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# Fano-chain: the Fano resonances in a nanoparticles chain

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We show that for a linear chain of nanoparticles the Fano resonances can be excited and tuned through particle number manipulation by adding or removing particles from the chain. Fano modes excited in the chain, the spectrally overlapped bright superradiant and dark subradiant modes, are presented with current flow pictures for the first time, which clearly reveal how each individual particle reacts to light and interacts with other particles in the chain. This work may help design new Fano resonances in plasmonic metamaterials and nanostructures.

**Keywords:** Fano resonance; core–shell metamaterial; nanoparticle



## 1. Introduction

Plasmonic meta-molecules, consisting of near-field interacting individual nanoparticles, have attracted tremendous interest recently as a result of intriguing features such as Fano resonances [1,2]. The Fano resonances result from the interferences of broad superradiant modes and narrower subradiant modes. In nanoplasmonic systems, Fano resonances have been attained with symmetry breaking [3,4], tuning of incidence angle [5] and light polarisation [6]. These asymmetric conditions allow high-order multipolar modes to couple directly with normal incident light, which leads to a destructive interference among the dark multi-polar and the bright dipolar modes for the Fano excitation [7]. Meanwhile, Fano resonances in symmetrical structures [8], such as dimmers [9], quadrumers [10] and heptamers [11–13], have been demonstrated via anti-parallel coupling of the dipolar modes. Mixing of dipole and high-order modes in symmetrical structures for Fano generation is less well known and remains to be addressed. In this paper, we show, for the first time, that the Fano resonances in a symmetric linear nanoparticles chain could be excited and tuned simply by adjusting the number of particles within the chain, making the high-order dark modes within the chain readily accessible for Fano resonances engineering.

## 2. Simulation

The linear chain structure consists of multiple close-contacting $Ag/SiO_2$ core–shell nanoparticles bonded in a single row, as illustrated in Figure 1. The simulation was performed using a finite integral technique (FIT). FIT provides a universal spatial discretisation scheme applicable to various electromagnetic problems, ranging from static field calculations to high frequency applications in time or frequency domains. Unlike most numerical methods, FIT discretises Maxwell's equation in an integral form rather than the differential ones. In this study, we have used triangular meshes in the simulation; it is naturally conformal to the circular boundary of a sphere, and has tight links with finite element methods (FEM) formulated in Whitney forms. A commercial FIT software package, CST Microwave Studio, was used. Each particle within the chain was discretised by tetrahedral meshes with a maximum edge length of $a/5$, where $a$ is the particle radius. The material properties of Ag and $SiO_2$ were taken from Palik [14]. The incident wave is a linearly polarised plane wave with electric vector directed along the particle chain axis. The retardation effect and contributions from all necessary orders of partial waves (dipole, quadrupole, ...) are inheritably considered in our modelling. To visualise different modes excited in the chain, electric fields and current flows were

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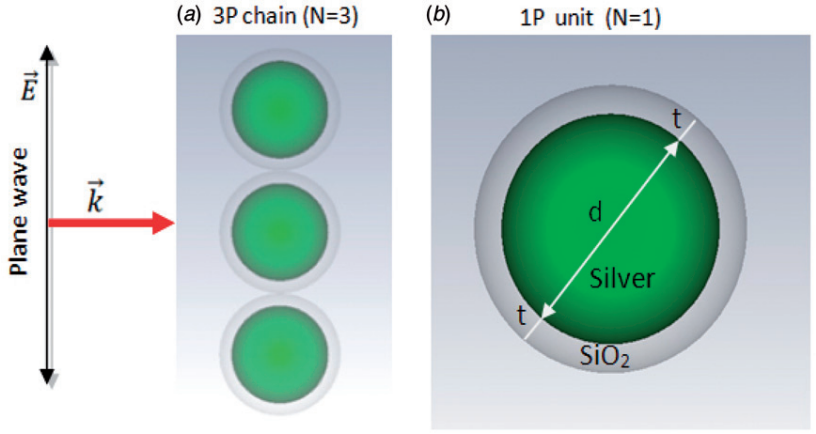


Figure 1. The Fano-chain system. (*a*) A representative example with three core–shell nanoparticles ($N=3$) arranged linearly. (*b*) Each meta-particle consists of a silver core with diameter $d$, and a silica shell coating with thickness $t$. The plane wave light source is incident from the left, and polarised along the chain axis. (The colour version of this figure is included in the online version of the journal).

