Supplemental Material for "Emergence of diffractive phenomena in finite arrays of subwavelength scatterers"

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S1. EIGENFREQUENCY ANALYSIS OF FINITE ARRAYS

Eigenfrequencies of the resonant states of the array within the developed CDA picture are given by complex-valued zeros of the inverse coupling matrix determinant:

$$\det \overset{\leftrightarrow}{\mathbf{M}}^{-1}(\omega) = 0. \tag{S1}$$

The coupling matrix $\overset{\leftrightarrow}{\mathbf{M}}$ itself is a function of frequency, thus Eq. (S1) expresses a nonlinear eigenvalue problem corresponding to a transcendental equation, which can only be solved numerically. By looking for solutions of this equation numerically using the Halley method [1] and Singular Value Decomposition for matrix in (S1), we obtain for each N a series of complex-valued roots. From each set, we select the root with the largest real part.

To complement the results obtained with the CDA-based model, we build a model for full-wave numerical FDTD simulations of finite arrays in COMSOL Multiphysics. The results shown in Fig. S1 represent the behavior of eigenfrequencies real and imaginary part with increasing number of array elements for both CDA model and COMSOL simulation. Both models converge to the frequency value for an infinite system. The numerical model shows smaller deviations around resonant frequency at $N = \infty$ with increasing number of array elements, which are caused mostly by perfectly matched layer boundary conditions errors. Due to the presence of contributions from the higher multipoles, the resonant frequency obtained by the COMSOL simulation will be slightly shifted from the one predicted by the CDA model, Fig. S1(a).

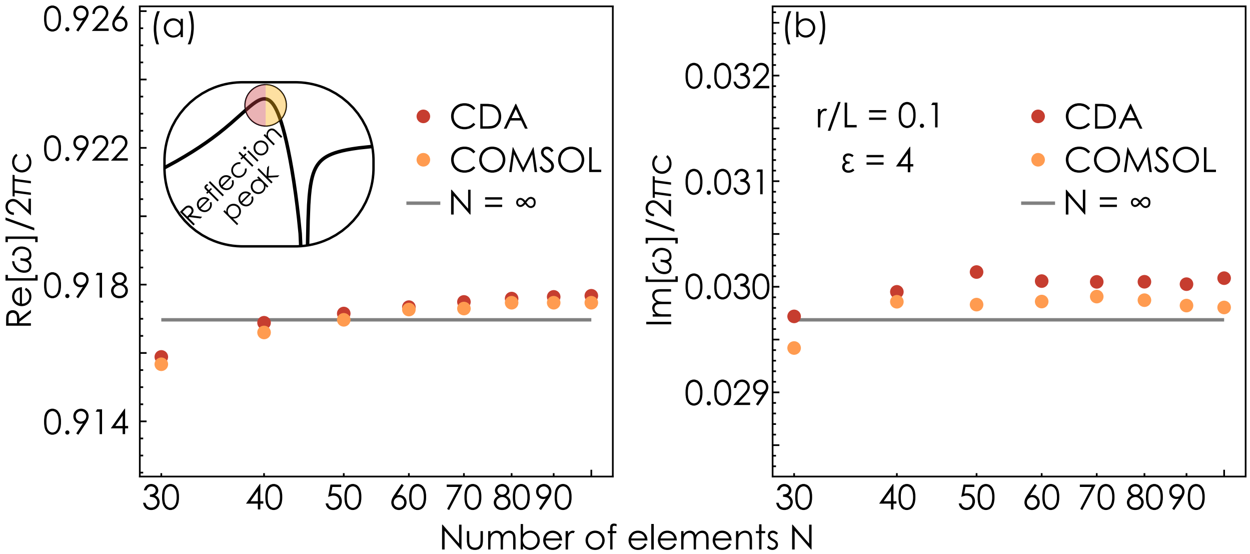

FIG. S1. Eigenfrequency analysis of finite arrays of dielectric circular cylinders ($\varepsilon = 4$, $r = 0.1L$). (a) Real and (b) imaginary parts of the lattice resonance eigenfrequency as a function of the number of array elements N predicted by the CDA model (red dots) and COMSOL Multyphysics simulations (orange dots). Grey lines represent the value of the infinite periodic array.

S2. CONVERGENCE OF DIPOLE MOMENTS TO THE CASE OF INFINITE ARRAY

In Fig. 5 of the main text we observed that the dipole moments of the cylinders located at the edges of the array differ substantially from those located in center of the array. This motivates us to analyze the behavior of the extinction efficiency of the central cylinder of finite arrays as a function of N.

