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Collective lattice resonances in arrays of dielectric nanoparticles: a matter of size

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Collective lattice resonances (CLRs) in finite-sized 2D arrays of dielectric nanospheres have been studied via the coupled dipole approximation. We show that even for sufficiently large arrays, up to 100 × 100 nanoparticles (NPs), electric or magnetic dipole CLRs may differ significantly from the ones calculated for infinite arrays with the same NP sizes and interparticle distances. The discrepancy is explained by the existence of a sufficiently strong cross-interaction between electric and magnetic dipoles induced at NPs in finite-sized lattices, which is ignored for infinite arrays. We support this claim numerically and propose an analytic model to estimate a spectral width of CLRs for finite-sized arrays. Given that most of the current theoretical and numerical researches on collective effects in arrays of dielectric NPs rely on modeling infinite structures, the reported findings may contribute to thoughtful and optimal design of inherently finite-sized photonic devices. © 2019 Optical Society of America

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All-dielectric nanophotonics is a rapidly growing field in modern physics [1] that provides a low-loss platform for an impressive number of applications such as color printing [2], biosensing [3–5], lasing [6], waveguiding [7–9], and flat [10,11] and nonlinear [12–14] optics. While even a single dielectric nanoparticle (NP) may exhibit extraordinary electromagnetic response [15,16], its periodic array possesses a richer variety of properties, extensively discussed recently [17–21]. Such interest in regular arrays of dielectric NPs is justified (among other factors) by the emergence of a tunable high-quality-factor lattice-mediated electromagnetic response that gives rise to collective lattice resonances (CLRs) [22–24]. CLRs originate from the strong electromagnetic coupling between NPs comprising the lattice, which usually occurs at wavelengths close to the Wood–Rayleigh anomalies [25,26] of the lattice. This

phenomenon has been extensively discussed for plasmonic NPs [27–33] with strong electric dipole (ED) resonances, and for all-dielectric NPs with ED and magnetic dipole (MD) optical resonances [34–37].

To date, the overwhelming majority of studies on CLRs deal with infinitely large arrays of NPs and ignore the presence of physical boundaries of arrays, either in full-field simulations [38–40] or dipole [41–44] and higher-order [45,46] semi-analytic approximations. It is commonly assumed that boundary effects are negligible for large arrays synthesized in experimental studies; thus, an infinite-array model is often considered as a satisfactory approximation. Nonetheless, the effects of the finite size have been thoroughly discussed for CLRs in regular nanostructures with Au [47–49], Ag [49–52], and graphene [49] constituents via the dipole approximation. Generally, one could expect the quality factor of CLRs in 20 × 20 and larger arrays of plasmonic NPs to be close to that of infinite arrays. However, in Refs. [47–51], NPs are considered as purely EDs, since ED oscillations predominate in plasmonic NPs. Thus, it is not obvious *a priori*, how CLRs in finite-sized arrays of dielectric NPs with strong ED and MD resonances differ from CLRs in infinite arrays, though brief discussions of up to 21 × 21 [17] and 30 × 30 [37] Si NP arrays have been reported recently. In this Letter, we address this problem and find regimes where the “infinite array” approximation is no longer reliable for CLRs in arrays of dielectric NPs with both ED and MD resonances.

Figure 1 shows a 2D array of $N_{\text{tot}} = N \times N$ identical spherical NPs embedded in a vacuum and illuminated by a plane wave with $\mathbf{E}_{\text{inc}}(\mathbf{r}) = \mathbf{E}_0 \exp(i\mathbf{k} \cdot \mathbf{r})$ and $\mathbf{H}_{\text{inc}}(\mathbf{r}) = \mathbf{H}_0 \exp(i\mathbf{k} \cdot \mathbf{r})$, where $\mathbf{E}_0 = (E_{0x}, 0, 0)$ and $\mathbf{H}_0 = (0, H_{0y}, 0)$ are amplitudes of the electric and magnetic fields, respectively, and \mathbf{k} is a wave vector. The time dependence $\exp(-i\omega t)$ is assumed and suppressed. Each NP is considered as a point dipole, so ED and MD moments \mathbf{d}_i and \mathbf{m}_i induced on the i -th particle are coupled to dipoles on other $j \neq i$ particles and to the incident

