Effective-medium description of a metasurface composed of a periodic array of nanoantennas coupled to a metallic film

P. T. Bowen, A. Baron, and D. R. Smith
Center for Metamaterials and Integrated Plasmonics and Department of Electrical and Computer Engineering, Duke University, Box 90291, Durham, North Carolina 27708
(Received 17 June 2016; published 20 March 2017)

We compute the reflectance properties of a metasurface that consists of a doubly periodic array of patch nanoantennas strongly coupled to a metallic film. Each plasmonic patch antenna can be accurately modeled as a polarizable, radiating, magnetic dipole. By accounting for interactions amongst the dipoles, an equivalent surface polarizability can be obtained, from which the effective surface impedance, reflectivity, and other homogenized quantities of interest can be obtained. When the metasurface is extremely close to the metal film, the interaction between constituent dipoles is dominated by surface plasmon mediation. We calculate analytically the dipole interaction constant by explicitly evaluating the infinite sum of fields from all the dipoles in the lattice. While a single film-coupled nanoparticle exhibits anomalous loss due to coupling to surface plasmons, we find that for the lattice of dipoles, the radiation reaction force due to the coupling to the surface plasmon modes is exactly canceled by the interaction constant; the lattice thereby conserves energy in the limit of zero Ohmic loss. When Ohmic losses are present, absorption to surface plasmons reemerges and can be compared with the losses to radiation and Ohmic absorption in the metasurface.

DOI: 10.1103/PhysRevA.95.033822

I. INTRODUCTION

Nanopatterned metasurfaces are of particular interest, as they offer a path to useful functionality while avoiding the large absorption often exhibited by volumetric metamaterials. Metasurfaces consisting of patterned slits or nanoantennas have been used to form a variety of holographic and diffractive optics, as well as surfaces that can absorb light over bandwidths selectable by design [1].

When metasurfaces involve plasmonic materials, field enhancement effects can become relevant, increasing the response of the scattering elements and introducing additional functionality. An important factor in controlling field enhancement is precise control over the gap dimension between nanometallic structures, since the magnitude of the field enhancement is typically a sensitive function of that spacing. One particular system that is relatively easy to fabricate and that allows excellent control over the gap dimensions is that of the nanopatch antenna, which consists of a nanoparticle with a planar facet (such as a cube, platelet or similar particle) separated by a dielectric layer from a metal film. With planar deposition techniques such as polymer self-assembly or atomic layer deposition, subnanometer accuracy of the insulating spacer layer can easily be achieved over large areas [2].

The nanopatch antenna is an especially convenient geometry for applying analytic methods. Similar to the patch antenna ubiquitous in radio frequency (RF) technology, the radiation, scattering, and many other properties of the nanopatch can be understood using relatively simple expressions. Because the nanopatch supports a transmissionlike resonance between the planar facet of the nanoparticle and the film [3] modified by the plasmonic response of the metalit can be effectively modeled as two polarizable magnetic dipoles [4,5]. For waves at normal incidence, the response of the nanopatch can be further simplified as a single magnetic dipole.

Unlike the lower frequency, RF patch antenna, a nanopatch resonant at optical wavelengths on a metal film can couple to surface plasmon modes, introducing an additional loss channel and compete with radiative losses. For many configurations of practical interest, it is desirable to maximize the radiative loss, such that the potential of surface plasmon coupling can be unwanted. In this work, we examine the role of the surface plasmons that are both emitted and reabsorbed by lattice, and compute the overall losses and coupling of the dipoles in the metasurface through surface plasmon modes using the framework of effective-medium theory.

Within effective-medium theory, materials and metamaterials are both defined as an ensemble of deeply subwavelength objects or elements, which under certain conditions will behave collectively as a homogeneous material. This ensemble of elements may be distributed randomly or periodically, and the elements that compose the material or metamaterial are assumed to be small enough to be well described as point dipoles. Lorentz was the first to propose in his doctoral thesis [6] in 1878 that a body of continuous material, as described by the macroscopic Maxwell's equations, should be described by point sources in vacuum which satisfy the microscopic Maxwell's equations, or Lorentz equations. According to Einstein, Lorentz thus famously "separated matter and ether" [7,8], providing a basic framework by which the effective material parameters used in the macroscopic Maxwell's equations might be derived from a given microscopic structure of point dipoles. Lorentz's early work was improved upon by Planck [8], Ewald [9], Madelung [10], Hoek [11], De Groot [12], and others who have collectively contributed to a long and rich history of relating the effective material parameters of a body to its microscopic structure. Ewald and Madelung in particular were the first to treat periodic crystals, while Lorentz, Planck, and Hoek were primarily concerned with gasses and amorphous solids. A good review of the early history and results of effective-medium theory is available in [8].

