Coupled electric and magnetic dipole formulation for planar arrays of dipolar particles: metasurfaces with various electric and/or magnetic meta-atoms per unit cell

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The optical properties of infinite planar array of scattering particles, metasurfaces and metagratings, are attracting special attention lately for their rich phenomenology, including both plasmonic and high-refractive-index dielectric meta-atoms with a variety of electric and magnetic resonant responses. Herein we derive a coupled electric and magnetic dipole (CEMD) analytical formulation to describe the reflection and transmission of such periodic arrays, including specular and diffractive orders, valid in the spectral regimes where only dipolar multipoles are needed. Electric and/or magnetic dipoles with all three orientations arising in turn from a single or various meta-atoms per unit cell are considered. The 2D lattice Green function is rewritten in terms of a 1D (chain) version that fully converges and can be easily calculated. Modes emerging as poles of such lattice Green function can be extracted. This formulation can be applied to investigate a wealth of plasmonic, all-dielectric, and hybrid metasurfaces/metagratings of interest throughout the electromagnetic spectrum.

I. INTRODUCTION

Planar arrays of resonant particles are attracting a great deal of attention nowadays. Widely known as metasurfaces (sub-wavelength lattice constant, thus in the non-diffraction spectral regime) and metagratings (diffraction being relevant), they exhibit fascinating properties that indeed hold promise of infinitely thin optical devices performing a wealth of functionalities [1–13]. Although consisting in the beginning of metallic meta-atoms [5] typically supporting localized plasmons (mostly electric dipole) resonances, they have been extended in recent years to include high-refractive-index (HRI) particles which possess Mie resonances with a (lowest-order) magnetic dipole character [14–20].

Furthermore, the unconventional optical properties of metasurfaces stem not only from the resonant properties of the meta-atoms themselves, but also from multiple scattering effects through coupling with guided-mode or lattice resonances [21–27]. Dealing with such complex interactions between particle and lattice resonances in planar infinite arrays by means of full wave numerical calculations is a formidable tasks even for common available solvers, which in turn cannot shed much light onto the underlying physics. In this regard, coupled-dipole formulations have been developed since long ago [28, 29], extended to a wealth of configurations typically involving a finite number of dipoles. In this regard, the widely employed discrete dipole approximation is an extension of such coupled-dipole formulations to deal with macroscopic objects discretized through volume (dipolar) elements [30, 31]. Nonetheless, very few works have investigated infinite dipolar arrays thoroughly, especially for 2D planar arrays involving both electric and magnetic dipole resonances [32–36], the latter crucial to account for lowest-order Mie resonances of HRI particles.

In this work we analyze analytically the reflection and transmission of two-dimensional lattices of one or various meta-atoms supporting electric and/or magnetic dipolar resonances with arbitrary orientation in- and out-of-plane. We develop a coupled electric and magnetic dipole (CEMD) formulation that fully accounts for the coupling between those electric and magnetic dipolar fields. In fact, this CEMD formulation has been successfully exploited to deal with HRI disk metasurfaces [35] and rod dimer arrays [36], but most details remain unpublished. Here we also incorporate a significant improvement, pertaining to the calculation of the so-called 2D lattice Green function (from which all relevant magnitudes are derived): rather than extracting it numerically through convergence, we rewrite it in terms of a 1D lattice Green function that can be easily evaluated. Finally, we also analyze the emergence of various lattice modes from the poles of the thus obtained Green function.

II. FORMULATION OF THE SCATTERING PROBLEM

Let us consider an infinite set of identical particles arranged in a rectangular array. Without loss of generality, the particle labeled as \((n, m)\) is placed at

\[
\mathbf{r}_{nm} = x_n \hat{x} + y_n \hat{y} = na \hat{x} + mb \hat{y},
\]

where \(a\) and \(b\) are the lattice constants along the \(x\) and \(y\) axis, respectively. The array is then illuminated by an external plane wave, \(\Psi^{(0)}(\mathbf{r})\), with incident wavevector \(\mathbf{k}^{(0)} = k_x^{(0)} \hat{x} + k_y^{(0)} \hat{y} + k_z^{(0)} \hat{z}\), while the time dependence \(\exp(-i\omega t)\) will be assumed for all the fields; \(\omega\) is the angular frequency, related to the modulus of the wavevector through \(k = \omega/c\), \(c\) being the speed of light.
Each particle in the array is excited by the external plane wave plus the waves scattered from the rest of the array. The self-consistent incident field, $\Psi_{\text{inc}}$, on the $(n,m) = (0,0)$ particle ($r_{00} = 0$), is then given by the solution of