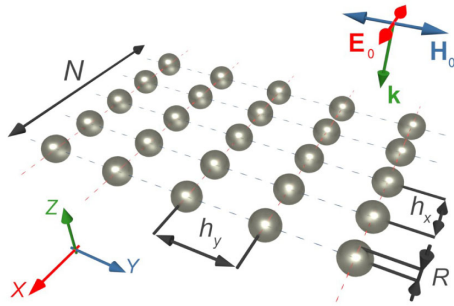


Fig. 1. Sketch of considered 2D array from $N \times N$ spherical NPs with radius R and center-to-center distances h_x and h_y along X and Y directions.

field [41,53,54]:

$$\mathbf{d}_i = \alpha^e \left(\mathbf{E}_{\text{inc}}(\mathbf{r}_i) + \sum_{j \neq i}^{N_{\text{tot}}} G_{ij} \mathbf{d}_j - \sum_{j \neq i}^{N_{\text{tot}}} \mathbf{g}_{ij} \times \mathbf{m}_j \right), \quad (1a)$$

$$\mathbf{m}_i = \alpha^m \left(\mathbf{H}_{\text{inc}}(\mathbf{r}_i) + \sum_{j \neq i}^{N_{\text{tot}}} G_{ij} \mathbf{m}_j + \sum_{j \neq i}^{N_{\text{tot}}} \mathbf{g}_{ij} \times \mathbf{d}_j \right), \quad (1b)$$

where $\alpha^{e,m}$ are ED and MD polarizabilities [55], and \times denotes a vector product. Tensor G_{ij} and vector \mathbf{g}_{ij} describe the interaction between i -th and j -th dipoles [41,53,54]. Note that G_{ij} is responsible for interaction between dipoles of the same kind (ED \leftrightarrow ED or MD \leftrightarrow MD), while \mathbf{g}_{ij} stands for ED \leftrightarrow MD cross-interaction.

The essence of CLR can be understood from a closed-form analytical solution of Eq. (1) obtained for the *infinite* array [29,41]. In this case, $\mathbf{d}_i = \mathbf{d} \parallel \mathbf{E}_0$ and $\mathbf{m}_i = \mathbf{m} \parallel \mathbf{H}_0$ for each NP [41]; therefore, the last terms in Eq. (1) vanish, since $\mathbf{E}_0 \perp \mathbf{H}_0$. Thus, for a special case of a regular 2D lattice illuminated with a normally impinging wave with $|\mathbf{E}_0| = E_{0x}$ and $|\mathbf{H}_0| = H_{0y}$, the non-zero components of \mathbf{d} and \mathbf{m} are

$$d_x = E_{0x} / (1/\alpha^e - G_{xx}^0), \quad m_y = H_{0y} / (1/\alpha^m - G_{yy}^0), \quad (2)$$

where G_{xx}^0 and G_{yy}^0 are diagonal elements of 3×3 tensor $G^0 = \sum_{j=2}^{\infty} G_{1j}$, and $(1/\alpha^{e,m} - G_{xx,yy}^0)^{-1}$ are *effective* electric and magnetic polarizabilities that capture the features of the NP's surrounding [33,41,47]. The summation in G^0 implies the use of the non-trivial Ewald method well known for 1D [56] and 2D [57] lattices, which thus has been implemented in this work.

