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# Waveguide and Radiation Applications of Modes in Linear Chains of Plasmonic Nanospheres

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**Abstract**—We apply an analytical procedure that uses a periodic Green's function based on the Ewald representation to compute the modes in a linear chain of plasmonic nanospheres, including the case of complex modal wave numbers. We analyze both transverse and longitudinal polarizations (with respect to the array axis) of the nanospheres' electric dipole moments. Among all the modes, we discuss those excitable and that can be used for wave guidance through bound modes or for radiation through leaky modes.

## I. INTRODUCTION

Linear chains of nanoparticles are one dimensional periodic arrays that have been studied to miniaturize photonic devices (e.g., biosensors [1]) and to efficiently transport electromagnetic energy (e.g., directive radiators [2], [3] and wave guiding structures [4]-[6]) required for the design of integrated photonic circuits. Linear chains reside their properties onto the excitation of *collective* resonances in periodic arrays with subwavelength inter-particle distance stemming from the resonance of the individual nanoparticles [7].

Over the years, researchers have tried to address the problem of mode propagation in linear chains of nanoparticles [8]-[33]. In particular, full characterization of the modes with real and complex wavenumber in the linear chain of plasmonic nanospheres has been provided in [23] and here briefly summarized. The inherent difficulty to handle the complex wave vector space in open cylindrical coordinates has also been discussed in [23], [34]. The modal classification here discussed provides with the knowledge of the physical bound (non-radiating) and leaky (radiating) modes excitable in the linear chain of plasmonic nanospheres. We then show in this paper how these modes can be used to obtain nano-waveguides and nano-antennas.

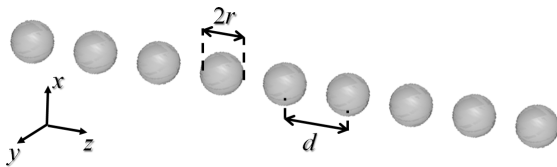


Fig. 1. Linear chain of plasmonic nanospheres (radius  $r$ , period  $d$ ) embedded in a homogeneous host environment with relative permittivity  $\epsilon_h$ . The linear chain is supposed to extend to infinity along the  $z$  direction.

## II. ELECTRODYNAMIC MODEL FOR THE COMPUTATION OF THE PHYSICAL MODES EXCITABLE IN LINEAR CHAINS OF PLASMONIC NANOSPHERES

Consider the linear chain of plasmonic nanospheres embedded in a homogeneous background with relative permittivity  $\epsilon_h$  in Fig. 1. Each nanosphere is described by a dipole-like electric polarizability (good approximation when the dipolar term dominates the scattered-field multipole expansion) and is placed at positions  $\mathbf{r}_n = z_n \hat{\mathbf{z}}$ , with  $z_n = nd$ ,  $n = 0, \pm 1, \pm 2, \dots$ , and  $d$  is the period of the chain.

Suppose that the array supports a mode with dielectric dipole moments equal to  $\mathbf{p}_n = \mathbf{p}_0 \exp(ik_z z_n)$  [the monochromatic time harmonic convention  $\exp(-i\omega t)$  is assumed], hence the field is periodic except for a phase shift described by the Bloch wavenumber  $k_z$  aligned with the chain axis, which also accounts for decay when  $k_z$  is complex. The induced electric dipole moment  $\mathbf{p}_0$  of the nanosphere at position  $\mathbf{r}_0$  is given by

$$\mathbf{p}_0 = \alpha_e \mathbf{E}^{\text{loc}}(\mathbf{r}_0), \quad (1)$$

where  $\alpha_e$  is its isotropic electric polarizability according to Mie theory [7]. The term  $\mathbf{E}^{\text{loc}}(\mathbf{r}_0)$  in (1) is the local electric field acting at  $\mathbf{r}_0$  produced by all the nanospheres of the array except the one at  $\mathbf{r}_0$ , and is given by