$$
\Psi_{\text{inc}}(0) = \Psi(0) + \sum_{n,m} k^2 \mathcal{G}_{nm} (r_{nm}) e^{i\phi_{nm}} \Psi_{\text{inc}}(r_{nm}),
$$

where $\sum_{nm} '$ means that the sum runs for all indices except for $(n,m) = (0,0)$. $\mathcal{G}$ and $\mathcal{A}$ are matrices representing the dyadic Green function and the dipolar polarizability of the particles, respectively, and their representations depend on the chosen basis to describe the electromagnetic fields, $\Psi$.

For a periodic array and plane wave illumination, the Bloch’s theorem holds, $\Psi_{\text{inc}}(r_{nm}) = \Psi_{\text{inc}}(0) \exp(ik_z^{(0)} na) \exp(ik_y^{(0)} mb) = \Psi_{\text{inc}}(0) e^{i\phi_{nm}}$, and the self-consistent incident field can be written as

$$
\Psi_{\text{inc}}(0) = \Psi(0) + k^2 \sum_{n,m} \mathcal{G}_{nm} (r_{nm}) e^{i\phi_{nm}} \mathcal{A} \Psi_{\text{inc}}(0).
$$

We have defined $\mathcal{G}_{b}$, the lattice ‘depolarization’ dyadic (or return Green function), as

$$
\mathcal{G}_{b} = \sum_{n,m} \mathcal{G}_{nm} (r_{nm}) e^{i\phi_{nm}}.
$$

$\mathcal{G}_{b}$ tells us about the coupling strength between particles, and is crucial to determine all the lattice properties. Next, the solution of the self-consistent equation can be formally written as a function of the external plane wave as:

$$
\Psi_{\text{inc}}(0) = \left[ I - k^2 \mathcal{G}_{b} \mathcal{A} \right]^{-1} \Psi(0).
$$

where $I$ is the unit dyadic.

Once we know the self-consistent incoming field, Eq. (5), the field scattered by the $(n,m)$ particle is given by

$$
\Psi_{\text{scat}}(r) = k^2 \mathcal{G}_{b} (r - r_{nm}) \mathcal{A} \Psi_{\text{inc}}(r_{nm}),
$$

and the total scattered field can be written as

$$
\Psi_{\text{scat-tot}}(r) = k^2 \sum_{n,m} \mathcal{G}_{nm} (r - r_{nm}) e^{i\phi_{nm}} \mathcal{A} \Psi_{\text{inc}}(0)
$$

$$
= k^2 \mathcal{G}_{b}^{\pm}(r) \mathcal{A} \Psi_{\text{inc}}(0),
$$

where the tensor lattice sum $\mathcal{G}_{b}^{\pm}(r)$ can be written as a sum over all diffracted spectral orders $(l,p = \cdots, -2, -1, 0, 1, 2 \cdots)$ as:

$$
\mathcal{G}_{b}^{\pm}(r) \equiv \sum_{nm} \mathcal{G}(r - r_{nm}) e^{i\phi_{nm}}
$$

$$
= \sum_{l,p} \mathcal{G}_{lp}^{\pm} \exp(ik_x l a) \exp(ik_y m b) \exp(ik_z^{(l,p)} z),
$$

$$
= \sum_{l,p} \mathcal{G}_{lp}^{\pm} e^{i\phi_{lp}},
$$

where, for $k_z^{(0)} > 0$, “+” (“−”) corresponds to upward scattered waves in the region $z > 0$ (downwards reflected waves in the region $z < 0$). $k_x^{(l)}$, $k_y^{(p)}$, and $k_z^{(l,p)}$ are the wavevectors of the diffracted orders

$$
k_x^{(l)} = k_x^{(0)} - \frac{2\pi l}{a}, \quad k_y^{(l)} = k_y^{(0)} - \frac{2\pi p}{b},
$$

$$
k_z^{(l,p)} = \sqrt{k^2 - (k_x^{(l)})^2 - (k_y^{(p)})^2}.
$$

Finally, using Eq. (5) in Eq. (7), the reflected and transmitted fields are then given by

$$
\Psi_{r}(r) = k^2 \mathcal{G}_{b}^{-} (r) \mathcal{A} \Psi(0),
$$

$$
\Psi_{t}(r) = k^2 \mathcal{G}_{b}^{+} (r) \mathcal{A} \Psi(0),
$$

where $\mathcal{A}$ is the renormalized (dressed) polarizability,

$$
\mathcal{A} = \mathcal{A} \left[ I - k^2 \mathcal{G}_{b} \right]^{-1} = \left[ \mathcal{A}^{-1} - k^2 \mathcal{G}_{b} \right]^{-1}.
$$

