Analytical Description of Fano Resonances in Plasmonic Nanostructures

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Abstract. We report on the derivation of analytical formulas for the lineshape of Fano resonances in plasmonic nanostructures as a function of their electromagnetic response. Contrary to the original work of Fano, the formalism proposed here includes losses in the materials composing the system. As a result, a more general formula is obtained for the response of the system and general conclusions for the determination of the resonance parameters are drawn, in particular on its width and asymmetry. The insights into the physical understanding of Fano resonances gained this way will be of great interest for the design of plasmonic sensing platforms and metamaterials.

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Asymmetric resonances display unique features, compared to their symmetric Lorentzian counterpart, and are currently the subject of considerable research efforts in photonic and plasmonic nanostructures. Fano resonances exhibit a very strong sensitivity to changes of the local environment as well as a sharp spectral dispersion [1, 2]. In plasmonics, they arise when a non-radiative (dark) mode interacts with a radiative (bright) mode. The control of their lineshape for each specific application remains a challenging task, and requires a theory to understand the underlying physical mechanisms. Numerical and experimental data are usually fitted and analyzed with the two coupled mechanical oscillators[3] or other intuitive phenomenological models[4]. As result, it is for example not well understood in a realistic plasmonic system composed of several interacting particles how the individual modes and their coupling affect the overall Fano–like resonance of the system. The quantum mechanical theory developed by Fano to explain autoionization of atoms provides a wave–like interpretation of asymmetric resonances[5], which can be adapted to a Lorentzian distribution of the continuum[6]. However, this approach cannot take into account intrinsic losses in the metallic structures that are characteristic of plasmonic structures.

In this work, we report on the derivation of an analytical theory of Fano resonances in plasmonic nanostructures from Maxwell's equations [7], and provide closed–form expressions for the resonance parameters. We finally numerically validate the analytical theory for dolmen and heptamers nanostructures supporting Fano resonances, which are currently under extensive investigation in the plasmonic and metamaterial communities [2].

The main results of the electromagnetic theory of Fano resonances are first summarized [7]. We consider electromagnetic scattering on a dielectric or metallic object in a dielectric background. The scatterer supports a non-radiative (dark) mode interacting with a continuum of radiative (bright) waves. A harmonic time-dependence for the fields $\mathbf{E} = \mathbf{E}_0 e^{-i\omega t}$ is assumed throughout. The relative dielectric permittivity $\varepsilon(\mathbf{r},\omega)$ is generally complex and has frequency dispersion. The frequency dependent electric field $\mathbf{E}$ satisfies the wave equation

$$\varepsilon^{-1}(\mathbf{r},\omega)\nabla\times\nabla\times\mathbf{E}(\mathbf{r},\omega) - \frac{\omega^2}{c^2}\mathbf{E}(\mathbf{r},\omega) = 0\,. \qquad (1)$$

To simplify notation, in the following the dependence of the electric field $\mathbf{E}$ on ω is kept implicit. Let us assume that the scatterer permittivity is given by a Drude model with plasma frequency ω_p; the scaling law of Maxwell's equations allows then to scale all frequency units by ω_p and length units by $2\pi c/\omega_p$. We introduce the generally complex and frequency dependent differential operator $\underline{\underline{\mathscr{M}}}_\omega$ defined by

$$\underline{\underline{\mathscr{M}}}_\omega\mathbf{E}(\mathbf{r}) = \frac{c^2}{\varepsilon(\mathbf{r},\omega)}\nabla\times\nabla\times\mathbf{E}(\mathbf{r})\,. \qquad (2)$$

The wave equation can be written for a vectorial wave function $|\mathbf{E}\rangle$

$$(\underline{\underline{\mathscr{M}}}_\omega - \omega^2\underline{\underline{I}})|\mathbf{E}\rangle = 0\,, \qquad (3)$$

where $\underline{\underline{I}}$ is the identity operator. The inner product is defined by

$$\langle\mathbf{E}_1|\mathbf{E}_2\rangle = \int \mathbf{E}_1^*(\mathbf{r})\cdot\mathbf{E}_2(\mathbf{r})d^3\mathbf{r}\,. \qquad (4)$$

Following Feshbach, Bhatia and Temkin, we introduce the orthogonal projection operators P and Q splitting

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the wave function into a radiative (bright) and a non-radiative (dark) part [8]. Any wave function $|\mathbf{E}\rangle$ can be decomposed as $|\mathbf{E}\rangle = Q|\mathbf{E}\rangle + P|\mathbf{E}\rangle$ where only $P|\mathbf{E}\rangle$ satisfies the radiation condition. Equation (3) becomes

$$(\underline{\underline{\mathscr{M}}}_{\omega} - \omega^2 \underline{\underline{I}})(Q|\mathbf{E}\rangle + P|\mathbf{E}\rangle) = 0\,. \tag{5}$$

