Opt Quant Electron (2016) 48:83
DOI 10.1007/s11082-015-0358-0

Analysis of transition from Lorentz resonance to Fano resonance in plasmon and metamaterial systems

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Received: 2 September 2015 / Accepted: 8 October 2015 / Published online: 12 January 2016

Abstract Fano resonance, viewed as a quantum interference between continuum and discrete states, demonstrates an asymmetric spectral line shape. Fano resonance is also observed in metamaterials and plasmonic nanostructures and could be explained by the coupling of two classical Lorentz oscillators. A unambiguous connection between Fano resonance and Lorentz resonance plays a vital role in the design and optimization of metamaterials and plasmonic materials for both mechanism understanding and applications. In this paper, a numerical method is employed to schematically investigate the parameters connection between Fano and Lorentz resonance. Both Fano resonant frequency and line-width are parabolic dependent with the coupling coefficient of the Lorentz oscillators. A distinct transition effect can be observed in the Fano parameters when the eigen-frequencies of Lorentz oscillators are tuned. Our results suggest that the controlling of Fano resonance can be done by designing of Lorentz resonance in metamaterials and plasmonic materials artificially, which sustains mimicking the quantum effect by classic systems.

Keywords Fano resonance · Lorentz resonance · Metamaterials · Plasmonic materials · Asymmetric spectral line shapes

This article is part of the Topical Collection on Micro/Nano Photonics for the International Year of Light 2015, Guest Edited by Yen-Hsun Su, Lei Liu, Xinlong Xu and Zhenhua Ni.

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1 Introduction

Spectral line shapes afford fundamental information for the physical processes in the scattering, fluorescence, absorption, and so on (Ott et al. 2013). The most common observed spectral line shapes are well-known symmetric Lorentzian line shapes, which can be explained by Lorentzian oscillators. However, in some atomic and optic systems, the asymmetric line shapes are usually observed, such as photoionization in atoms and Wood anomalies in gratings (Miroshnichenko et al. 2010). The theory breakthrough with a superposition principle from quantum mechanics was put forward by Ugo Fano in 1935, who suggested unique interference phenomena between a discrete state and a continuum state in atomic physics (Miroshnichenko et al. 2010). Unlike the Lorentzian resonance which can be fitted by a Lorentz formula, a Fano formula should be used for the asymmetric spectral line shape.

Recently, the blooming of asymmetric spectral line shapes in the transmission/absorption spectra in metamaterials as well as the scattering spectra in plasmonic systems regain the vitality of Fano resonance in optic systems. For instance, sharp Fano resonances have been observed in metamaterials with weak asymmetric split ring resonators (Luk'yanchuk et al. 2010; Singh et al. 2011). Fano resonances have also been observed in a plenty of novel plasmonic nanostructures such as plasmonic oligomers, heptamer, nanoclusters, nanocubes as well as the nanocavities (Luk'yanchuk et al. 2010; Fan et al. 2010a; Fang et al. 2011; Hao et al. 2008, 2009; Lassiter et al. 2010; Mirin et al. 2009; Sonnefraud et al. 2010; Verellen et al. 2009; Ye et al. 2012; Zhang et al. 2011). In physics, these structures can be designed and achieved quality factors of approximate 50 with good geometrical and chemical tunability. In applications, these sharp Fano resonances compared with Lorentz resonances could be exploited for notch filters, highly selective narrowband photo-emitters, biological and chemical sensors, and slow-light devices (Rahmani et al. 2013; Yanik et al. 2011; Fedotov et al. 2007). The most promising applications among them are the ultrasensitive sensing devices due to Fano resonances are highly sensitive to the dielectric environment. These also give us a chance to improve the surface enhanced infrared absorption (SEIRA) and surface enhanced Raman scattering (SERS) (Lee et al. 2007; Hao et al. 2008; Lal and Halas 2010; Banholzer et al. 2008; Liu et al. 2009) by the designed enhanced local electric field (ELEF) (Xu et al. 2011). As such, much effort has been taken for further excavate the Fano resonances as well as the applications based on both intensity change and phase shift in Fano resonances (Ott et al. 2013; Genet et al. 2003; Riffe 2011; Fano 1961).

