambda_1}{\chi_1^2 + \lambda_1^2} + \frac{\Gamma_2\lambda_2}{\chi_2^2 + \lambda_2^2}, \tag{39}$$

$$\beta = \frac{\Gamma_1\chi_1}{\chi_1^2 + \lambda_1^2} + \frac{\Gamma_2\chi_2}{\chi_2^2 + \lambda_2^2}, \tag{40}$$

where

$$\Gamma_k = \frac{|\langle \mathbf{E}_{d_k}|\mathbb{M}_\omega|P\mathbf{E}_b\rangle|^2}{2\omega_k} \tag{41}$$

k	λ_k, THz^2	Γ_k, THz^2	q'_k	ω_k, THz	Δ_k, THz
1	55452	309	451158	2297	0.778
2	216955	1428	449113	2342	0.913

TABLE I. The parameters obtained by the least-squares optimization fitting of Eq. (43) to the numerical simulation data by Dana and Bahabad [29].

and

$$\chi_k = \omega^2 - \omega_k^2 - \omega_k\Delta_k. \tag{42}$$

Following Huang *et al.* [46], we assume that the asymmetry parameters q_k are real. With account of this, we can substitute Eqs (38), (39), (40) in Eq. (35) and use Eq. (28) to obtain formula

$$\sigma = \frac{1}{\Xi}\left[\left(1 + \frac{\Gamma_1\chi_1 q_1}{\chi_1^2 + \lambda_1^2} + \frac{\Gamma_2\chi_2 q_2}{\chi_2^2 + \lambda_2^2}\right)^2 + \left(\frac{\Gamma_1\lambda_1 q_1}{\chi_1^2 + \lambda_1^2} + \frac{\Gamma_2\lambda_2 q_2}{\chi_2^2 + \lambda_2^2}\right)^2\right], \tag{43}$$

where

$$\Xi = \frac{(\Gamma_1 + \lambda_1)^2}{\chi_1^2 + \lambda_1^2} + \frac{(\Gamma_2 + \lambda_2)^2}{\chi_2^2 + \lambda_2^2} + \frac{(\chi_1\chi_2 - \lambda_1\lambda_2 + 2\Gamma_1\Gamma_2)(\chi_1\chi_2 + \lambda_1\lambda_2)}{(\chi_1^2 + \lambda_1^2)\,(\chi_2^2 + \lambda_2^2)}. \tag{44}$$

The parameters in Eq (43), which determine the resonance shape, depend on the physical nature of the transition described by the operator T.

D. Resonance parameters

The formula for the optical response of the system to an external excitation, Eq (43) can be represented in the classical form, Eq. (4). However, in this case the parameters which enter Eq. (4) would be frequency-dependent, and hence the resonance profile given by Eq (43) would differ from that given by Eq. (4). This difference is illustrated in Figure 1, where the transmission profile in a plasmonic double grating structure, obtained by numerical simulation by Dana and Bahabad [29] is fitted by both Eq. (43) and Eq. (4).

In principle, it is possible to calculate the parameters in Eq. (43) using various model approaches. For example, Gallinet and Martin [42] derive closed–form expressions for the parameters of the formula for single Fano resonance in the particular case when the bright mode is assumed to generate a continuum of radiative waves $|P\mathbf{E}_b\rangle$ with the Lorentzian distribution

$$|P\mathbf{E}_b(\omega)\rangle = \frac{\Gamma_b\,|P\mathbf{E}_b(\omega_b)\rangle}{\omega^2 - \omega_b^2 + i\Gamma_b}, \tag{45}$$

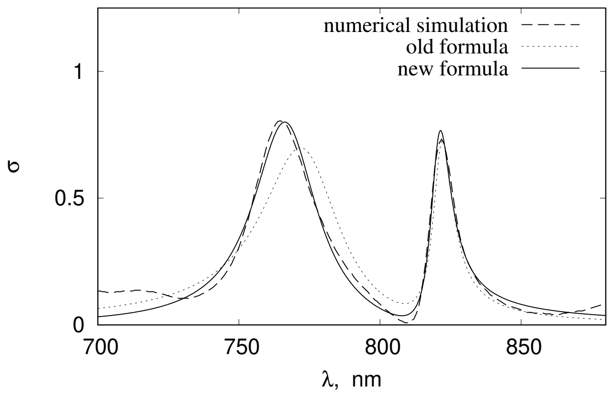

FIG. 1. The results of the numerical simulation of the transmission profile in a plasmonic double grating structure, presented by Dana and Bahabad [29] (the dashed line) fitted by Eq. (43) (the continuous line, the parameters are listed in Table I). The dotted line represents the best-fit line shape obtained by Dana and Bahabad [29] using Eq. (4).

where ω_b is the frequency of highest amplitude and Γ_b the width of the distribution. In the case of double Fano resonance, the derivation is applicable to each dark mode separately. As a result, the parameters in Eq. (43) are given by formulas

$$q_k = \frac{\omega_k^2 - \omega_b^2}{\Gamma_b}, \tag{46}$$

$$\Delta_k = \frac{c_k^2(\omega_k^2 - \omega_b^2)\Gamma_b}{2\omega_k^2\left[(\omega_k^2 - \omega_b^2)^2 + \Gamma_b^2\right]}, \tag{47}$$

$$\Lambda_k = \frac{4\gamma_k\left[(\omega_k^2 - \omega_b^2)^2 + \Gamma_b^2\right]\omega_k^2}{c_k^2(\omega_k^2 - \omega_b^2)^2}, \tag{48}$$

$$\Gamma_k = \frac{c_k^2\Gamma_b^2}{2\omega_k\left[(\omega_k^2 - \omega_b^2)^2 + \Gamma_b^2\right](1 - \Lambda_k)}, \tag{49}$$

where

$$c_k = |\langle P\mathbf{E}_b(\omega_b)|\mathbb{M}_\omega|\mathbf{E}_k\rangle| \tag{50}$$

are the coupling strengths between the bright mode and the kth dark mode.

III. CONCLUSION

We have generalized the electromagnetic theory for Fano resonances in plasmonic nanostructures and metamaterials by Gallinet and Martin [23] to the case of double Fano resonances. Using Fano–Feshbach partitioning formalism, we have obtained the formula, Eq. (43), for the spectral line shape of the system in which two uncoupled non-radiative modes interfere with a broad radiative mode, and derived expressions for the parameters in terms of the transition operator which describes the optical response of the system. The more accurate fit of the numerical simulation data by Dana and Bahabad [29], presented in Figure 1, illustrates that the result in Eq. (43) can go beyond the double Fano result known in the literature and be applied to the realistic systems with material losses not necessarily small. In principle, our approach can be used to further generalize the theory to include more than two resonances.

The results of this work, aimed at facilitating control of double Fano resonances, can potentially be useful for design of plasmonic nanostructures and metamaterials with the desired properties.

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