From the analysis of Eq. (2), one could expect to observe resonances if $\text{Re}(1/\alpha^{e,m} - G_{xx,yy}^0)$ vanishes for either ED or MD moments. Indeed, Fig. 2(a) shows that the dimensionless representation of the above parameter becomes zero near $\lambda \approx h_y$ and $\lambda \approx h_x$ for d_x and m_y , respectively, which corresponds to $(0, \pm 1)$ and $(\pm 1, 0)$ Wood-Rayleigh anomalies. Note that in the general case of $h_x \neq h_y$ considered here, a simple rotation of the incident field polarization, e.g., $(E_{0x}, 0, 0) \rightarrow (0, E_{0y}, 0)$, does not yield the interchange between ED and MD CLR spectral positions, since it implies only the interchange $G_{xx}^0 \leftrightarrow G_{yy}^0$ in Eq. (2), which will likely violate the $\text{Re}(1/\alpha^{e,m} - G_{xx,yy}^0) = 0$ condition

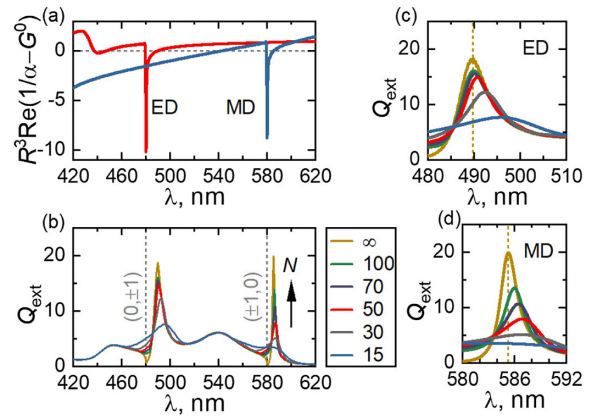


Fig. 2. (a) Real parts of normalized denominators of Eq. (2), which correspond to d_x (ED) and m_y (MD); (b) extinction efficiency for infinite (∞) and for $N \times N$ finite-sized arrays. Dashed vertical lines show the spectral positions of $(0, \pm 1)$ and $(\pm 1, 0)$ Wood-Rayleigh anomalies; (c), (d) zoomed-in spectra for ED and MD CLR, respectively. Dashed vertical lines indicate the position of the CLR peak for the infinite array. Arrays from Si NPs (refractive index from [58]) with $R = 65$ nm, $h_x = 580$ nm, and $h_y = 480$ nm are considered.

due to $G_{xx}^0 \neq G_{yy}^0$ and non-trivial wavelength dependence of polarizabilities $\alpha^{e,m}(\lambda)$ (Fig. 4 in [41]).

To characterize the electromagnetic response of the finite-sized array, we use the extinction efficiency [41,54]

$$Q_{\text{ext}}^{\text{fin}} = \frac{4k}{|\mathbf{E}_0|^2 N_{\text{tot}} R^2} \text{Im} \sum_{i=1}^{N_{\text{tot}}} [\mathbf{d}_i \cdot \mathbf{E}_{\text{inc}}^*(\mathbf{r}_i) + \mathbf{m}_i \cdot \mathbf{H}_{\text{inc}}^*(\mathbf{r}_i)], \quad (3)$$

where the asterisk denotes a complex conjugate, and \mathbf{d}_i and \mathbf{m}_i are defined from the solution of Eq. (1). For an infinite array, after substituting Eq. (2) in Eq. (3), one gets

$$Q_{\text{ext}}^{\text{inf}} = \frac{4k}{R^2} \text{Im} \left[(1/\alpha^e - G_{xx}^0)^{-1} + (1/\alpha^m - G_{yy}^0)^{-1} \right]. \quad (4)$$

We are now ready to consider Q_{ext} for infinite and finite-sized arrays. Figure 2(b) shows that extinction spectra for finite-sized arrays gradually approach the spectrum for the infinite lattice as N increases, which is consistent with reported trends for arrays of plasmonic NPs [47,49]. Indeed, ED CLR at $\lambda \approx 490$ nm for arrays with $N_{\text{tot}} > 50 \times 50$ becomes almost indistinguishable from one for the infinite array, as it is clearly seen in Fig. 2(c). Of note, for plasmonic NP arrays, the corresponding “threshold,” when Q_{ext} becomes almost the same for finite and infinite lattices, is $\approx 20 \times 20$ NPs [47]. Analogously, Q_{ext} for an MD CLR at $\lambda \approx 586$ nm in finite-sized arrays becomes similar to the infinite case if N grows, as shown in Fig. 2(d). However, what is really surprising and unexpected is that Q_{ext} of finite-sized arrays is noticeably different even for the $N_{\text{tot}} = 100 \times 100$ case. Moreover, the Fano-type profile for CLR [30] in Fig. 2(d) is significantly different for infinite and finite-sized arrays near $\lambda \approx h_x$, which implies the existence of non-negligible electromagnetic interaction emerging in finite-sized arrays.