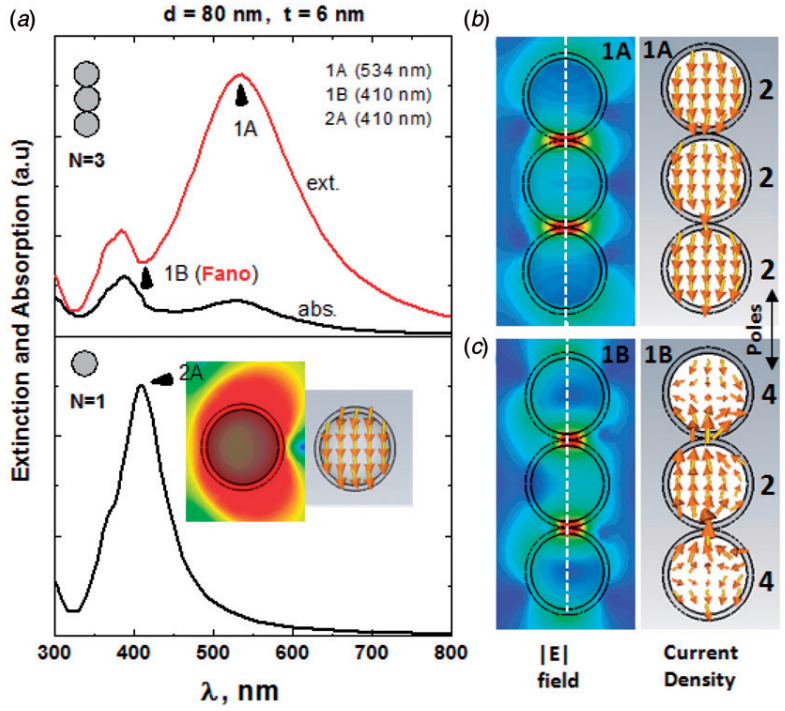


Figure 2. (*a*) Extinction and absorption spectra for 3P ($N=3$, top panel) and 1P ($N=1$, bottom panel) core-shell nanoparticles. A clear Fano dip, 1B, is observed in the 3P chain. Near-field and current density distributions of the 3P chain at (*b*) resonance peak 1A and (*c*) Fano dip 1B. (The colour version of this figure is included in the online version of the journal).

both presented. Noting the current flow illustrations is a new way to illustrate the Fano resonance coupling, in addition to the recent strong efforts to decode the Fano resonances in systems where several nanoparticles are interacting [15–17].

## 3. Results and discussion

Figure 2 demonstrates the excitation of Fano resonance in a three particles (3 P) chain; each particle has a core diameter $d=80$ nm, and a shell thickness $t=6$ nm. Compared with a single particle that has a

single dipole peak at 410 nm (label 2A, and the insert), the 3 P chain shows a clear Fano dip profile at 410 nm (label 1B), and a symmetric dipole resonance peak at 534 nm (label 1A). The near-field plots of the electric field and current density distributions in Figure 2(*b*)–(*c*) reveal the underlying mechanism: at 534 nm (label 1A), all three particles in the chain are oscillating in dipole mode and in-phase, constructing a collective resonance mode which is bright and superradiant. The resonance is red-shifted and broadened compared to that of the single particle dipole resonance (label 2A), due to the increasing of radiative damping for larger net dipole moments in the 3P chain resulted from strong near-field coupling between plasmonic core-shell nanoparticles [18]. The two hot spots inside the gaps are symmetrical with respect to the chain axis (dotted line in Figure 2(*b*)) – a signature of pure dipole resonances in all particles.