More recently, interest in effective-medium theory has revived with the popularization of metamaterals, which has brought new challenges to the classical homogenization approaches that were developed in the late 19th and early 20th centuries to model natural materials. Classical homogenization techniques were very commonly based on the assumption, which is originally attributed to Lorentz, that there exists a length scale Δ over which one might average the electric field, which is both much smaller than the wavelength λ and much larger than the lattice spacing a between the atoms [8,13], i.e.,

$$a \ll \Delta \ll \lambda. \tag{1}$$

However, metamaterials are designed to be resonant, and many metamaterial elements are resonant at wavelengths where $\lambda/10 < a < \lambda/2$ [2,4] since it can be difficult to design resonators that operate at a wavelength that is more than an order of magnitude larger than the physical dimension of the metamaterial element. In this regime spatial dispersion becomes an important effect, and the classical Lorentz-Lorenz relation will not apply, which has led authors to develop exact formulas for the interaction constant and homogenization of metamaterials and metasurfaces that have a larger lattice spacing relative to the wavelength [14–16]. These formulas are not only useful for the modeling of metamaterials [16–18], but also for the extraction of the exact polarizability of metamaterial elements from full-wave simulations [19].

In this work we focus on the homogenization of metasurfaces consisting of nanoparticles tightly coupled to a metallic film. Metasurfaces in this geometry are of significant interest in optics as absorbers [2], fluorescence enhancing surfaces [20], and single photon sources [21]. In each of these applications, a metasurface is close enough to a metal film to where the dipole elements that compose the metasurface couple to the surface through evanescent near fields. When a metasurface is placed a shorter distance from a metal film than the distance between the elements of the metasurface, the interaction between the metasurface and the film can no longer be treated with a transfer-matrix formalism based on the homogenized parameters of the metasurface, because the evanescent near fields of the dipoles will interact with the surface. In this case, the microscopic details of the metasurface need to be taken into account. When this happens, an additional loss mechanism is made available through surface plasmons, and it is no longer clear how the forces that the dipoles exert on one another will be modified when the interaction is mediated by surface plasmon modes. The question that this paper seeks to address is, how are the interaction constants between dipoles in a metasurface modified when a metasurface is tightly coupled to a metal film that supports surface plasmons?

We begin with a brief overview of the effective-medium theory framework that we will be using, presented in Sec. II. In Sec. III we explore a particular geometry of current interest in optics, which is a single metamaterial element with a magnetic response coupled to a metal film. An exact expression for the surface plasmon contribution to the interaction constant of a film-coupled metasurface is derived in Secs. IV and V, and it is shown that the interaction constant perfectly cancels the radiation reaction damping force due to the surface plasmon coupling. Although the radiative damping force due to the surface plasmon is perfectly canceled in the limit of no Ohmic losses, the interaction between the metamaterial elements produces a resonance frequency shift, which is given by the real part of the interaction constant. The resonance frequency shift is compared against full-wave simulations in Sec. VI by examining a perfect absorber made of a metasurface of patches that are coupled closely to a metal film, and it is thereby shown that the surface plasmon interaction dominates the coupling between the metamaterial elements. The theory also predicts the existence, depth, and position of Wood's anomalies, which are also compared with full-wave simulation results in Sec. VI.

II. EFFECTIVE-MEDIUM THEORY FRAMEWORK

There is a sense in which the polarizability of a dipole itself is not an inherent property of the dipole, but depends on the environment, and therefore may be considered a nonlocal property. Even vacuum is no exception, since the vacuum itself places certain requirements on what values the polarizability of a dipole may take. From the perspective of quantum electrodynamics, any geometry interacts with a dipole through vacuum states, which cause the dipole to spontaneously emit and therefore decay.

This phenomenon is not, however, unique to quantum electrodynamics, and can also be seen in the classical realm. Here we derive the complex polarizability of a point dipole, following a treatment similar to what is presented in Refs. [13,22]. Consider a single dipole that is placed at position $\mathbf{r}_0$ in an environment that is described by a Green's function $\mathbf{G}(k,\mathbf{r},\mathbf{r}')$, and imagine that the environment is illuminated by some incident electric field $\mathbf{E}_0$. The total field in the environment $\mathbf{E}$ at wave number $k = \omega/c$ will be

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_0(\mathbf{r}) + \epsilon_0^{-1}\mathbf{G}(k,\mathbf{r},\mathbf{r}_0)\mathbf{p}. \tag{2}$$