Writing $\mathcal{G}_{b}^{\pm}(r)$ as a sum over diffracted spectral orders, the field scattered into each diffractive mode is

$$
\Psi_{r}(l,p) (r) = k^2 \mathcal{G}_{b}^{-} (r) \mathcal{A} \Psi(0) e^{-i\phi_{lp}},
$$

$$
\Psi_{t}(l,p) (r) = k^2 \mathcal{G}_{b}^{+} (r) \mathcal{A} \Psi(0) e^{i\phi_{lp}}.
$$

III. LATTICE DEPOLARIZATION GREEN FUNCTION FOR ARBITRARY 2D ARRAYS

The optical properties of periodic arrays are then described by the lattice depolarization Green function, $\mathcal{G}_{b}$, that accounts for the electromagnetic field scattered by all the array over its own particles. The evaluation of $\mathcal{G}_{b}$ can be done in real space, but the convergence is in general very low. Although there are mathematical techniques to improve the convergence, [37], it is more convenient to transform the sum from the real to the reciprocal space. For example, for complex frequencies the sum cannot be evaluated in the real space. Actually, the techniques to improve the convergence, [37], it is more convenient to transform the sum from the real to the reciprocal space. For example, for complex frequencies the sum cannot be evaluated in the real space. Actually, the (complex) resonant frequencies of the metasurface can be only found in the reciprocal space, which in turn yields more physical insights and approximate expressions close to the Rayleigh-Wood anomalies. To simplify the expressions, the sum for a 2D array of particles will be described below as that for a 1D array, namely, a chain of particles. To this end, let us first study the scattering properties of a chain of particles.
A. Scattered field by a chain of particles

The scattering properties of an individual particle are derived from the scalar Green function, \( g(\mathbf{r} - \mathbf{r}') \), defined as the solution of the Helmholtz equation with a point source located at \( \mathbf{r} = \mathbf{r}' \):

\[
\nabla^2 g(\mathbf{r} - \mathbf{r}') + k^2 g(\mathbf{r} - \mathbf{r}') = -\delta(\mathbf{r} - \mathbf{r}'),
\]

(15)

where \( \mathbf{r} \) is the observation point, \( \mathbf{r}' \) is the position of the emitter/source, and \( k \) is the wavevector in the media. The scalar Green function in 3D is a spherical wave that propagates away from its origin

\[
g(\mathbf{r} - \mathbf{r}') = \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|} = \int \frac{dQ_x dQ_y e^{iQ_x(x-x')} e^{iQ_y(y-y')}}{4\pi^2} e^{i|\mathbf{r}-\mathbf{r}'|},
\]

\( q = \sqrt{k^2 - Q_x^2 - Q_y^2}, \)

(16)

wherein we have used the Weyl expansion to express it as a sum of plane waves. The dyadic Green function, \( \mathbf{G}(\mathbf{r} - \mathbf{r}') \), is obtained from \( g(\mathbf{r} - \mathbf{r}') \) by applying a linear differential operator, \( \mathbf{L} \), that depends on the basis chosen to describe the electromagnetic fields.

Now let us consider a periodic chain of particles along the \( x \) axis located at the position \( \mathbf{r}_n \), \( a \) being the separation between particles. Upon the incidence of an external plane wave (with incident wavevector, \( \mathbf{k}^{(0)} = k_x^{(0)} \hat{x} + k_y^{(0)} \hat{y} + k_z^{(0)} \hat{z} \)), the scattering properties of the chain of particles are defined by the next sum in the real space:

\[
\sum_n \mathbf{G}(\mathbf{r} - \mathbf{r}_n) e^{ik_x^{(0)}na} = \mathbf{L} \sum_n g(\mathbf{r} - \mathbf{r}_n) e^{ik_x^{(0)}na},
\]

(18)

where \( k_x^{(0)} \) is the projection of the incident wavevector along the \( x \) axis. The linear differential operator is made of spatial derivatives, independent of the summation variable \( n \), so it can be removed from the summation. After some algebraic manipulations (using the Weyl representation), the sum in the real space can be rewritten in the reciprocal space as:

\[
\sum_n g(\mathbf{r} - \mathbf{r}_n) e^{ik_x^{(0)}na} = \sum_l e^{ik_l^{(l)}x} \frac{1}{4a} H_0(k_l^{(l)} \rho),
\]