Let's now look at the Fano dip occurring at 410 nm (label 1B) for the 3 P chain. Since such a Fano dip is absent in the single particle spectrum, it must be the result of multiple chain particles interaction. From the optical near-fields at this dip wavelength (Figure 2(*c*)), we can see that a dark chain mode exists (quadrupole–dipole–quadrupole, i.e. 4-2-4 mode) that is a mixture of dipole (the centre particle) and quadrupole (two edged particles) resonance modes. The dipole in the middle appears to be dominant over edge quadrupoles in terms of the strength (longer arrows as in the plot). This dark subradiant mode overlaps with the bright superradiant dipole modes (label 1 A) as shown above, causing the formation of Fano dip in the spectrum. One can also see that an absorption peak (Figure 2(*a*), top panel), although quite weak, appears at the Fano dip wavelength, which serves a strong evidence of Fano nature of the dip [19]. It is also noted that the two hot spots appear to be slightly asymmetrical with respect to the chain axis (see dotted line in Figure 2(*c*)), which could be regarded as a signature of the involvement of high-order quadrupole modes.

As particle number increases, more dark modes could be supported by the chain and thus more Fano resonances could be excited and seen in the extinction spectrum of the Fano-chain. Figure 3 shows that five nanoparticles (5P, $d = 80$ nm) chain produces two Fano resonance dips at 463 nm (label 3A) and 406 nm (label 3B), respectively, when $t = 6$ nm. The dark mode at 463 nm (label 3A) illustrated in Figure 3(*b*) is a mixture of dipole and high-order quadrupole modes in the chain (2-4-2-4-2 mode), similar to the 3 P case in Figure 2(*c*). Again the oscillating strength is dominated by the central dipole particle, causing the near-field hot spots in the middle gaps to be more pronounced than those at the edges. The dark mode at 406 nm (label 3B) is new and not observed in the previous 3P chain.

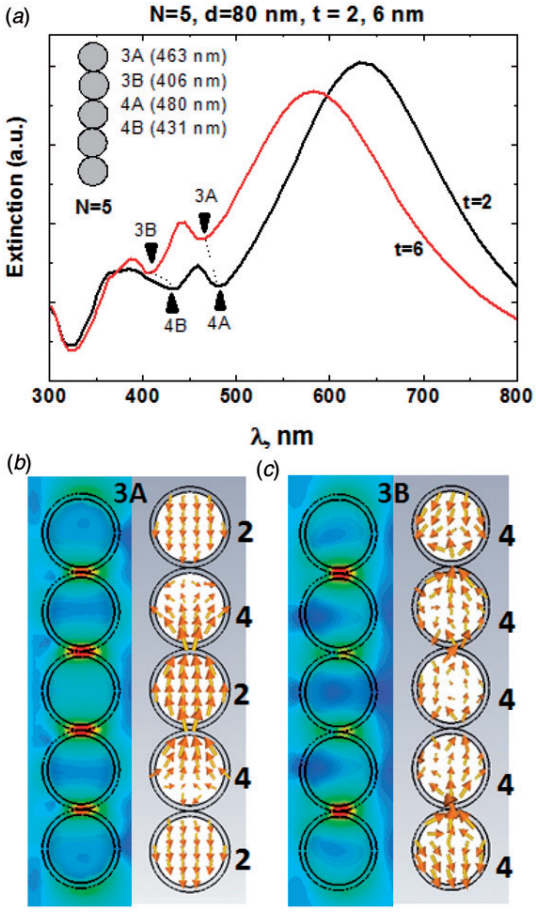


Figure 3. Additional Fano resonances can be excited in the chain structures by adding more particles. (*a*) Double Fano dips in a 5P ($N = 5$) chain at $t = 2$ and $t = 6$ nm. (*b*), (*c*) The corresponding near-field and current density distributions at Fano frequencies 3A and 3B. (The colour version of this figure is included in the online version of the journal).