We consider a unique non-radiative mode $|\mathbf{E}_d\rangle$, defined to be eigenfunction of the projector to non-radiative modes $Q|\mathbf{E}_d\rangle = |\mathbf{E}_d\rangle$, and to satisfy $Q\underline{\underline{\mathscr{M}}}_{\omega_d} Q|\mathbf{E}_d\rangle = z_d^2|\mathbf{E}_d\rangle$ and $|\langle \mathbf{E}_d|\mathbf{E}_d\rangle|^2 = 1$. Taking material losses into account, the quantity $z_d = \omega_d + i\gamma_d$ is generally complex. Its real part ω_d is the mode resonance frequency, and γ_d its intrinsic damping. The radiative (bright) wavefunction $|P\mathbf{E}_b\rangle$ is defined to satisfy the following homogeneous wave equation in the radiative region:

$$(P\underline{\underline{\mathscr{M}}}_{\omega} P - \omega^2 \underline{\underline{I}})|P\mathbf{E}_b\rangle = 0\,. \tag{6}$$

Let us define the shift from the dark mode's resonance position ω_d:

$$\Delta = -\langle \mathbf{E}_d|\underline{\underline{\mathscr{M}}}_{\omega} P \underline{\underline{G}}_b P \underline{\underline{\mathscr{M}}}_{\omega}|\mathbf{E}_d\rangle/\omega_d\,, \tag{7}$$

the intrinsic damping parameter:

$$\Gamma_i = \frac{|\langle \mathbf{E}_d|\underline{\underline{\mathscr{M}}}_{\omega}|P\mathbf{E}_b\rangle|^2 \gamma_d \omega_d}{\omega(\omega_d^2 - \omega^2 + \omega_d\Delta)^2}\,, \tag{8}$$

the resonance width:

$$\Gamma = \frac{|\langle \mathbf{E}_d|\underline{\underline{\mathscr{M}}}_{\omega}|P\mathbf{E}_b\rangle|^2}{2\omega(1-\Gamma_i)}\,, \tag{9}$$

and the reduced frequency:

$$\kappa = (\omega^2 - \omega_d^2 - \omega_d\Delta)/\Gamma\,. \tag{10}$$

The system is studied in the vicinity of the resonance frequency ω_d. Most plasmonic nanostructures and metamaterials are embedded in a dielectric medium, allowing us to assume that the permittivity is real and non dispersive in the radiative region. Considering these assumptions, the ratio σ/σ_b of the optical response of the total field $|\mathbf{E}\rangle$ to the one of the continuum $|P\mathbf{E}_b\rangle$ satisfies:

$$\frac{\sigma}{\sigma_b} = \frac{(\kappa+q)^2 + b}{\kappa^2 + 1}\,. \tag{11}$$

The parameter q is given by the ratio between the optical response of the perturbed non-radiative mode and the continuum and describes the degree of asymmetry of the resonance [5]. Equation (11) introduces a family of lineshapes as shown in Fig. 1, with an additional parameter b describing the screening of the resonance by intrinsic losses [7].

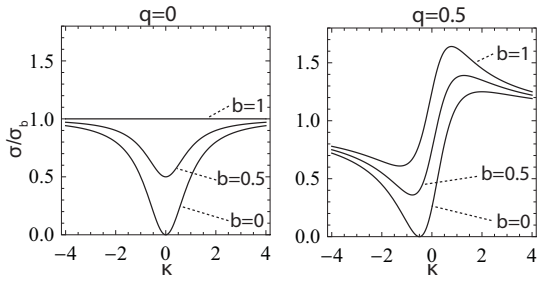

FIGURE 1. Resonance shape function σ/σ_b as a function of the reduced frequency $\kappa = (\omega^2 - \omega_d^2 - \omega_d\Delta)/\Gamma$ for different values of the asymmetry parameter q and the screening parameter b [Eq. (11)].

We now consider the particular case where the continuum of radiative waves $|P\mathbf{E}_b\rangle$ is generated from a bright plasmon mode satisfying a lorentzian resonance lineshape:

$$\sigma_b = \frac{A\Gamma_s^2}{(\omega^2 - \omega_s^2)^2 + \Gamma_s^2}\,, \tag{12}$$

where ω_s is the bright mode's frequency resonance and Γ_s its spectral width. In this case, each resonance parameter in Eq. (11) has a closed–form expression. It is assumed that all the parameters are independent of the frequency in a spectral region around the resonance, and can be evaluated at ω_d. The Fano resonance frequency shift from ω_d is given by:

$$\Delta = \frac{c^2(\omega_d^2 - \omega_s^2)\Gamma_s}{2\omega_d^2[(\omega_d^2 - \omega_s^2)^2 + \Gamma_s^2]}\,, \tag{13}$$

where $c = |\langle P\mathbf{E}_b(\omega_s)|\underline{\underline{\mathscr{M}}}|\mathbf{E}_d\rangle|$ is the coupling strength between the dark and bright modes. The sign of Δ is determined by the frequency difference between the two modes, and its magnitude linearly depends on the coupling strength, which is a signature of weak coupling. From Eqs. (8) and (13), the intrinsic damping parameter Γ_i becomes:

$$\Gamma_i = \frac{4\gamma_d[(\omega_d^2 - \omega_s^2)^2 + \Gamma_s^2]\omega_d^2}{c^2(\omega_d^2 - \omega_s^2)^2}\,. \tag{14}$$