Figure S2 shows the contributions of the central cylinder of the finite array (normalized to the unit cell period L) to the total extinction and compares that to the extinction efficiency of the whole array. As one can see, for relatively small arrays the contribution of the central cylinder deviates substantially from the extinction efficiency of the array as a whole, while for large arrays ($N = 100$) the extinction of the whole array converges to that of the middle cylinder.

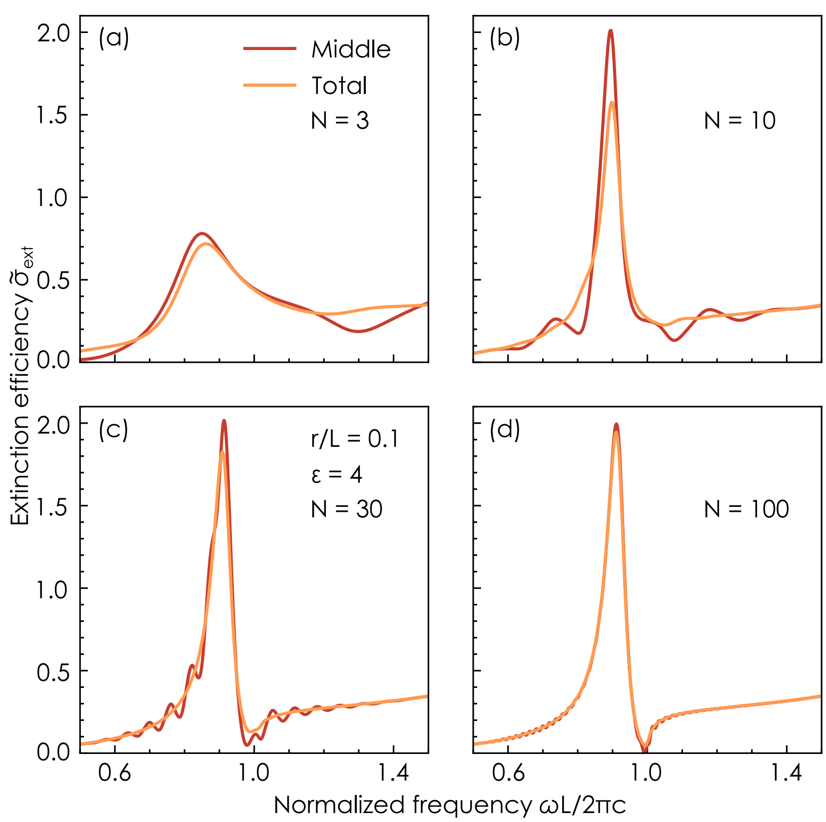

FIG. S2. Extinction efficiency spectra for finite arrays of (a) $N = 3$, (b) $N = 10$, (c) $N = 30$, (d) $N = 100$ cylinders with $r = 0.1L$, $\varepsilon = 4$. Red line illustrates contribution of the middle cylinder of the array; orange line shows total extinction efficiency of the array as a whole.

S3. CONNECTION OF EXTINCTION EFFICIENCY WITH FORWARD TRANSMISSION

Per-unit-area extinction σ/A of a truly infinite periodic metasurface can be expressed as [2]:

$$\sigma/A = 2\,\mathfrak{Re}(1 - t), \tag{S2}$$

where t is the complex-valued zero-order (forward) transmission amplitude of the periodic system.

At the lattice resonance of an infinite array of subwavelength rods CDA model predicts zero forward transmission amplitude $t = 0$, Fig. S3(a). Correspondingly, the per-unit-area extinction reaches 2, Fig. S3(b). This regime already develops for $N = 30$ cylinders, where the extinction efficiency approaches 2, Fig. S3(b).

Conversely, at the frequency of the Rayleigh anomaly forward transmission amplitude $t = 1$ with zero imaginary part, $\mathfrak{Im}\ t = 0$, yielding zero extinction efficiency in the limit of infinite array.