It is the pure mixture of quadrupole modes within all chain particles (4-4-4-4-4 mode), as revealed by the current density plot in Figure 3(*c*). The resonance is dominant, as can see by the near-field hotspots, by the particles sitting on the chain ends and its neighbours, instead of the central particle in the middle.

The observed Fano resonances in the core–shell chain could be tuned via the parameter of shell thickness $t$. In Figure 3(*a*), the spectrum for $t = 2$ nm, $d = 80$ nm is also shown; the two Fano dips are now located at wavelengths of 480 nm (label 4A) and 431 nm (label 4B), respectively. Both Fano dips (3A vs. 4A, 3B vs. 4B) and main dipole peaks are red-shifted when compared to the $t = 6$ nm case, due to the stronger near-field coupling in the chain with thinner shells.

Figure 4 illustrates Fano resonances in the chain with even numbers of particles $N = 6$, 8, and 10. For the

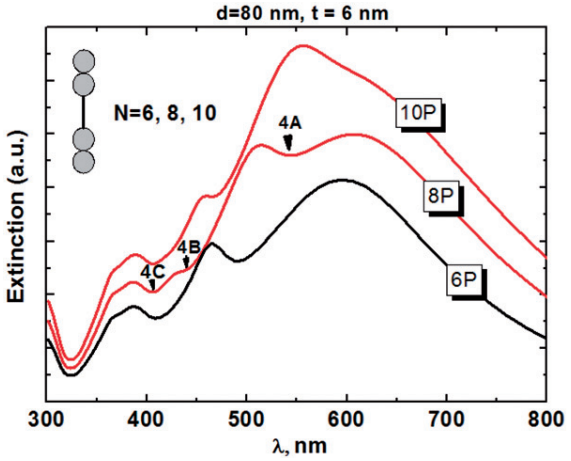


Figure 4. Fano-chain with even numbers of particles $N = 6$, 8, and 10. (The colour version of this figure is included in the online version of the journal).

6 P chain ($N = 6$), the spectrum is close to that of 5P shown in Figure 3(*a*), while the main dipole peak (bright mode: 2-2-2-2-2-2) and two Fano dips (dark modes: 2-4-2-2-4-2 and 4-4-4-4-4-4) are slightly red-shifted. For the 8P chain ($N = 8$), the Fano dip at 547 nm (label 4A) strongly modulates the main dipole peaks, due to the close spectral overlapping of dipole mode (2-2-2-2-2-2-2-2) and dark mode (2-2-4-2-2-4-2-2). The 4C Fano dip has a dark mode of pure quadrupoles (4-4-4-4-4-4-4-4). A new Fano peak, although quite weak, can be seen at 438 nm (label 4B), which corresponds to a dark mode (2-4-4-2-2-4-4-2). At $N = 10$, the mixture of the first Fano dip and the main dipole peak has led to the blue-shift as well as the asymmetric profile of the dipole peak.

Note that the present study has focused on $Ag/SiO_2$ core–shell nanoparticles. For Ag nanoparticles chains without shell layers, we also observed the presence of Fano resonances, but with relatively weak dips and shifted positions. In addition to the far-field Fano spectra due to the particle number effect in the chain, as shown above, one may refer to a previous paper by the authors [20] on the influence of number of particles within the chain on optical near-fields inside the gaps of the chain, which is important for applications in surface enhanced Raman scattering (SERS).

## 4. Conclusions

In summary, we have shown that Fano resonances can readily be excited and engineered through particle number engineering in a strongly coupled linear nanoparticles chain consisting of $Ag/SiO_2$ core-shell nanoparticles bonded in a row; the excitation of different dark modes within the chain of different number of particles, could spectrally overlaps with the fundamental bright superradiant dipoles modes of the chain, leading to the generation of Fano resonances. We have also demonstrated that current flows pictures are valuable for visualising the Fano modes. This work may help design new Fano resonances in plasmonic metamaterials and nanostructures.

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