(19)

where \( H_0 \) is the 0th-order Hankel function of the first type with \( \rho = (y^2 + z^2)^{1/2} \) in its argument being the radial distance to the chain of particles; \( k_l^{(l)} \) and \( k_x^{(l)} \) are the wavevector components of the diffracted waves

\[
k_l^{(l)} = \sqrt{k^2 - (k_x^{(l)})^2}, \quad k_x^{(l)} = k_x^{(0)} - \frac{2\pi}{a} l.
\]

(20)

The scalar Green function in 2D with translational symmetry along the \( x \) axis (i.e., for an infinitely long cylinder where the \( x \) axis is the cylinder axis) is

\[
g_{2D}(\mathbf{r} - \mathbf{r}_n) = \frac{1}{4} H_0 \left( \sqrt{k^2 - k_x^2} |\mathbf{r} - \mathbf{r}_n| \right) e^{ik_x x}.
\]

(21)

Thus, Eq. (19) can be written as:

\[
\sum_n g(\mathbf{k}, \mathbf{r} - \mathbf{r}_n) e^{ik_x^{(0)}na} = \sum_l \frac{1}{a} g_{2D}(\mathbf{k}, k_x^{(l)} \mathbf{r} - \mathbf{r}_n),
\]

(22)

where we have explicitly added the wavevector as an argument in the scalar Green functions (normally this is omitted).

Therefore, from Eq. (22) we can infer that a chain of particles behaves effectively as an infinitely long cylinder that is however excited by both propagating and evanescent plane waves. There is always a propagating wave that coincides with an incident external plane wave, while the rest of propagating waves appears as a diffraction phenomenology when the lattice constant \( a \) exceeds the incoming wavelength \( \lambda = 2\pi/k \). Thus, only terms with \( \text{Im}[k_l^{(l)}] = 0 \) survive in the far field, whereas in the near field there are contributions from all waves.

The other key element to describe the optical response of a chain of particles is the lattice depolarization Green function, that is defined for this system as

\[
\mathbf{G}_{b-C} (\mathbf{r}, \mathbf{k}, k_x^{(0)}) = \mathbf{L} \sum_n g(\mathbf{r} - \mathbf{r}_n) e^{ik_x^{(0)}na}.
\]

(23)

Importantly, \( \mathbf{G}_{b-C} \) can be expressed in terms of analytical functions called polylogarithm functions.

B. Rectangular arrays

Now we have the tools to tackle the problem of the two dimensional rectangular array of particles. By using \( \mathbf{L} \), Eq. (4) can be rewritten as:

\[
\mathbf{G}_b = \sum_{nm} \mathbf{G}(\mathbf{r}_{nm}) e^{i\phi_{nm}} = \mathbf{L} \sum_{nm} g(\mathbf{r}_{nm}) e^{i\phi_{nm}}.
\]

(24)

From Eq. (22) we learn that a 2D array of particles can be seen as a 1D array of chains of particles. Assuming that the chains are along the \( x \) axis, the effective cylinders (that the chains represent) are placed at \( \mathbf{r}_{nm} = m\hat{y} \). Within this convention, it is straightforward to show that

\[
\mathbf{G}_b = \mathbf{G}_{b-C} + \frac{1}{a} \left( \sum_l \mathbf{G}_{b-1D}^{(l)} \right),
\]

(25)

where \( \mathbf{G}_{b-C} \) is the ‘depolarization’ dyadic of a chain of particles defined in Eq. (23) and \( \mathbf{G}_{b-1D}^{(l)} \) is the ‘depolarization’ dyadic of a 1D array of cylinders (with their axis
along the $x$ axis):
\[
\mathcal{G}_{b-1D}^{(l)}(b, k, k_0^x, k_0^y, r) = \mathcal{L} \sum_m \mathcal{G}_{2D}(k, k_0^x, -r_m) \mathcal{e}^{ik_0^y m b}. \quad (26)
\]

In both cases all arguments of the functions are shown explicitly. The importance of writing $\mathcal{G}_b$ as shown in Eq. (25) is that analytical expressions are available for Eq. 23 and Eq. 26 in the reciprocal space. Also, although the summation in Eq. 25 runs over infinite diffraction orders $l$, only a few orders are needed to achieve a good convergence.