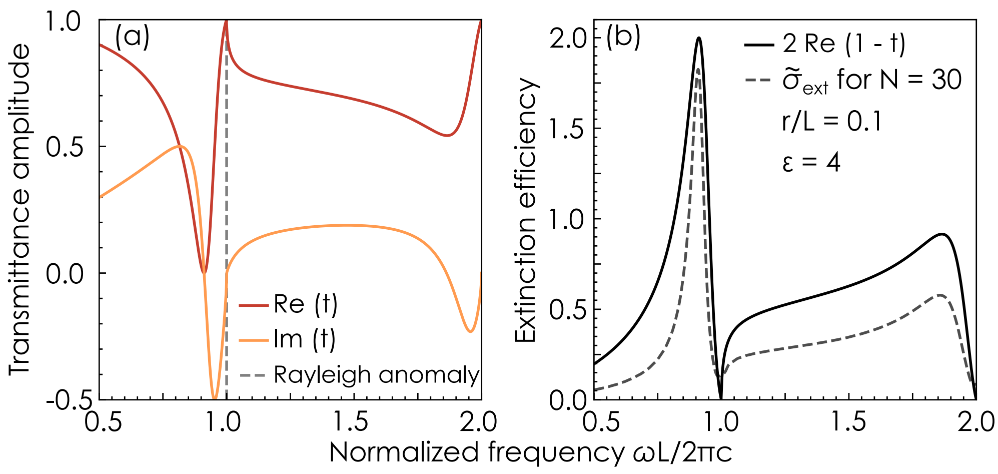

FIG. S3. (a) Complex transmission amplitude $\mathfrak{Re}(t)$ (red line) and $\mathfrak{Im}(t)$ (orange line) of the infinite array of $\varepsilon = 4$, $r = 0.1L$ circular cylinders obtained with the CDA model. (b) Extinction efficiency of finite array of $N = 30$ $\varepsilon = 4$, $r = 0.1L$ circular cylinders (dashed), and per-unit-area extinction $2\mathfrak{Re}\ (1 - t)$ of the corresponding infinite array (solid).

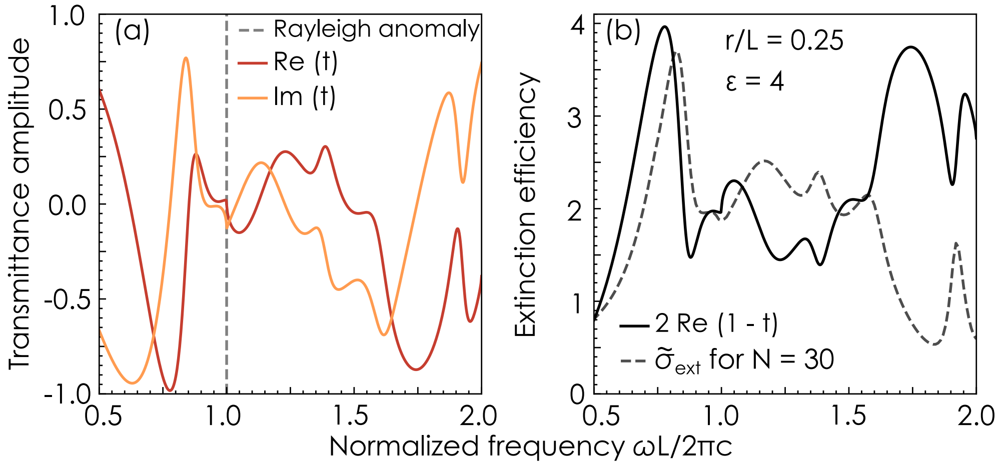

FIG. S4. (a) Complex transmission amplitude $\mathfrak{Re}(t)$ (red line) and $\mathfrak{Im}(t)$ (orange line) of the infinite array of $\varepsilon = 4$, $r = 0.25L$ circular cylinders simulated with RCWA. (b) Extinction efficiency of finite array of $N = 30$ $\varepsilon = 4$, $r = 0.25L$ circular cylinders (dashed), and per-unit-area extinction $2\ \mathfrak{Re}(1 - t)$ of the corresponding infinite array (solid).

Another interesting regime occurs in arrays of thicker cylinders, $r = 0.25L$, presented in Fig. 7 of the main text. CDA model is no longer valid, and all scattering amplitudes should be calculated using full-wave numerical model. In this case forward transmission amplitude reaches $t = -1$ at the Fano resonance below the first diffraction threshold, Fig. S4(a). Correspondingly, per-unit-area extinction approaches 4 at the Fano resonance of the finite array, Fig. S4(b).

[1] L. Yau and A. Ben-Israel, The newton and halley methods for complex roots, The American Mathematical Monthly **105**, 806 (1998).

[2] M. Gustafsson, I. Vakili, S. E. B. Keskin, D. Sjoberg, and C. Larsson, Optical theorem and forward scattering sum rule for periodic structures, IEEE transactions on antennas and propagation **60**, 3818 (2012).