$$\mathbf{E}^{\text{loc}}(\mathbf{r}_0) = \tilde{\mathbf{G}}^\infty(\mathbf{r}_0, \mathbf{r}_0, k_z) \cdot \mathbf{p}_0, \quad (2)$$

where  $\tilde{\mathbf{G}}^\infty(\mathbf{r}_0, \mathbf{r}_0, k_z)$  is the electric field periodic dyadic Green's function (GF) for the phased periodic array of electric dipoles, without considering the self coupling (the reader is addressed to [23] for more details). We employ the Ewald method for fast computation of the regularized GF in (2) because it provides with the analytic continuation of  $k_z$  into the complex wavenumber space, and the expressions for the required spatial and spectral terms have been reported elsewhere [23]. Furthermore, the Ewald representation has the spatial singularity explicitly shown, which makes it simple to regularize by subtracting the self term from the periodic GF.

By combining (2) with (1), one obtains a linear system from which one could compute the modal  $k_z$  wavenumber by solving

$$\det \left[ \mathbf{I} - \alpha_c \tilde{\mathbf{G}}^\infty(\mathbf{r}_0, \mathbf{r}_0, k_z) \right] = 0 \quad (3)$$

for complex  $k_z$ .

The field relative to a mode in the linear chain is expressed in terms of spatial Floquet waves as

$$\mathbf{E}^{\text{mode}}(\mathbf{r}, k_z) = \sum_{p=-\infty}^{+\infty} \mathbf{e}_p^{\text{mode}}(x, y, k_z) e^{ik_{z,p}z}, \quad (4)$$

where  $k_{z,p} = k_z + 2\pi p/d = \beta_{z,p} + i\alpha_z$  are the Floquet wavenumbers,  $p$  is the order of the Floquet harmonic, and  $\mathbf{e}_p^{\text{mode}}$  is the transverse eigenvector of the  $p$ -th Floquet harmonic. Moreover, each Floquet wavenumber has the same attenuation constant  $\alpha_z$  and periodic (in the complex wavenumber domain) propagation constant  $\beta_{z,p}$ , with period  $2\pi p/d$ . Due to this periodicity, a mode will be described by the wavenumber of its Floquet wave in the fundamental Brillouin zone (BZ), defined as  $-\pi/d < \beta_{z,0} < \pi/d$ . Here we assume here that the wavenumber  $k_z$  is the one that lies in the fundamental BZ, i.e.,  $k_z = k_{z,0}$ . Furthermore, the radial wavenumber is  $k_{\rho,p} = \sqrt{k^2 - k_{z,p}^2} = \beta_{\rho,p} + i\alpha_{\rho,p}$ , where  $k = \omega\sqrt{\epsilon_0\epsilon_h\mu_0}$  is the wavenumber in the host material. Proper waves, i.e., those that vanish for  $\rho = \sqrt{x^2 + y^2} \rightarrow \infty$ , are defined as those with  $\alpha_{\rho,p} > 0$ . Improper waves, i.e., those that grow for  $\rho \rightarrow \infty$ , are those with  $\alpha_{\rho,p} < 0$ .

TABLE I  
CLASSIFICATION OF PHYSICAL MODES WITH COMPLEX WAVENUMBER OF THE FUNDAMENTAL FLOQUET HARMONIC

	Forward Wave $\beta_{z,0}\alpha_z > 0$	Backward Wave $\beta_{z,0}\alpha_z < 0$
<b>Slow Wave</b>	$ \beta_{z,0}  > k$ (proper, bound) $\alpha_{\rho,0} > 0$	$ \beta_{z,0}  > k$ (proper, bound) $\alpha_{\rho,0} > 0$
<b>Fast Wave</b>	$ \beta_{z,0}  < k$ (improper, leaky) $\alpha_{\rho,0} < 0$	$ \beta_{z,0}  < k$ (proper, leaky) $\alpha_{\rho,0} > 0$