C. 2D arrays with arbitrary lattice symmetry

For completeness, let us next consider a generic 2D array of particles defined by the lattice constants $a$ and $b$ with corresponding lattice vectors forming an angle $\theta$ between them. Then, if the primitive vector associated to the lattice constant $a$ is taken along the $x$ axis, the position of the particle labeled as $(n, m)$ becomes
\[
r_{nm} = (na + m \cos \theta) \hat{x} + m \sin \theta \hat{y}. \quad (27)
\]

For example, the rectangular lattice is recovered for $\theta = \pi/2$, while $\theta = \pi/3$ and $a = b$ yield a triangular lattice. Using this description the lattice depolarization dyadic, $\mathcal{G}_b$, follows the same expression shown in Eq. (25) but with some changes in the arguments of the functions:
\[
b \to b \sin \theta, \quad \quad \quad (28)
\]
\[
k_y^{(0)} \to k_y^{(0)} - \frac{2\pi}{a} l \frac{\cos \theta}{\sin \theta}. \quad (29)
\]

Thus, $\mathcal{G}_{b-C}^{CH}$ does not change
\[
\mathcal{G}_{b-C}^{CH}(a, k, k_0^{(0)}) \to \mathcal{G}_{b-C}^{CH}(a, k, k_0^{(0)}) \quad (30)
\]

while the arguments of $\mathcal{G}_{b-1D}$ are modified
\[
\mathcal{G}_{b-1D}^{(l)}(b, k, k_0^x, k_0^y, r) \to \mathcal{G}_{b-1D}^{(l)}(b \sin \theta, k, k_0^y - \frac{2\pi}{a} l \frac{\cos \theta}{\sin \theta}, k_0^x). \quad (31)
\]

Alternatively, it is possible to define the chains of particles along the direction $\hat{u} = \cos \theta \hat{x} + \sin \theta \hat{y}$.

D. Complex unit cells

In general, the unit cell may in turn be composed of more than one particle. The self-interaction between the particles of the same kind is still described by $\mathcal{G}_b$, but it is necessary to also account for the interaction between the different particles within the unit cell. Interestingly, this interaction is easy to express in the reciprocal space through the tensor lattice sums by
\[
\mathcal{G}_{ij}^{CH} = \left[ \mathcal{G}_b^{(0)}(r_i - r_j) + \mathcal{G}_b^{(0)}(r_i - r_j) \right]/2, \quad \text{where } r_i \text{ and } r_j \text{ are the positions of particles } i \text{ and } j \text{ within the unit cell, respectively. Nonetheless, if two different particles are in the same } xy \text{ plane, the convergence is slow, but it can be improved using convergence techniques.}
\]

IV. RESONANCES AND BOUND STATES IN THE CONTINUUM IN METASURFACES

In order to find the resonant states of the metasurfaces we need to find solution to Eq. (5) in the absence of the external wave. At the condition $\Psi^{(0)} = 0$, Eq. (5) becomes a homogeneous linear system of equations that supports solutions only when
\[
\left| \mathbf{T} - k^2 \mathcal{G}_b \mathbf{\alpha} \right| = \left| \frac{1}{k^2 \mathbf{\alpha}} - \mathcal{G}_b \mathbf{\alpha} \right| = 0. \quad (32)
\]

The complex frequencies at which Eq. (32) is satisfied are the eigenfrequencies, denoted by $\nu$. In the latter eigenmode equation, it is more convenient to use the second expression than the first one. Also, in this context, $k_x^{(0)}$ and $k_y^{(0)}$ are the in-plane wavevector components of the surface wave represented by the resonant mode. The eigenmode equations is written in the case of one particle per unit cell. For complex unit cells, $\mathbf{\alpha}$ is a matrix with the polarizability terms of all particles. In addition, $\mathcal{G}_b$ must be replaced by a matrix that contains $\mathcal{G}_b$ and also the interaction matrices $\mathcal{G}_{ij}$ (the specific form of these matrices to be determined by the basis chosen to describe the fields). Since $\mathcal{G}_b$ and $\mathcal{G}_{ij}$ can be expressed in the reciprocal space, Eq. (32) can be thus employed to solve for the resonant modes of the metasurface.