The polarizability of a dipole is the tensor that defines the proportionality between the dipole moment and the field. However, there are two possible ways in which this polarizability might be defined. The polarizability might be expressed as the proportionality with the total field experienced by the dipole, $\mathbf{p} = \bar{\alpha}_e^0\mathbf{E}$. We define $\bar{\alpha}_e^0$ as the inherent polarizability of the dipole, since all interactions with the environment are contained in $\mathbf{E}$ rather than in the polarizability, and therefore $\bar{\alpha}_e^0$ does not change when the environment changes. The alternative definition of the polarizability is $\mathbf{p} = \bar{\alpha}_e\mathbf{E}_0$, which is the effective polarizability of the dipole, since it is a quantity that is dependent on the environment in which the dipole is placed. The effective polarizability can be found directly from Eq. (2),

$$\bar{\alpha}_e = \bar{\alpha}_e^0\left[1 - \epsilon_0^{-1}\mathbf{G}(k,\mathbf{r}_0,\mathbf{r}_0)\bar{\alpha}_e^0\right]^{-1}. \tag{3}$$

The real part of Green's tensor at the origin is generally singular or undefined. A good discussion of the nature of the singularity of Green's functions is available in [23–25]. In this work, we disregard the real part of Green's tensor at the origin for a dipole in free space, since it does not lead to any restrictions on the range of values that the effective polarizability may take, and hence makes it impossible to observe a difference between the inherent and effective polarizability due to the real part of the Green's function. In Ref. [13] it was pointed out that the real part may be ignored by renormalization, and that only the imaginary part is of physical significance.

The imaginary part of Green's tensor at the origin, however, is always finite, and according to Poynting's theorem corresponds to the power loss of fields radiated by the dipole. A careful calculation of the limiting form of Green's tensor at the origin for a dipole in free space shows that [26]

$$\mathbf{G}(k,\mathbf{r}_0,\mathbf{r}_0) = -i\frac{k^3}{6\pi}\mathbf{I}, \tag{4}$$

and so the effective polarizability of a dipole in free space is

$$\bar{\alpha}_e = \bar{\alpha}_e^0\left(1 + ik^3\bar{\alpha}_e^0/6\pi\epsilon_0\right)^{-1}. \tag{5}$$

This is the well-known radiation reaction correction, which corrects the polarizability in order to account for the force that a radiating dipole exerts on itself so that its amplitude decays in time according to the energy that is radiated from the dipole.

Similar to the manner in which an effective polarizability might be formed for a single dipole, an effective polarizability might be formed by any arrangement of dipoles where there is sufficient symmetry in the system and incident field $\mathbf{E}_0$ to require that the dipole moments of these dipoles must be equal. Under this assumption, the total field incident on the ith dipole can be written as the sum of the incident field plus the sum of the fields radiated by all the dipoles in the space,

$$\mathbf{E}(\mathbf{r}_i) = \bar{\alpha}^{-1}\mathbf{p}_i = \mathbf{E}_0(\mathbf{r}_i) + \epsilon_0^{-1}\sum_j \mathbf{G}(\mathbf{r}_j - \mathbf{r}_i)\mathbf{p}_j, \tag{6}$$

where the $j = i$ term in the sum represents the self-interaction of the dipole. The Green's function here has been reduced to a function of a single argument of the distance between dipoles, which can be done when the dipoles are placed in free space. All of the $\mathbf{p}_i$ terms may be collected to give

$$\left(\bar{\alpha}_e^{-1} - \epsilon_0^{-1}\mathbf{G}(\mathbf{0})\right)\mathbf{p}_i = \mathbf{E}_0(\mathbf{r}_i) + \epsilon_0^{-1}\sum_{j\neq i} \mathbf{G}(\mathbf{r}_j - \mathbf{r}_i)\mathbf{p}_j. \tag{7}$$

Moreover, if it is known by the symmetry of the problem that $\mathbf{p}_j = \mathbf{p}_i$ for all j, then the equation may be rewritten in the form,

$$\mathbf{p}_i = \left(\bar{\alpha}^{-1} - \epsilon_0^{-1}\sum_j \mathbf{G}(\mathbf{r}_j - \mathbf{r}_i)\right)^{-1}\mathbf{E}_0(\mathbf{r}_i). \tag{8}$$

The quantity in the parentheses becomes the new effective polarizability, and the infinite sum over the Green's function is typically defined as the interaction constant [14,16,27],

$$\mathbf{C} = \sum_j \mathbf{G}(\mathbf{r}_j - \mathbf{r}_i). \tag{9}$$

Thus we have that

$$\bar{\alpha}_{\text{eff}} = \bar{\alpha}(1 - \mathbf{C}\bar{\alpha}/\epsilon_0)^{-1} \tag{10}$$

is the effective polarizability of any arrangement or lattice of dipoles that exhibits sufficient symmetry for the dipole moments to be equal.

