Regimes of optical mode coupling: from core-shell single particle to dimer

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Abstract. We study a transformation of a core-shell dielectric rod into a dimer by pulling the core rod out of the shell. We present simulated scattering spectra of two infinite dielectric rods with dipole Mie resonances tailored to the same frequency by choice of the refractive indices ratio. We identify a transition between weak and strong coupling regimes by examining the peak splitting of the dipole Mie resonance. We find that the splitting increases as the distance between the rod centres decreases. This behaviour is kept for all configurations: core-shell, eccentrically embedded rod and dimer.

1. Introduction

Photonic systems support a lot of resonances, which may couple in different regimes [1]. Here we discuss two opposite cases: resonances that exist in a single particle and those that involve a complex of separate particles. The first case is realized in a core-shell particle, where the coupling of resonances is manifested by effects like scattering cancellation, making it possible to achieve invisibility [2]. An example of the second case is a photonic oligomer [3], which in the simplest case is a dimer. The modes in the oligomer might hybridize leading to a peak splitting effect [4].

Here we consider a smooth transition between these two cases by pulling the core of a core-shell particle outside of the shell so that the two separated particles form a dimer. To

![Figure 1. A sketch of the system under consideration.](image-url)
demonstrate this transition, we study the simplest two-dimensional problem of scattering on infinite dielectric rods.

2. Simulation of scattering spectra

We consider scattering of a plane wave by the system of two parallel infinite dielectric rods placed along the direction of incidence (see Figure 1). One of the rods has the radius $R$ and the refractive index $n_1$. The second one has the radius $r < R$ and the refractive index $n_2 > n_1$. We adjust the system parameters to make the frequency of the dipole Mie resonance to be the same for both rods. In our study we take $R = 3r$, $n_2 = 10 = 3n_1$ and the TM polarization is considered where the electric field vector is directed along the axes of the rods.

We examine the scattering spectra of this system in a dependence on the distance $d$ between the rod centres. We consider three cases: $d = 0$ where the rods are placed coaxially and form a core-shell particle (Figure 1a); $d \leq R - r$ where the small rod is embedded eccentrically into the larger one (Figure 1b); and $d \geq R + r$ where the rods are separated by an air gap transforming

![Figure 2](image-url).

**Figure 2.** Scattering spectra in cases of dimer, embedded rod and core-shell particle. (a) Dimer case. At infinitely large distance (labelled $d \to \infty$) the rods scatter light independently. The single peak at the size parameter of $kR = 0.25$ corresponds to degenerated dipole Mie resonances, which are tailored to the same frequency for both rods. At distances from $25r$ to $1000r$ (see the curve labelled $d = 100R$) the scattering spectra demonstrate fringes, which correspond to Fabry–Perot-like modes appearing between the rods. At distances from $d = 4r$ (touching rods) to $d = 25r$ the spectra demonstrate a peak splitting into two hybrid modes. This splitting effect is due to the transition from weak to strong coupling regime between dipole modes. The lower peak corresponds to the symmetric hybridized mode, while the higher one is the antisymmetric mode. (b) Embedded rod and core-shell particle cases. The distances from $d = 0$ to $2r$ correspond to the configuration when the smaller rod is embedded into the larger one. Here the spectra shown by dotted curves exhibit even stronger splitting of the resonant modes. When $d = 0$, the rods are arranged coaxially to form a core-shell particle. The analysis of peak position reveals that the change in the configuration from the dimer (a) to the embedded case (b) does not alter the splitting effect. The grey curves are guide to the eyes only.
the system into a dimer configuration (Figure 1c).

As in our previous study [5], we use the multiple scattering theory (MST) to obtain the amplitudes of scattered fields. MST is a rigorous coupled multipole method that takes into consideration the interactions between all scatterers – that is, waves scattered by a rod at a point \( A \) become incident on other rods at \( B, C, \ldots \). This is achieved by rewriting the scattered field, which is expressed in terms of cylindrical harmonics with a pole at \( A \) in terms of cylindrical harmonics with poles at \( B, C, \ldots \), so that a closed-form system of equations on the multipole amplitudes can be obtained. We extend this idea to multiple rods that are embedded into a bigger rod and formulate a generalized Lorentz–Mie theory for such kind of a complex. To do that, we rewrite the incident and scattered fields for embedded rods in terms of cylindrical harmonics with a pole at the centre of the enclosing rod.

To calculate the scattering cross-section from the scattering amplitudes we utilize the 2D optical theorem [5], which differs from its 3D analogue:

\[
C_{\text{ext}} = 2 \sqrt{\frac{\pi}{k}} (\text{Im}\{f(0)\} - \text{Re}\{f(0)\}),
\]

where \( f(0) \) is the normalized forward scattering amplitude and \( k \) is the wave vector.

3. Results
We show the scattering spectra simulated for different distances in Figure 2. As the distance \( d \) decreases, the weak-to-strong coupling transition occurs, which is manifested by splitting of the dipole resonance. The splitting increases with decreasing \( d \).

This behaviour is kept when the smaller rod is embedded into the bigger one. In this regime we observe even stronger splitting of the dipole resonance. We note that the frequency of the symmetric mode demonstrates little change with \( d \). This is explained by absence of a zero in the symmetric mode, thus the relative placement of the rods becomes almost irrelevant, provided that they are close enough. The frequency remains close to the Mie resonance of the large rod, because only small fraction of it becomes replaced with a material with higher refractive index.

The distance \( d = 0 \) corresponds to the core-shell particle. We note that in this regime the names “symmetric” and “antisymmetric” modes lose sense, as they both become symmetric. The difference is that the “antisymmetric” mode has a zero, while the “symmetric” mode does not have one.
To verify the validity of our analytical results, we have compared them to ones performed with a finite-element method. Scattering spectra obtained with both methods are shown in Figure 3 and they demonstrate an excellent agreement.

4. Conclusion
We have performed analytical and numerical simulations of scattering spectra of two infinite dielectric rods with different radii and same frequency of the dipole Mie resonance as the distance between their centres is varied.

At large distances the rods are coupled weakly, which is manifested by presence of a single peak corresponding to the Mie resonance and fringes that are due to the Fabry–Perot-like modes. At small distances the rods demonstrate strong coupling which is manifested through the splitting of the Mie resonance. This splitting increases as the distance between the centres of the rods decreases, and this behaviour is kept after one rod is embedded into another, to the point where distance becomes zero and the rods form a core-shell particle. Thus, we have demonstrated a smooth transition between a core-shell particle and a dimer by “pulling out” the core from the shell for the case of infinite dielectric rods tuned to the same Mie resonance frequency.

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