On one hand, Fano resonances in metamaterials and plasmonic materials can be explained by the coupling of two classical Lorentzian oscillators with electromagnetic waves as driving force (Joe et al. 2006). On the other hand, Fano resonances suggest a good approximation of constructive and destructive interference of discrete states and continuum states [viewed as dark and bright states (Fan et al. 2010a)]. However, few works have been done on the transition from Lorentz resonances to Fano resonances. As Lorentz resonances can be tuned easily and understood well in metamaterials and plasmonic systems by geometry design, the Lorentz spectral parameters can be used to tune the Fano spectral parameters such as Fano line shape, Fano resonant frequency, as well as the Fano linewidth artificially.

In this paper, the relationships of Lorentz parameters and Fano parameters have been studied. It is revealed that the influence of the damping constant of the Lorentz resonance is an approximate parabolic dependence with Fano spectral line shape parameter, Fano resonant frequency, and Fano line-width in the Fano resonance. Both Fano resonant frequency and line-width are parabolic dependent with the coupling coefficient of the Lorentz oscillators. However, Fano spectral line shape parameter demonstrates a saturation effect with the Lorentz coupling coefficient. A distinct transition can be observed in the Fano parameters when we tune the eigen-frequencies of the coupled Lorentz oscillators. Our results suggest that the controlling of Fano resonance can be done by the artificial designing of Lorentz resonance in metamaterials and plasmonic materials.

2 Coupling Lorentzian oscillators and Fano formula

2.1 Coupling Lorentzian oscillators

As a classic description, two coupled oscillators can be used to describe the Fano resonance. These coupled oscillators are equivalent to a discrete state and a continuum state in a quantum description. The coupled oscillators under the driving of external electromagnetic wave can be written as:

$$\begin{aligned} x'' + \gamma_1 x_1' + \omega_1^2 x_1 + \upsilon_{12} x_2 &= Ae^{i\omega t} \\ x'' + \gamma_2 x_2' + \omega_2^2 x_2 + \upsilon_{21} x_1 &= 0 \end{aligned} \tag{1}$$

where ω_1 and ω_2 are the eigen-frequency of independent oscillators. γ_1 and γ_2 represent the damping constants, and v_{12} describes the coupling coefficient of the two oscillators. The amplitude of the first oscillator can be expressed as follows (Joe et al. 2006):

$$c_1 = A\frac{\omega_2^2 + i\omega\gamma_2 - \omega^2}{\left(\omega_1^2 + i\omega\gamma_1 - \omega^2\right)\left(\omega_2^2 + i\omega\gamma_2 - \omega^2\right) - v_{12}^2} \tag{2}$$

In the region near ω_1, the spectral response still shows a Lorentzian spectral line (Joe et al. 2006). However, in the region near ω_2, the spectral response first goes into an anti-resonance near the ω_2 due to the destructive interaction (Fig. 1). Then the spectral response goes into a peak position at an eigen-mode of the coupled system (Fig. 1).

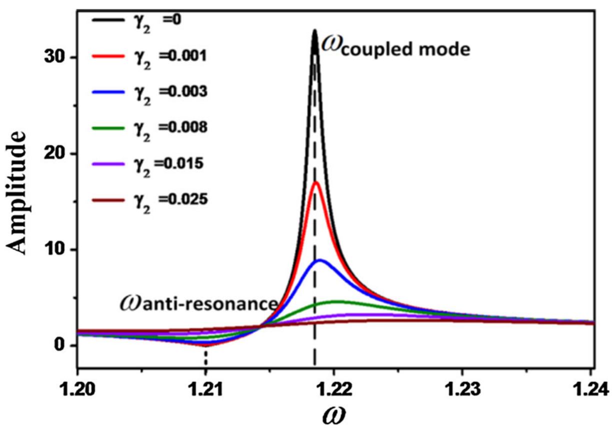

Fig. 1 Fano resonance line shape change with the damping constant γ_2

A Lorentz oscillator (Xu et al. 2006) is usually used for the localized response. In the classic analogy of Fano resonance (Joe et al. 2006), a continuum response is usually introduced by $\gamma_2 = 0$. However, in the case of $\gamma_2 \neq 0$, Fano resonance can also happen as this case corresponds to the interaction of a discrete state with a quasi-continuum state. As shown in Fig. 1, when $\gamma_2 \neq 0$, the amplitude spectra is still asymmetric. However, the resonances become blur and broad with the increasing of γ_2. As Fano resonances in plasmonic systems (Fan et al. 2010b) are usually broader than that in atomic systems (Ott et al. 2013), this suggests that Fano resonances in plasmonic systems can be viewed more likely the interaction of a discrete state with a quasi-continuum state.