Once the effective polarizability is known, the effective-medium properties of the lattice are immediately available. The trivial example is the single point dipole in free space, where the interaction constant is $C = C^{0D} \equiv -i\frac{k^3}{6\pi}$, and therefore the effective polarizability of the point dipole is given by Eq. (5). If the set of dipoles are arranged in a column in one dimension with a lattice constant $a < \lambda/2$ then they form a line source with a polarizability per unit length of $\chi = \alpha_{\text{eff}}/a$, since $(\alpha_{\text{eff}}/a)\mathbf{E}$ will be equal to the average dipole moment per unit length. Similarly, if the dipoles are arranged in a two-dimensional plane with a lattice constant a, then the surface susceptibility will be $\chi = \alpha_{\text{eff}}/a^2$, and the volumetric susceptibility of a three-dimensional lattice will be $\chi = \alpha_{\text{eff}}/a^3$.

We end this section on a final note regarding the energy dissipation of resonant dipoles. If the inherent polarizability of the dipole $\bar{\alpha}_e$ happens to follow a Lorentzian line shape, i.e.,

$$\bar{\alpha}_e^0 = \frac{\epsilon_0 A\omega_0^2}{\omega_0^2 - \omega^2 + i\omega_0^2/Q_\Omega}, \tag{11}$$

where A is an amplitude coefficient that has units of volume, ω_0 is the resonance frequency, and Q_Ω is the Ohmic Q factor, then the effective polarizability will also be a Lorentzian, but with a resonance frequency shift in proportion to the real part of the Green's function, and an added loss term through the imaginary part of the Green's function. This is explicitly given by

$$\bar{\alpha}_{\text{eff}} = \frac{\epsilon_0 A\omega_0^2}{\tilde{\omega}_0^2 - \omega^2 + i\omega_0^2/Q}, \tag{12}$$

where

$$\tilde{\omega}_0 = \omega_0\sqrt{1 - \text{Re}\{C(\omega)A\}} \approx \omega_0(1 - \text{Re}\{C(\omega_0)A/2\}), \tag{13}$$

$$1/Q \approx 1/Q_\Omega - \text{Im}\{C(\omega_0)\}A, \tag{14}$$

where we have assumed that the interaction constant doesn't vary significantly as a function of frequency near the resonance of the dipole, i.e., $C(\omega) \approx C(\omega_0)$. When the geometry within which a dipole is placed is modified, the resonance frequency and quality factor of the dipole's resonance are both modified as the Green's function is changed.

III. THE FILM-COUPLED MAGNETIC DIPOLE

In this section, the contribution to the radiation reaction force experienced by a single dipole due to the coupling to a surface plasmon mode in a metal film is calculated, as shown in Fig. 1(a). In particular, we are interested in magnetic dipoles that are oriented parallel to the surface of a metal film, and separated by some distance d from the film along the z axis. The radiation reaction force for any dipole is given by the imaginary part of the Green's function evaluated at the location of the dipole. One of the standard approaches for computing the Green's function in any waveguidelike geometry is to expand the field into a set of bound modes and radiation modes [28]. For a dipole in free space, there are no bound modes, and so the Green's function for a dipole in free space can be computed using only radiation modes. However, for a dipole placed near a metal film, there is a set of bound surface modes, which are surface plasmons. Here we show that the coupling of the dipole to surface plasmon modes yields an imaginary part of the Green's function at the location of the dipole that corresponds to the power loss of the dipole into surface plasmon modes.

The coupling to the surface plasmon is found using a modified formulation of coupled mode theory, adapted particularly for expansions of the field into a basis of cylindrical