To understand and explain these trends, we recall the difference between Eqs. (1) and (2), i.e., the last terms of Eqs. (1a) and (1b), which, respectively, provide the electric field at the i -th NP mediated by MDs on other $j \neq i$ NPs and, vice versa, the

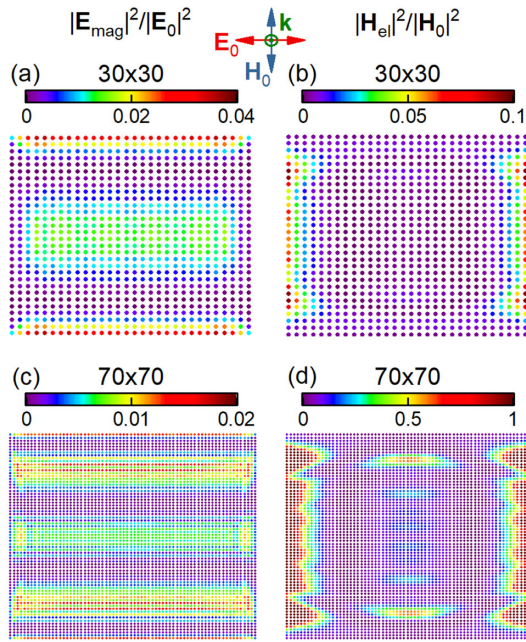


Fig. 3. Normalized intensities of electric field induced by MDs (left) and of magnetic field induced by EDs (right) for $N \times N$ arrays at wavelengths that correspond to peaks of ED (left) and MD (right) CLRs [see Figs. 2(b)–2(d) for details]: (a) 493 nm, (b) 588 nm, (c) 490 nm, (d) 586.5 nm. Each dot represents the NP, and the actual sizes of arrays vary for different $N \times N$.

magnetic field at the i -th NP mediated by EDs. Figure 3 shows the corresponding intensities, i.e., $|\mathbf{E}_{\text{mag}}|^2$ and $|\mathbf{H}_{\text{el}}|^2$, for each NP in the array. It can be seen that the normalized intensity of the electric field induced by MDs is quite small compared to the incident field, and increases only at the boundaries of the array, which again agrees well with results for plasmonic NPs [49]. The maximum value of $|\mathbf{E}_{\text{mag}}|^2/|\mathbf{E}_0|^2$, which is already quite small for 30×30 arrays in Fig. 3(a), gradually decreases for larger arrays, and almost vanishes for the 70×70 array in Fig. 3(c), thus providing a negligible difference for ED CLRs of infinite and sufficiently large finite-sized arrays in Fig. 2(c). On the contrary, the maximum intensity of the magnetic field induced by electric dipoles, i.e., $|\mathbf{H}_{\text{el}}|^2/|\mathbf{H}_0|^2$, increases for larger arrays, and again a divergence takes place near the boundaries of the array. Although the overall contribution of cross-interaction between EDs and MDs to $Q_{\text{ext}}^{\text{fin}}$ gradually decreases as N grows, the “boundary effect” is pronounced even for sufficiently large arrays, and thus cannot be completely ignored in this case. In other words, for MD CLR, the last term in Eq. (1b) has to be taken into account to get a reliable estimate of the extinction efficiency, which is clearly justified by the discrepancy between Q_{ext} for infinite and finite arrays in Fig. 2(d).