Among all the mathematical solutions of (4), only a subset represents physical waves, i.e., those that can be excited by a localized source, a defect, or array truncation. Note that modes that are not classified as physical in this paper may however be excited by much more complicated source distributions, though this study is not within the scope of this paper. The physical waves are summarized in Table I based on the

complex wavenumber of the fundamental Floquet harmonic in the first BZ, i.e., the one with  $p=0$ . Modes are classified as backward when  $\beta_z\alpha_z < 0$  and forward when  $\beta_z\alpha_z > 0$ ; bound when  $|\beta_z| > k$  (slow wave) and leaky when  $|\beta_z| < k$  (fast wave). The periodic condition  $k_{z,p} = k_z + 2\pi p/d$  would determine the behavior of Floquet harmonics with wavenumbers in other BZs. More details about classification of physical modes can be found in [23].

### III. DISPERSION DIAGRAMS

We show the dispersion diagrams  $(\beta_z, \alpha_z) - k$ , for both transverse (T-pol, Fig. 2) and longitudinal (L-pol, Fig. 3) polarization states relative to the physical modes excitable in a linear chain of silver nanospheres embedded in free space with  $\epsilon_h = 1$ . The reader is addressed to [23] for a detailed modal description, including nonphysical modes and modal wavenumber frequency evolution in the complex  $k_z$  plane. The radius of the nanospheres is  $r = 35$  nm, the relative permittivity of silver is described by a tabulated measured dielectric function [35], and the period is  $d = 75$  nm.

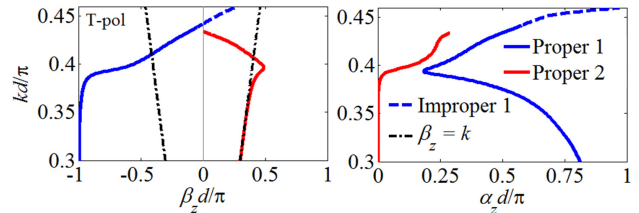


Fig. 2. Dispersion diagram showing the physical modes for T-pol. (a) Real part and (b) imaginary part of the wavenumber of the fundamental Floquet wave  $k_z = \beta_z + i\alpha_z$ . Mode ‘Proper 2’ is physical only when  $\beta_z > k$ , i.e., under the light line.

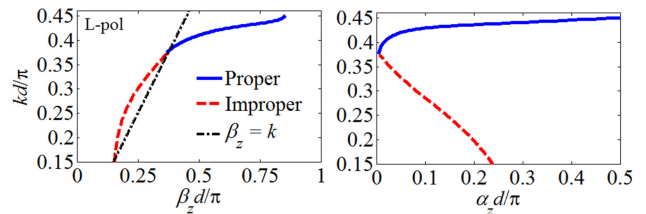


Fig. 3. As in Fig. 2, for L-pol. Mode ‘Improper’ is physical only when  $\beta_z < k$ , i.e., above the light line.

Modes ‘Proper 2’ (T-pol) and ‘Proper’ (L-pol) are good candidates for the development of nano-waveguides because they exhibit a small attenuation constant  $\alpha_z$  for some frequency ranges (refer to Fig. 2 and Fig. 3); analogously, mode ‘Improper’ (L-pol) may be used for the design of directive nano-antennas. Indeed, it is well-known that a small attenuation constant  $\alpha_z$  is a required condition for long mode propagation or directive radiation. The attenuation constant  $\alpha_z$  can be further lowered by optimizing the chain dimensions [23], [28] or by employing active gain materials

[36]-[43]. For example, the latter method may be used to lower the attenuation constant of mode ‘Proper 1’ (T-pol) whose minimum value is now limited to  $\alpha_z d / \pi \approx 0.18$ .