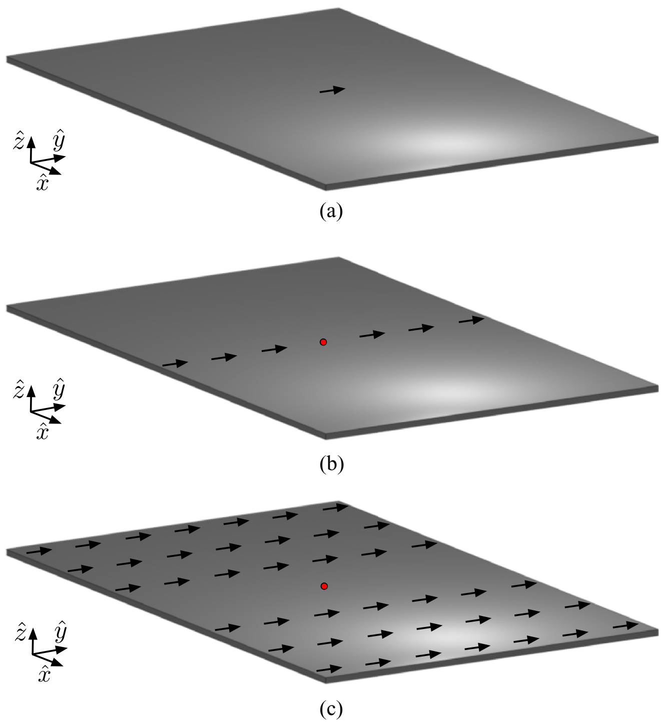

FIG. 1. Illustration of the dipoles summed to produce the (a) $C^{0\text{D}}$, (b) $C^{1\text{D}}$, and (c) $C^{2\text{D}}$ components of the interaction constant. The interaction constant is found by computing the fields of the dipoles at the location of the red dot, which designates the origin.

Hankel functions, i.e., by expanding the field in a sum of modes,

$$\mathbf{E} = \sum_{\mu\nu} A^{+}_{\mu\nu} \mathbf{E}^{+}_{\mu\nu}, \tag{15a}$$

$$\mathbf{H} = \sum_{\mu\nu} A^{+}_{\mu\nu} \mathbf{H}^{+}_{\mu\nu}, \tag{15b}$$

where $\mathbf{H}^{+}_{\mu\nu}$ and $\mathbf{E}^{+}_{\mu\nu}$ are the outgoing cylindrical Hankel basis defined in Appendix B. The Hankel basis is a convenient choice for this problem, because there is only one bound cylindrical wave that a magnetic dipole can excite when it is oriented parallel to the surface of the metal film. However, unlike most of the bases used in coupled mode theory, which assume that the basis is a set of source-free solutions to Maxwell's equations, it is shown in Appendix A that the Hankel functions are not source-free solutions to Maxwell's equations, since they imply the existence of a delta-function source at the origin. The modification of the coupled mode theory equations due to this source is taken into account in Appendix A, and the final expression for the amplitude $A^{+}_{\mu\nu}$ of an outgoing cylindrical Hankel wave $\{\mathbf{E}^{+}_{\mu\nu}, \mathbf{H}^{+}_{\mu\nu}\}$ is

$$A^{+}_{\mu\nu} = \frac{ik^2}{4L\epsilon_0(1+\delta_{\nu 0})} \int \mathbf{P}\cdot(\mathbf{E}^{+}_{\mu\nu} + \mathbf{E}^{-}_{\mu\nu}) - \mu_0 \mathbf{M}\cdot(\mathbf{H}^{+}_{\mu\nu} + \mathbf{H}^{-}_{\mu\nu})dV, \tag{16}$$

where $\{\mathbf{E}^{-}_{\mu\nu}, \mathbf{H}^{-}_{\mu\nu}\}$ is the incoming Hankel basis, and L is a normalization constant that is described in Appendix B. This equation is in disagreement with the expressions given in [29], and in agreement with the expressions in the supplementary material presented in [30], although no rigorous proof was provided in [30] for Eq. (16), and Refs. [29,30] both treated the Hankel basis as source-free.

Consider a magnetic dipole sitting at some distance d along the z axis from a metal film with relative dielectric constant ϵ, the surface of which is on the xy plane. Then in Eq. (16), we have that $\mathbf{M} = m_y \hat{\mathbf{y}} \delta(z-d)\delta(r)/2\pi r$. A careful calculation shows that

$$H^{\text{TM}+}_{\mu\nu y}(d\hat{\mathbf{z}}) + H^{\text{TM}-}_{\mu\nu y}(d\hat{\mathbf{z}}) = \frac{-i}{Z_0} Z^{\text{TM}}_{\mu}(d)\delta_{\nu 1}, \tag{17a}$$

$$H^{\text{TE}+}_{\mu\nu y}(d\hat{\mathbf{z}}) + H^{\text{TE}-}_{\mu\nu y}(d\hat{\mathbf{z}}) = \frac{i}{Z_0 k}\frac{d}{dz} Z^{\text{TE}}_{\mu}(d)\delta_{\nu 1}, \tag{17b}$$

where $Z^{\text{TM}}_{\mu}(z)$ and $Z^{\text{TE}}_{\mu}(z)$ are the profiles of the TE and TM modes in the z direction, with mode numbers μ, as defined in Appendix B. The mode amplitudes excited by this source are, therefore,

$$A^{\text{TM}c}_{\mu\nu} = \frac{-m_y k^2 Z_0}{4L} Z^{\text{TM}}_{\mu}(d)\delta_{\nu 1}, \tag{18a}$$

$$A^{\text{TM}s}_{\mu\nu} = 0, \tag{18b}$$

$$A^{\text{TE}c}_{\mu\nu} = 0, \tag{18c}$$

$$A^{\text{TE}s}_{\mu\nu} = \frac{m_y k Z_0}{4L}\frac{d}{dz} Z^{\text{TE}}_{\mu}(d)\delta_{\nu 1}. \tag{18d}$$