2.2 Fano formula

In a quantum description, the couple of a continuum state with a discrete state gives rise to the destructive and constructive phenomena (Fano 1961; Miroshnichenko et al. 2010; Luk'yanchuk et al. 2010), which gives the asymmetric spectral line shape as follows (Miroshnichenko et al. 2010):

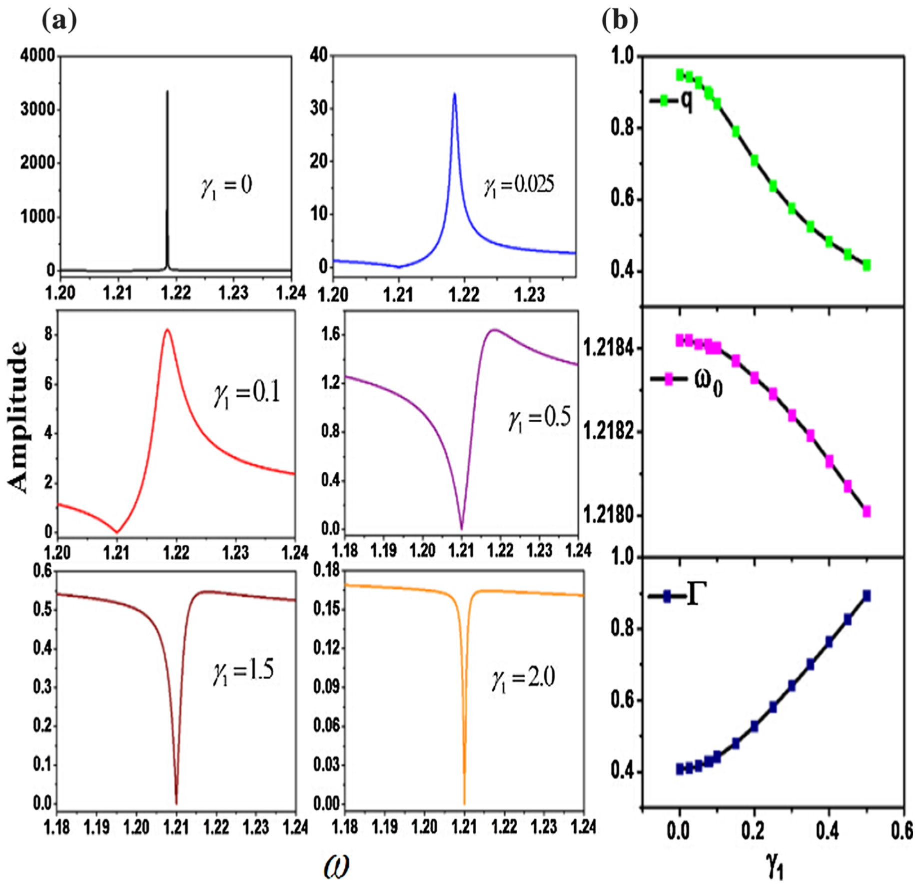

Fig. 2 **a** Resonant behavior of the coupled system under different γ_1. **b** Mapping of Fano parameters q, ω_0, Γ with the change of γ_1

$$\sigma = \frac{(\varepsilon + q)^2}{1 + \varepsilon^2} \tag{3}$$

where q is a phenomenological spectral line shape parameter representing the excitation probability ratio between the continuum and discrete state. It depends on the phase angle ϕ as $q(\varphi) = -\cot(\varphi)$ (Giannini et al. 2011). The lower the value of q is, the higher the asymmetry of line shape is. In the extreme case, when q drops to zero, the line shape becomes a symmetric anti-resonance (Riffe 2011; Mirin et al. 2009). ε is the reduced energy, which can be expressed as:

$$\varepsilon = \frac{E - E_0}{\left(\frac{\Gamma}{2}\right) \times \hbar} \tag{4}$$

ε depends on the energy of the incident electromagnetic wave ($E = \hbar\omega$), the Fano resonant energy ($E_0 = \hbar\omega_0$) and its spectral line-width Γ. The Fano resonance mode is related to the discrete state (ω_1) plus a shift $\omega_0 = \omega_1 + \Delta$ (where Δ is due to the interaction with the continuum state ω_2) (Chang et al. 2005). The reciprocal of Γ is the lifetime of the Fano resonance.