Below the light line (and below diffraction), the solutions of Eq. (32) are real and determine the dispersion relation of guided modes that propagate along the metasurface. Opposite, above the light line the solutions are normally given by complex frequencies. The quality factor of the resulting mode is defined as the ratio between the real and the imaginary parts of the frequency, informing us on how fast the system leaks energy out to the continuum of radiation. However, it is also possible to find real solutions in this region, called bound states in the continuum [35, 36](BICs). Although they are embedded in the continuum of radiation, for symmetry reasons or interference effects these state remain localized within the metasurface without emitting energy to the far field [38].
V. PRACTICAL CASE: SQUARE ARRAY OF DIELECTRIC SPHERES

Let us consider a specific case: a square array of dielectric spheres of constant dielectric permittivity \( \epsilon = 3.5 \) (similar to that of Si in the visible and near-IR), with normalized lattice constant \( a / R = b / R = 4 \), where \( R \) is the sphere radius. To describe the electromagnetic field, we choose the following basis:

\[
\Psi(r) = \begin{bmatrix} E(r) \\ ZH(r) \end{bmatrix}, \quad E(r) = \begin{bmatrix} E_x(r) \\ E_y(r) \end{bmatrix}, \quad H(r) = \begin{bmatrix} H_x(r) \\ H_y(r) \end{bmatrix},
\]

(33)

\( E(r) \) and \( H(r) \) being the electric and magnetic vector fields defined in Cartesian coordinates and \( Z = (\mu_0 / \epsilon_0)^{1/2} \) the vacuum impedance. The linear differential operator \( \mathcal{L} \) takes the form

\[
\mathcal{L} = \begin{pmatrix} I + \frac{\nabla}{\epsilon} & i \frac{\nabla}{\epsilon} \\ -i \frac{\nabla}{\epsilon} \times I & I + \frac{\nabla}{\epsilon} \end{pmatrix},
\]

(34)

We assume that the sphere electrodynamical response can be fully described by its electric and magnetic dipolar contributions in terms of a polarizability tensor \([39, 40]\), \( \tilde{\alpha} \):

\[
\tilde{\alpha} = \begin{pmatrix} \alpha^{(e)} & 0 \\ 0 & \alpha^{(m)} \end{pmatrix},
\]

(35a)

\[
k^2 \alpha^{(e)} = \frac{6\pi}{k} a_1 \mathbf{T}, \quad k^2 \alpha^{(m)} = \frac{6\pi}{k} b_1 \mathbf{T},
\]

(35b)

where \( \alpha^{(e)} \) and \( \alpha^{(m)} \) are the electric and magnetic polarizabilities, and \( a_1 \) and \( b_1 \) are the (dimensionless) Mie coefficients [29].

Within this description and for incidence along the \( x \) axis, the specular reflectance, \( R_0 \), for both \( p \)- and \( s \)-polarized fields is:

\[
R_0^{(p)} = \left( \frac{k^2}{2kab \cos \theta_0} \right)^2 \left| \gamma^{(p)} \left( \frac{\alpha_y^{(m)}}{\alpha_z^{(e)}} \right) \frac{\sin^2 \theta_0}{\cos^2 \theta_0} \right|^2,
\]

(36a)

\[
R_0^{(s)} = \left( \frac{k^2}{2kab \cos \theta_0} \right)^2 \left| \gamma^{(s)} \left( \frac{\alpha_y^{(e)}}{\alpha_z^{(m)}} \right) \sin^2 \theta_0 \right|^2,
\]

(36b)

where \( \theta_0 \) is the angle of incidence \( (k_x^{(0)} = k \cos \theta_0, k_z^{(0)} = k \sin \theta_0) \), and the renormalized polarizability terms in \( \tilde{\alpha} \) are:

\[
k^2 \alpha_z^{(e)} = \frac{1}{k^2 \alpha_z^{(e)} - G_{bi}}^{-1},
\]

(37a)

\[
k^2 \alpha_z^{(m)} = \frac{1}{k^2 \alpha_z^{(m)} - G_{bi}}^{-1},
\]

(37b)

with

\[
\gamma^{(p)} = \frac{1}{1 - k^4 G_{bi}^2 \alpha_z^{(m)} \alpha_z^{(e)}},
\]

(38a)

\[
\gamma^{(s)} = \frac{1}{1 - k^4 G_{bi}^2 \alpha_z^{(e)} \alpha_z^{(m)}},
\]

(38b)

\( G_{bi} \) and \( G_{bxz} \) being the matrix elements of \( \tilde{\alpha} \). The polarization is defined in such away that \( p \) (respectively, \( s \)) stands for TM (respectively, TE). It should be noted that this convention is the opposite of that in Ref. [25], where the "transverse" polarization was defined for the sake of convenience with respect to the cylinder axis, rather than with respect to the plane of incidence.