The superscripts "c" and "s" refer to modes that have an angular dependence that goes as $\cos(\nu\theta)$ and $\sin(\nu\theta)$, respectively. In the particular case of the geometry where there is only a single interface between a metal and a dielectric, there is only one bounded TM mode, and there are no bounded TE modes, and so the TE mode amplitudes become irrelevant. For the single bounded TM mode, an expression for $Z^{\text{TM}}_{\mu}(z)$ is given in Eq. (B8).

Using the excited mode amplitudes in Eqs. (18a)–(18d), together with the mode definitions provided in Eqs. (B11e) and (B11f), the y component of the magnetic field excited by the dipole is shown to be

$$H_y(r,\theta,z) = \frac{-i m_y \beta^3\sqrt{-\epsilon}}{4(1-\epsilon)} e^{-k_z^+(d+z)} \times\left[H_0^{(2)}(\beta r) - \cos(2\theta)H_2^{(2)}(\beta r)\right], \tag{19}$$

where $k_z^+ = ik/\sqrt{\epsilon+1}$ and $\beta = k\sqrt{\epsilon/(\epsilon+1)}$ is the surface propagation constant. Taking the limit as $r \to 0$, the real part of Eq. (19) becomes singular, as it is for a dipole in free space. The imaginary part, however, is simply $\text{Im}\{H_y(0)\} = \frac{-m_y\beta^3\sqrt{-\epsilon}}{4(1-\epsilon)} e^{-2k_z^+ d}$. According to Poynting's theorem, the power dissipated by the horizontal magnetic dipole into the surface plasmon is given by $P_{\text{sp}} = (-\omega/2)\text{Im}\{\mathbf{m}^*\cdot\mathbf{H}\}$, and therefore the power dissipated into the surface plasmon is

$$P_{\text{sp}} = \omega|m_y|^2 \text{Re}\left\{\frac{\beta^3\sqrt{-\epsilon}}{4(1-\epsilon)} e^{-2k_z^+ d}\right\}. \tag{20}$$

Moreover, the coupling factor due to the radiation reaction from the SPP mode is, then,

$$C^{0D} = H_y(0)/m_y = \frac{-i\beta^3\sqrt{-\epsilon}}{4(1-\epsilon)} e^{-2k_z^+ d}. \tag{21}$$

IV. ONE-DIMENSIONAL ARRAY OF FILM-COUPLED MAGNETIC DIPOLES

Consider a one-dimensional array of magnetic dipoles placed along the y axis, oriented in the y direction, separated by some distance a_y from each other, and placed at a distance d over a metal film that lies in the xy plane. Moreover, assume that the one-dimensional array is illuminated by a TM plane wave with a free-space wave vector of $\mathbf{k} = (k_x, k_y, k_z)$, with $k_z = \sqrt{k^2 - k_x^2 - k_y^2}$ and polarized with the magnetic field oriented in the y direction. The phase of the moments of the dipoles that comprise the one-dimensional array will therefore be related by the phase of the illuminating plane wave, such that dipole $\mathbf{m}_i = m_i \hat{\mathbf{y}}$ at location $\mathbf{r}_i$ will have dipole moment $m_i = m_y e^{-i\mathbf{k}\cdot\mathbf{r}_i}$.

The dipole at the origin is excluded when computing the C^{1D} interaction constant, as illustrated in Fig. 1(b). The effective polarizability of the magnetic dipoles in the array is determined by the fields that the dipoles exert on each other. The field experienced by the magnetic dipole at the origin due to all the other dipoles is given by

$$H_y^{1D}(0) = \frac{-i m_y \beta^3 \sqrt{-\epsilon}}{2(1-\epsilon)} e^{-2k_z^+ d} \sum_{\mu=-\infty}^{\infty}{}' \frac{H_1^{(2)}(\beta|\mu a_y|)}{\beta|\mu a_y|} \times e^{-ik_y \mu a_y}. \tag{22}$$