Finally, to get even deeper insight, we provide the following analytical considerations. For the electromagnetic field confined in a finite volume, the corresponding wave vector is also distributed in a finite volume of the reciprocal space: $\Delta r \Delta k_r \gtrsim 1$ [59]. In our case, the finiteness of the lattice mode in space is determined by the lattice size $\Delta r \approx Nh_{x,y}$, where N and $h_{x,y}$ correspond to the direction *perpendicular* to the polarization of the respective component of the electromagnetic field (i.e., Nh_x for \mathbf{H}_0 , and Nh_y for \mathbf{E}_0). Thus, the confinement of the wave vector in the reciprocal space is $\Delta k_r \approx 2\pi \Delta\lambda_r/\lambda^2$, which yields

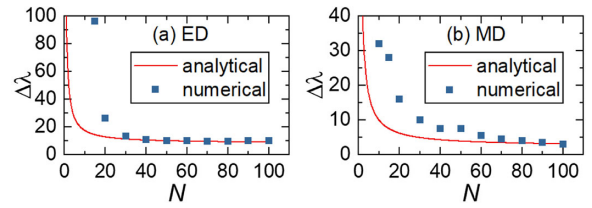


Fig. 4. (a) ED and (b) MD CLRs spectral width $\Delta\lambda$ calculated with Eq. (5) (analytical) and from data in Fig. 2(b) (numerical).

$$\Delta\lambda_r \gtrsim \frac{h_{x,y}}{2\pi N} \quad (5)$$

for CLRs coupled with the $(\pm 1, 0)$ or $(0, \pm 1)$ Wood–Rayleigh anomaly with $\lambda \approx h_x$ and $\lambda \approx h_y$, respectively. Therefore, for a given spectral width $\Delta\lambda_{\text{inf}}$ of the CLR for the infinite array [which is readily obtained via Eq. (4)], one can immediately get its size-dependent counterpart with $\Delta\lambda = \Delta\lambda_{\text{inf}} + \Delta\lambda_r$ without extensive simulations of finite-sized arrays.

Figure 4 compares analytical estimates of $\Delta\lambda$ with the corresponding numerical data from Fig. 2(b). One can see that, indeed, Eq. (5) provides reliable estimates of $\Delta\lambda$ for sufficiently large arrays ($N_{\text{tot}} > 30 \times 30$ and $N_{\text{tot}} > 70 \times 70$ for ED and MD, respectively). It is worthwhile to emphasize that the pronounced discrepancy between analytic approximation and numerical calculations for smaller arrays supports the claim that cross-interaction terms, ignored in Eq. (5), indeed matter for CLRs in finite-sized arrays, especially for the MD case.

Here, we have considered arrays of NPs embedded in a homogeneous environment under normal illumination via the coupled dipole approximation, which is a quite insightful approach valid for experimentally feasible setups [11]. Qualitatively similar effects are expected in homogeneous media with refractive index $\neq 1$ or under oblique incidence, though the position of the CLRs will be shifted due to the change in G^0 and/or $\alpha^{e,m}$ [11,30]. We also anticipate that reported finite-sized effects will likely emerge in a more sophisticated manner for higher-order electromagnetic interactions [46,60,61] or in non-homogeneous environments [62–65]. Even though we have limited the discussion to Si NPs, the obtained results are qualitatively valid for appropriately scaled arrays of dielectric particles from other materials [66] at corresponding frequencies, as long as CLRs are emerged. For instance, it is a well-known practice to verify concepts of all-dielectric nanophotonics with millimeter-sized ceramic particles under microwave illumination [7,21].

To conclude, we have shown that the *finite* size of arrays of dielectric NPs plays an important role for the emergence of both ED and MD CLRs. We have demonstrated that ED \leftrightarrow MD cross-interactions significantly contribute to both types of CLRs, even in sufficiently large NP arrays, where such interaction is usually considered to be negligible. While ED CLRs in finite-sized arrays converge to the infinite-array model for $\approx 50 \times 50$ NPs, MD CLRs in finite-sized arrays are quite different from the ones of infinite arrays even for 100×100 NPs; thus, the common use of numerical and theoretical models for *infinite* arrays should be handled with great caution. Given that a significant number of works on CLRs in all-dielectric nanostructures deal with numerical or theoretical considerations of *infinite* arrays, we believe that the reported results may lead to deeper understanding and more thoughtful research of

electromagnetic phenomena in this rapidly developing field of nanophotonics.

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