#### IV. PROPAGATION LENGTH FOR WAVEGUIDE APPLICATIONS

Considering exciting a wave travelling as  $\exp(ik_z z)$  along the linear chain with wavenumber  $k_z$ , we estimate its propagation length as  $L = 1/\alpha_z$  ( $1/e$  criterion), reported in Fig. 4 normalized to the free space wavelength  $\lambda_0 = 2\pi\sqrt{\epsilon_h}/k$  for both T- and L-pol states.

We note that mode ‘Proper 2’ (T-pol) is able to propagate very large distances for a large frequency range. A fairly large propagation distance is travelled also by both modes for L-pol around 750 THz. Mode ‘Proper 1’ (T-pol) can propagate, in the best case, a length of  $L \approx 0.34\lambda_0$  at about 788 THz in the analysed linear chain.

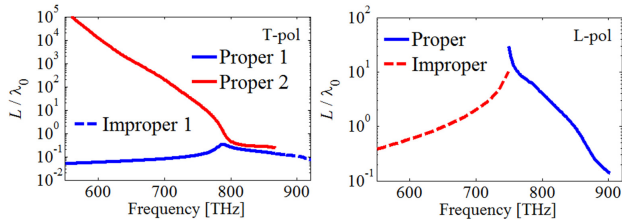


Fig. 4. Propagation length  $L = 1/\alpha_z$  normalized to the free space wavelength  $\lambda_0$  relative to the linear chain used in Fig. 2 and Fig. 3.

#### V. LEAKY MODES FOR DIRECTIVE RADIATION

We apply array factor theory [44], [45] to determine the radiation pattern of  $|E_\theta|$  in Fig. 5 of the ‘Improper’ (L-pol) forward leaky mode excited in a finite chain of 20 elements, along positive  $z$ , to achieve radiation at a certain angle  $\theta$  (the angle from the  $z$  axis in Fig. 1) from the end-fire direction.

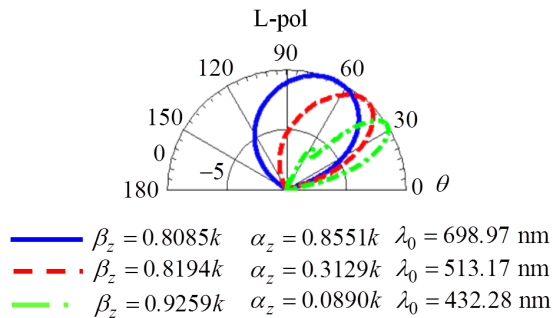


Fig. 5. Radiation pattern of  $|E_\theta|$  relative to the excitation of the ‘Improper’ (L-pol) forward leaky mode estimated using array factor theory at the three frequencies in the legend. The leaky wave parameters  $\beta_z$  and  $\alpha_z$  are also provided in the legend.

We have chosen three frequencies pertaining to the red dashed dispersion modal curve in Fig. 3. From the dispersion curve we note that an increase in frequency determines an increase of the propagation constant  $\beta_z$  and a decrease of the

attenuation constant  $\alpha_z$ . This will in turn determine the beam to approach a pencil beam shape as well as to point at a smaller angle, as can be clearly seen by looking at the solid blue, dashed red and dashed-dotted green curves in Fig. 5.

#### VI. CONCLUSION

The strength of the shown analytical procedure based on a periodic Green’s function is that it allows for the determination of the physical modes in linear chains of plasmonic nanospheres excitable by a localized source, a defect, or array truncation. The Ewald representation of the periodic GF is very suitable for linear arrays because a fully spectral representation cannot be used when the observer is on the array axis, and representations based on poly-logarithmic functions [8], [9], [13] render the classification of complex modes in their Riemann sheets more difficult. Classification is important for determining if a mode can be excited (physical), and if it is proper/improper, bound/leaky, forward/backward. Complex mode analysis enables the use of the described method for designing nano-waveguides and nano-antennas. Future developments will consider the excitation of a linear chain with finite extent through a dipole source.

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