This sum converges quickly, but a simpler expression for the real part of the sum, which corresponds to the power loss due to radiation into surface plasmons, can be found by applying Poisson's summation formula [27]. The Poisson summation formula states that

$$\sum_{\mu=-\infty}^{\infty} f(\mu a) = \frac{1}{a} \sum_{\mu=-\infty}^{\infty} F\left(\frac{2\pi\mu}{a}\right), \tag{23}$$

where $F(\omega)$ is the Fourier transform of $f(t)$. We are interested in applying this formula to aid in evaluating the infinite sum,

$$\begin{aligned} \sum_{\mu=-\infty}^{\infty}{}' \frac{H_1^{(2)}(\beta|\mu a_y|)}{\beta|\mu a_y|} e^{-ik_y\mu a_y} &= -\lim_{z\to 0} \frac{J_1(z)}{z} + \sum_{\mu=-\infty}^{\infty} \frac{J_1(\beta|\mu a_y|)}{\beta|\mu a_y|} e^{-ik_y\mu a_y} \\ &\quad -i \sum_{\mu=-\infty}^{\infty}{}' \frac{Y_1(\beta|\mu a_y|)}{\beta|\mu a_y|} e^{-ik_y\mu a_y} \\ &= \frac{-1}{2} + \sum_{\mu=-\infty}^{\infty} \frac{J_1(\beta|\mu a_y|)}{\beta|\mu a_y|} e^{-ik_y\mu a_y} \\ &\quad - i \sum_{\mu=-\infty}^{\infty}{}' \frac{Y_1(\beta|\mu a_y|)}{\beta|\mu a_y|} e^{-ik_y\mu a_y}. \end{aligned} \tag{24}$$

Using the Fourier transform,

$$\mathscr{F}\left\{\frac{J_1(\beta|t|)}{\beta|t|}\right\} = \begin{cases} \frac{2}{\beta^2}\sqrt{\beta^2 - \omega^2} & \omega < |\beta|, \\ 0 & \text{otherwise} \end{cases} \tag{25}$$

we can transform the infinite sum over the Bessel function of the first kind as

$$\sum_{\mu=-\infty}^{\infty} \frac{J_1(\beta|\mu a_y|)}{\beta|\mu a_y|} e^{-ik_y\mu a_y} = \sum_{\mu\in U} \frac{2\Gamma_\mu}{\beta^2 a_y}, \tag{26}$$

where

$$\Gamma_\mu = \sqrt{\beta^2 - (2\pi\mu/a_y - k_y)^2}. \tag{27}$$

The sum is evaluated over all of the Γ_μ modes that are *propagating*, which satisfy the relationship $|2\pi\mu/a - k_y| < |\beta|$. We define the set U as the set of all mode numbers μ such that Γ_μ is propagating:

$$U = \{\mu\ ||2\pi\mu/a - k_y| < |\beta|\}. \tag{28}$$

Then the total magnetic field experienced by the dipole at the origin is expressed as

$$H_y^{1D}(0) = \frac{m_y\sqrt{-\epsilon}}{(1-\epsilon)} e^{-2k_z^+ d} \left[\frac{i\beta^3}{4} - \sum_{\mu\in U} \frac{i\beta\Gamma_\mu}{a_y} - \beta^3 \sum_{\mu=1}^{\infty} \frac{Y_1(\beta\mu a_y)}{\beta\mu a_y} \cos(k_y\mu a)\right]. \tag{29}$$

Let $C^{1D} = H^{1D}(0)/m_y$ be defined as the part of the interaction constant due to all of the dipoles along the y axis, excluding the dipole at the origin. The total interaction constant for the one-dimensional array of dipoles lying along the y axis and oriented in the y direction is $C = C^{0D} + C^{1D}$, where C^{1D} is given by

$$C^{1D} = \frac{\sqrt{-\epsilon}}{(1-\epsilon)} e^{-2k_z^+ d} \left[\frac{i\beta^3}{4} - \sum_{\mu\in U} \frac{i\beta\Gamma_\mu}{a_y} - \beta^3 \sum_{\mu=1}^{\infty} \frac{Y_1(\beta\mu a_y)}{\beta\mu a_y} \cos(k_y\mu a)\right]. \tag{30}$$

In the limit that β is purely real, the final sum on the right-hand side of Eq. (30) is purely real, and all losses are due to the two purely imaginary terms, and these two terms therefore represent the radiative damping force. As was the case for the one-dimensional array of dipoles in free space, the dipoles in the column exert a force on each other that cancels the force proportional to $i\beta^3/4$ that they exert on themselves due to the radiation reaction, and replaces it with a force proportional to the sum of the energy carried in all surface plasmon diffraction orders that are radiated by the line of dipoles.