On the other hand, Eq. (32) can be used to find the resonant modes supported by the metasurface. For those modes propagating along the \( x \) axis \( (k_x^{(0)} \neq 0 \) and \( k_y^{(0)} = 0) \), although in this case the wavevector is not related to any incident external plane wave, Eq. (32) reduces to

\[
\left| \eta_x^{(e)} \right| \times \left| \eta_x^{(m)} \right| \times \left| \eta_y^{(em)} \right| \times \left| \eta_y^{(me)} \right| = 0,
\]

(39)

with

\[
\eta_x^{(e)} = \frac{1}{k^2 \alpha_x^{(e)}}, \quad \eta_y^{(em)} = \frac{1}{k^4 \alpha_y^{(e)} \alpha_z^{(m)}}, \quad G_{byz}^2,
\]

(40)

Each term in Eq. 39 is associated to a different resonant surface mode. The solutions of \( \eta_x^{(e)} \) and \( \eta_x^{(m)} \) represent coherent oscillations of electric and magnetic dipoles along the \( x \) axis, respectively. Since the imaginary part of \( 1/\tilde{\alpha}_z^{(e,m)} \) (for lossless particles) vanishes only at \( k_x^{(0)} \approx k \), they can never lead to a BIC; inside the continuum of radiation they represent broad resonant (leaky) modes that radiate energy to the far field. More interesting are the terms \( \eta_y^{(em)} \) and \( \eta_y^{(me)} \). They represent hybrid modes where electric (magnetic) dipoles along the \( y \) axis are coupled with magnetic (electric) dipoles along the \( z \) axis. These terms can yield BICs due to the mutual interference between the different dipolar modes, although in general they correspond to broad resonant modes. Nonetheless, at \( k_x^{(0)} = 0 \), both \( G_{byz} = 0 \) and the imaginary part of \( 1/\tilde{\alpha}_z \) are zero. Then, the dipolar modes are decoupled and the metasurface can support a BIC given by the in-phase oscillation of dipoles along the \( z \) axis. This BIC is the typical one used in several applications []. In addition, all terms can support guided modes in the region defined by \( k_x^{(0)} \geq k \) and \( k_x^{(0)} \leq 2\pi/\omega - k \) (with \( k \geq 0 \) and \( k_x^{(0)} \geq 0 \)), where the imaginary part (for lossless particles) of Eq. 39 is identically zero.

To show the interplay of the resonant mode on the properties of the metasurface we study the specular reflectance, \( R_0 \), for both polarizations. First, in Fig. 1a) the specular reflectance for TM polarized light and the dispersion relation of the resonant modes are shown as a
function of the normalized frequency and angle of incidence. Due to the symmetry of the resonant modes not all of them can be exited at a given polarization (keep in mind that $k_z^{(0)} = 0$), so we only show the modes related to the zeros of $\eta_x^{(e)}$ and $\eta_{yz}^{(me)}$. Since the incident polarization determines the nature of the mode (electric or magnetic), for the sake of clarity the superscript is replaced by a number that label the mode solution. As expected, the resonances of the reflectance coincide with dispersion relation of the surface modes. In addition, their widths agree with the Q-factor of the modes, displaying in Fig. 1b). The Q-factor is calculated as the ratio between the real and imaginary part of the eigenfrequency, $\nu = \nu' + i\nu''$. For simplicity we only represent the modes in the non-diffracting region (delimited by the white dashed line), but Eq. 39 still have solutions in this region.

Around $ka/(2\pi) = 0.56$ there is the $\eta_{yz}^{(1)}$ resonant (leaky) surface mode. Its associate resonance in the reflectance spectra is broad at normal incidence, and it becomes narrower as long as the angle of incidence increases. The Q-factor of the leaky surface mode diverges at $k_z^{(0)} = k$, point where the leaky mode becomes a guided mode. Later, as the frequency increases in the reflectance we find a narrow resonance around $ka/(2\pi) = 0.72$, related to the $\eta_{yz}^{(2)}$ surface mode. At normal incidence this mode represents a symmetry protected BIC (in-phase oscillation of electric dipoles along the z axis) that becomes broader as the angle of incidence increase. However, due to diffraction, the dispersion relation of the modes stops at the diffraction line. Finally, the last surface mode encloses in the studied frequency windows is $\eta_x^{(1)}$. The width of the surface resonance in almost constant as a function of the angle of incidence and as before its dispersion relation stops at diffraction.