3 Transition from Lorentz resonance to Fano resonance

Both classic (Lorentz) and quantum (Fano) models can be used to describe the asymmetric spectral line shapes (Gallinet and Martin 2011). The connection of q, ω_0, Γ with the γ_1, ν_{12}, ω_1, ω_2, would be important for tuning and manipulating classic system to mimick the quantum phenomena in metamaterial and plasmonic materials. Numerical method is used to find the intrinsic relationship between them.

Figure 2a demonstrates the resonant behavior in the coupled oscillator system with different damping constant value γ_1, while keeps the other parameters unchanged. It is evident that both anti-resonance and Fano resonance appear when $\gamma_1 \neq 0$. With the increasing of γ_1, the intensity of anti-resonance increases, while the intensity of Fano resonance decreases. Although the frequency of anti-resonance (ω_2) does not change anymore, the frequency of Fano resonance redshift with the increasing of γ_1. Due to the coupling, the Fano resonance becomes broad gradually with the increasing of γ_1. As the first oscillator (discrete state) sufferred a much stronger damping leading to a lower efficiency of coupling with the second oscillator (continuum state), the Fano resonance becomes broader at the same time. After numerical fitting with Fano formulas (3) and (4), we draw out the connections of q, ω_0 and Γ of Fano resonances with γ_1 (Fig. 2b). The q demonstrates nonlinear decrease with the increasing of damping constant γ_1, which follows an approximately parabolic function. The resonant frequency ω_0 decreases with the increasing of γ_1, which can be described as a parabolic function. However, the line-width of ω_0 increases with the increasing of γ_1. These results are consistent with the spectral line-shape change in Fig. 2a. In one extreme case $\gamma_1 = 0$, there just exist two coupled continuum states, which is symmetric in the spectral line shape. In another extreme case $\gamma_1 \to \infty$, the spectral line shape becomes a symmetric anti-resonance (Mirin et al. 2009). These suggest that we can observe a gradual transition not only from a symmetric line shape to an asymmetric line shape but also from a resonance to an anti-resonance by tuning γ_1. These afford a playground for mimicking quantum phenomenas by the classic system design.

Figure 3a demonstrates the resonant behavior of the coupled system under different coupling coefficients of the Lorentz oscillators ν_{12}, while keeps the other parameters constant. It is shown that Fano resonant frequency moves to high frequency region, while the width becomes broader with the increasing of ν_{12}. In the extreme case $\nu_{12} = 0$, the discrete state does not couple to the continuum state with the spectral line shape as a Lorentzian symmetry (Riffe 2011). The relationship between ν_{12} and q, ω_0, Γ are plotted in Fig. 3b. It is evident that q is increasing with the increasing of ν_{12} in the low value region, but it will saturate when we further increases the ν_{12}. This means that the asymmetric spectral line-shape could reach the maximum, when the two states are most widespread overlap (Rau 2004). At the same time, Fano resonant frequency moves to high frequency (blue shift) with a parabolic dependence. The line-width of the Fano resonance also increases with the increasing of the coupling strength and can be described as a parabolic function. The results suggested that there exists a moderate coupling strength for better Fano resonance design.

Figure 4a shows the Fano resonant behavior of the coupled oscillators with the change of ω_1. It is evident that there is a transition when ω_1 moves close to ω_2 as the Fano line-width increases firstly and then decreases when ω_1 passes a transition position. The anti-resonance frequency also change as a dip on the left side of Fano resonance before $\omega_1 = 1.21$ to a right side of the Fano resonance after $\omega_1 = 1.21$. At the resonance position $\omega_1 = \omega_2 = 1.21$, the spectral line shapes show more Lorentz symmetry likely. Figure 4b shows the relationship between ω_1 and q, ω_0, Γ, which is also in accordance with Fig. 4a. When ω_1 approaches ω_2 from the low-frequency part, there is little change of the q, ω_0, Γ with ω_1. However, when ω_1 is close to ω_2, it can be regarded as a superposition of the two states and the spectral line shape is Lorentz symmetry likely. As ω_1 moves away from ω_2, the overlap of the coupled oscillators decrease and the values of q, ω_0, Γ recover to Fano