The magnitude of Γ_i is driven by the ratio γ_d/c^2, meaning that the effect of intrinsic losses is critical if the coupling between the dark and bright modes is not sufficient. From Eq. (9), the resonance width becomes:

$$\Gamma = \frac{c^2\Gamma_s^2}{2\omega_d[(\omega_d^2 - \omega_s^2)^2 + \Gamma_s^2](1-\Gamma_i)}\,. \tag{15}$$

It is determined by the coupling strength between the modes and also affected by the intrinsic damping parameter Γ_i. The asymmetry parameter q depends on a

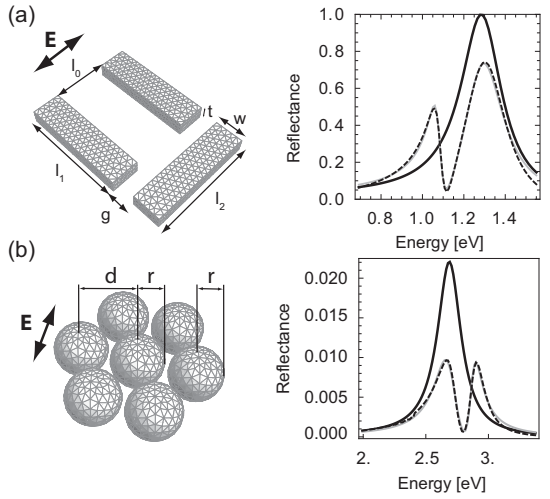

FIGURE 2. (a) Reflectance of gold dolmen nanostructures at normal illumination, arranged in a two–dimensional array of period 500 nm and placed in vacuum. The material is chosen to satisfy Drude model with plasma frequency $\omega_p = 1.37 \times 10^{16} \mathrm{s}^{-1}$ and damping γ. The structure dimensions are $w = 40$ nm, $l_0 = 160$ nm, $t = 80$ nm, $g = 30$ nm and $l_2 = 300$ nm. (b) Reflectance of silver plasmonic heptamers at normal illumination, arranged in a two–dimensional array of period 1400 nm and placed in vacuum. The structure dimensions are $r = 30$nm and $d = 65$nm. Experimental data for silver[9] has been taken for the particles material. In (a) and (b): black dashed–numerical simulations; gray–fit with Eq. (11); black–background resonance with parameters A, ω_s and Γ_s extracted from the fit.

transition element T, which we consider from now on to describe the reflectance of an array of nanostructures. In these conditions, the dark mode is characterized by $\langle g|T|\mathbf{E}_d\rangle = 0$ and the asymmetry parameter becomes:

$$q = (1-\Gamma_i)\frac{\omega_d^2 - \omega_s^2}{\Gamma_s}, \tag{16}$$

which is also a function of the frequency detuning between the two modes. In addition, the parameter Γ_i is responsible for damping in case of high losses or low coupling. Other components of intrinsic losses are described by the screening parameter b:

$$b = 4\frac{\gamma_d^2 q^2}{\Delta^2}. \tag{17}$$

The screening parameter is mainly influenced by the ratio γ_d^2/c^4. If the coupling between the two modes is too weak compared to intrinsic losses, the parameter b increases, which in turn screens the Fano resonance (Fig. 1).

In Fig. 2, the optical properties of dolmen and heptamer plasmonic nanostructures are numerically computed with a surface integral formulation [10, 11] and compared to the analytical formula (11). A perfect agreement is obtained, which shows that the lineshape of these nanostructures can be described by a set of four independant parameters (Δ, Γ, q and b). The control of the lineshape is made possible using the analytical expressions (13) to (17). They predict a behavior of the lineshape parameters that was verified in Ref. [7].

In summary, we have derived from Maxwell's equations an analytical expression for Fano resonances in plasmonic nanostructures and metamaterials using Feshbach formalism. This theory relies on the interference between a radiative (bright) mode and non-radiative (dark) mode established in the entire system. The analytical theory has been verified by fitting the analytical formula to numerical simulations in dolmen and heptamers nanostructures. The insights into the physical understanding of Fano resonances gained this way will be of great interest for the design of plasmonic sensing platforms and metamaterials.

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