The agreement between the dispersion relation of the surface resonant modes and the resonances in the reflectance spectra is further confirmed for TE incident waves, as it can be seen in Fig. 2. Now, for this polarization $\eta_x^{(m)}$ and $\eta_{yz}^{(em)}$ are the relevant modes that can be excited by the incident external wave. Around $ka/(2\pi) = 0.57$, at normal incidence there are two modes, $\eta_x^{(1)}$ and $\eta_{yz}^{(1)}$. The characteristics of $\eta_x^{(1)}$ are similar that the ones observer in TM polarization its electric counterpart. The mode is relative broad and presents low dispersion in frequency that end up at the diffraction line. Opposite, $\eta_{yz}^{(1)}$ posses more interesting features. First, at normal incidence it represents a symmetry protected BIC given by in-phase oscillation of magnetic dipoles along the z axis. As $k_z^{(0)}$ increases the surface mode becomes broader and evolves until a minimum in the Q-factor. From this point, the mode becomes narrower again and the Q-factor finally diverges around $\theta = 45^{\circ}$; the surface modes turns into an accidental BIC given by the destructively interference at the far field between the emission of the electric dipoles along the y axis and the magnetic dipoles along the z axis. Lastly, the Q-factor decreases to another minimum and diverges once again at $\theta = 90^{\circ}$, where the surface mode becomes a guided mode. For the sake of completeness, the last surface mode shown in Fig. 2 is $\eta_{yz}^{(2)}$, placed around $ka/(2\pi) = 0.75$. This mode is much boarder than $\eta_{yz}^{(1)}$, although both modes come from to the same term ($\eta_{yz}^{(em)}$). Also, its dispersion relation stops at the diffraction line.

The mode $\eta_{yz}^{(1)}$ that comes from $\eta_{yz}^{(em)}$ is very narrow in all regions, so the their features on the reflectance spectra Fig. 2a) are hidden by the dashed line that marks the dispersion relation. Thus, lets take a closer view of this region in Fig. 3a), where a zoom on the reflectance for TE polarization is done. Strong asymmetry Fano resonances in the reflectance can be appreciated through out all angles of incidence. The asymmetry of the resonance will...
FIG. 3. (a) Zoom to the reflectance for TE polarization from Fig. 2 in the region of the accidental BIC. The white dashed lines delimit the diffractive region. (b) Imaginary part of the eigenvalue of the narrow $\eta_{yz}^{(em)}$ mode.

depend on the interference given by the rest of surface modes present in the metasurface. Also, the resonance shows vanishing features distinctive of BIC at normal incidence, around $\theta = 45^\circ$ and at grazing incidence, that correspond to the symmetry protected BIC, the accidental BIC and the connection to the guided mode, respectively.

In order to characterize the surface hybrid mode, Fig. 3b) shows the imaginary part of the eigenvalue (inversely proportional to the Q-factor), whose zeros coincide with the BICs (and with the guided mode). In addition, the color of the line represents the eigenvector of the mode. The red color means that the mode is made purely of magnetic dipoles along the $z$ axis, while the line turns into blue as long as the nature of the mode becomes more hybrid. As predicted, the eigenvalue of the symmetry protected BIC has no $p_y$ component, it is formed only by the oscillation of magnetic $m_z$ dipoles. Contrary, the accidental BIC is a hybrid mode, where the mutual interference between the emission of $p_y$ and $m_z$ cancels out at that specific configuration.

VI. CONCLUSIONS

We have developed a coupled electric and magnetic dipole (CEMD) analytical formulation to describe the reflection and transmission of planar arrays of electric and/or magnetic particles, including specular and diffractive orders, and modes emerging as poles of such lattice Green function can be extracted. The formulation is largely simplified by rewriting the 2D lattice Green function in terms of a 1D (chain) version that fully converges. Electric and/or magnetic dipoles with all three orientations arising in turn from a single or various meta-atoms per unit cell are considered. Analytical expressions for the emergence of either guided or resonant modes are given, along with corresponding Q-factors, which allow us to identify bound states in the continuum. By way of example, both symmetry-protected and accidental BICs are identified for a square array of all-dielectric spheres with constant dielectric permittivity close to that of Si in the visible and near-IR. Despite limited to meta-atoms where there optical response is basically dipolar, this formulation can be exploited to deal with metasurfaces/metagratings of interest throughout the electromagnetic spectrum, bearing in mind that most plasmonic, all-dielectric, and/or hybrid meta-atoms, either at or out of resonance, behave in many spectral regimes as a combination of electric and magnetic dipoles.

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