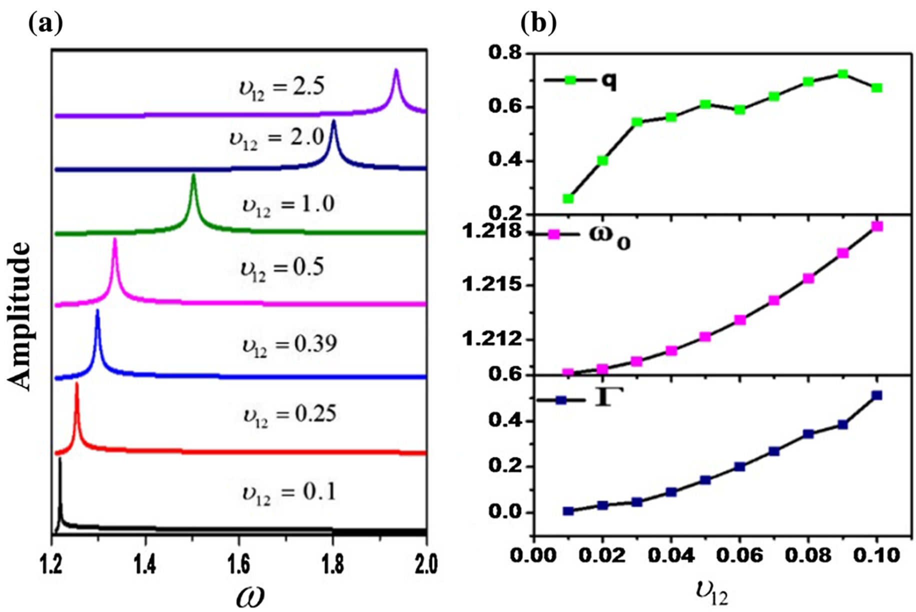

Fig. 3 **a** Resonant behavior of the coupled system under different ν_{12}. **b** Mapping of Fano parameters q, ω_0, Γ with the change of ν_{12}

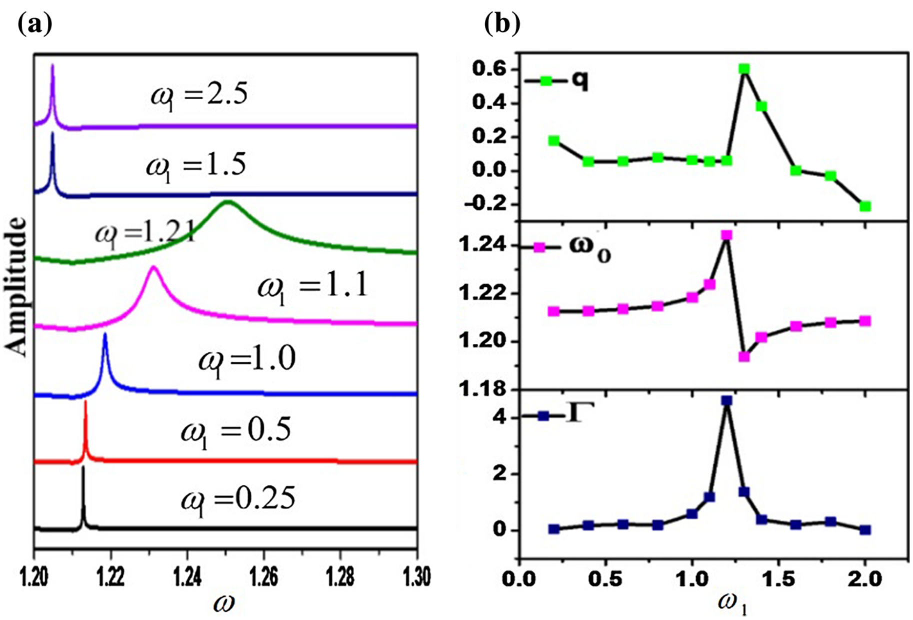

Fig. 4 **a** Resonant behavior of the coupled system under different ω_1. **b** Mapping of Fano parameters q, ω_0, Γ with the change of ω_1

symmetry likely. It is also clearly that there exists an anti-crossing of Fano resonance with the ω_1. At this state, the q and Γ demonstrate a peak with ω_1. All these variations suggest that the transition from Lorentz resonance to Fano resonance (Sheikholeslami et al. 2011), which can be designed with the symmetry breaking. This is important as the plasmonic system can be used to mimic the transition effect as tuning ω_1 by changing geometry size and geometric symmetry.

Similar to the tuning of ω_1, we can also tune ω_2 as shown in Fig. 5a. It is obvious that the anti-resonance locates at the right-side of the Fano resonance before $\omega_2 = 1.0$ and then shifts to the left-side as we further tune ω_1. Fano resonant frequency is blue-shifted when the ω_2 increases. In this process, the line-width of the Fano resonance has a maximum. Figure 5b shows the relationship between ω_1 and q, ω_0, Γ, which is in accordance with the change in Fig. 5a. The spectral line parameter q and the line-width Γ firstly increases with the increasing of ω_2 and then decreases after they pass the transition position at $\omega_1 = \omega_2$. However, the Fano resonant frequency always increases with the increasing of ω_2 as a linear response. These also demonstrate that the Lorentz resonant frequency can be used to mimic the transition from Lorentz resonances to Fano resonances.

4 Conclusions

In summary, we carry out a numerical method to schematically investigate the transition from Lorentz resonances to Fano resonances. It is revealed that the influence of the damping constant of the Lorentz resonance is an approximate parabolic dependence with Fano spectral parameters. Both Fano resonant frequency and line-width are parabolic

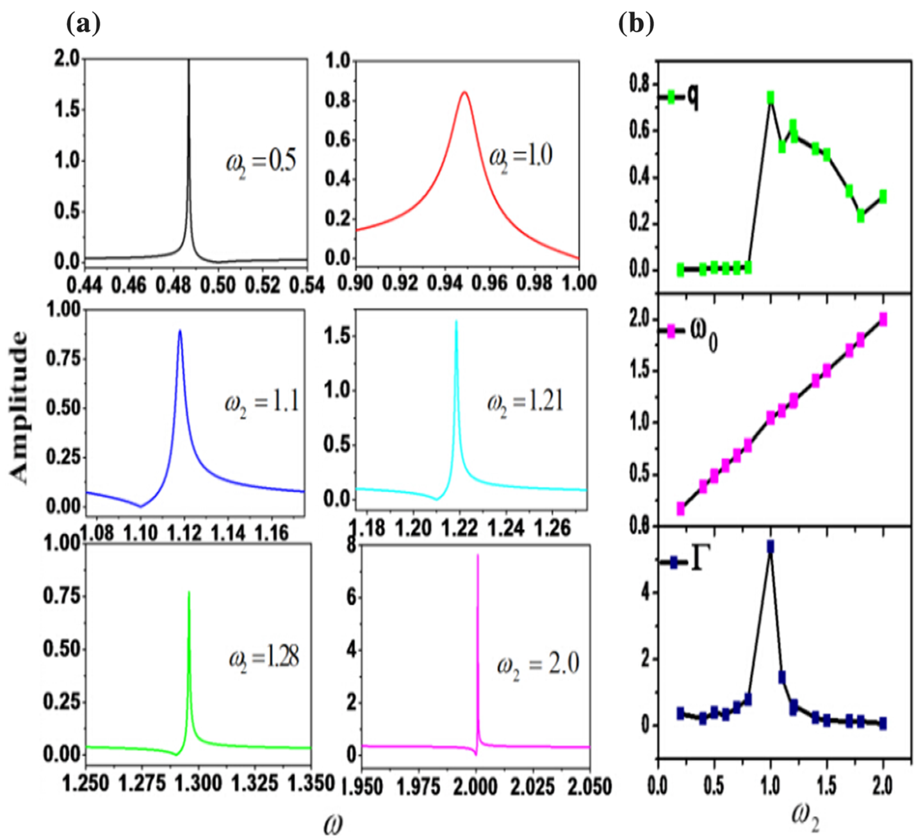

Fig. 5 **a** Resonant behavior of the coupled system under different ω_2. **b** Mapping of Fano parameters q, ω_0, Γ with the change of ω_2

dependence with the coupling coefficient of the Lorentz oscillators. However, Fano spectral line shape parameter demonstrates a saturation effect with the Lorentz coupling coefficient. A distinct transition can be observed in the Fano parameters when we tune the eigen-frequencies of the coupled Lorentz oscillators. Our results suggest that the artificial controlling of Fano resonance can be done by designing of Lorentz resonance in meta-materials and plasmonic materials.

Acknowledgments This work was supported by National Science Foundation of China (No. 11374240), Natural Science basic Research Plan in Shannxi Province of China (No. 2012KJXX-27), Ph.D. Programs Foundation of Ministry of Education of China (No. 20136101110007), Key Laboratory Science Research Plan of Shannxi Education Department (13JS101), National Key Basic Research Program (2014CB339800).

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