V. TWO-DIMENSIONAL ARRAY OF FILM-COUPLED MAGNETIC DIPOLES

Now consider a two-dimensional lattice of dipoles oriented in the y direction with lattice spacing a_x and a_y in the x and y directions, excluding the line of dipoles along the y axis, as illustrated in Fig. 1(c). The two-dimensional lattice may be thought of as a set of lines of dipoles parallel to the y axis, and at positions na_x along the x axis. The total field of the lattice is the sum of the fields radiated by the lines of dipoles, and so we first compute the field radiated by a single line of dipoles lying along the y axis and oriented in the y direction. Directly summing the magnetic fields of this lattice would be cumbersome because the field in the Hankel basis is given in cylindrical coordinates, and the redefinition of the cylindrical unit vectors would need to be taken into account for each dipole in the lattice. Instead of summing the magnetic fields, we compute the total z component of the electric field, and the total electric field from all of the dipoles can be easily summed since $\hat{z}$ is translationally invariant. Then the y component of the magnetic field can be found using

$$H_y = \frac{ik}{Z_0\beta^2}\frac{\partial}{\partial x}E_z. \tag{31}$$

which is valid when the field in the entire surface is assumed to vary as $e^{-k_z^+ z}$, and the field is purely transverse magnetic [28].

The total z component of the electric field radiated by a single line of dipoles, which is denoted by $E_z^{1\mathrm{D}}$, is given by the infinite sum of the field radiated by each of the individual dipoles. Using the same methods outlined in Sec. III and Appendix A, the z-component electric field in the surface plasmon mode radiated by a single magnetic dipole placed over a metal surface is

$$E_z = \frac{-m_y Z_0\beta^4\sqrt{-\epsilon}}{2k(1-\epsilon)}e^{-k_z^+(z+d)}\cos(\theta)H_1^{(2)}(\beta r), \tag{32}$$

and therefore the total electric field radiated by a line of dipoles along the y axis is

$$E_z^{1\mathrm{D}} = \frac{-m_y Z_0\beta^4\sqrt{-\epsilon}}{2k(1-\epsilon)}e^{-k_z^+(z+d)} \times \sum_{\mu=-\infty}^{\infty}\frac{xH_1^{(2)}(\beta\sqrt{x^2+(y-\mu a_y)^2})}{\sqrt{x^2+(y-\mu a_y)^2}}e^{-ik_y\mu a_y}. \tag{33}$$

Applying Poisson's summation technique to the sum in Eq. (33), the total field is

$$E_z^{1\mathrm{D}} = \frac{-im_y Z_0\beta^3\sqrt{-\epsilon}}{ka_y(1-\epsilon)}e^{-k_z^+(z+d)}e^{-ik_y y} \times \sum_{\mu=-\infty}^{\infty}\mathrm{sgn}(x)e^{-i|x|\Gamma_\mu}e^{-i(2\pi\mu/a_y)y}, \tag{34}$$

where Γ_μ is given in Eq. (27), and the Fourier transform,

$$\mathscr{F}\left\{\frac{H_1^{(2)}(\beta\sqrt{x^2+(y-t)^2})}{\sqrt{x^2+(y-t)^2}}\right\} \tag{35}$$

$$= \frac{2i}{\beta|x|}e^{-i|x|\sqrt{\beta^2-(\omega-k_y)^2}}e^{-i(\omega-k_y)y}, \tag{36}$$

was used [31]. If the distance between the dipoles is less than the surface plasmon wavelength, then only the $\mu = 0$ mode will be propagating.

The total electric field generated by all of the lines of dipoles in the lattice together, $E_z^{2\mathrm{D}}$, excluding the line of dipoles at $x = 0$, is the sum of the electric field radiated by each line of dipoles individually:

$$E_z^{2\mathrm{D}} = \frac{-im_y Z_0\beta^3\sqrt{-\epsilon}}{ka_y(1-\epsilon)}e^{-k_z^+(z+d)}e^{-ik_y y} \times \sum_{\mu=-\infty}^{\infty}\sum_{\nu=-\infty}^{\infty}{}' \,\mathrm{sgn}(x-\nu a_x) \times e^{-i|x-\nu a_x|\Gamma_\mu}e^{-ik_x\nu a_x}e^{-i(2\pi\mu/a_y)y}. \tag{37}$$

If we restrict ourselves to considering the region of space where $|x| < a_x$, then

$$E_z^{2\mathrm{D}} = \frac{-2m_y Z_0\beta^3\sqrt{-\epsilon}}{ka_y(1-\epsilon)}e^{-k_z^+(z+d)}e^{-ik_y y} \times \sum_{\mu=-\infty}^{\infty}e^{-i(2\pi\mu/a_y)y}\sum_{\nu=1}^{\infty}e^{-i\Gamma_\mu\nu a_x}\sin(\Gamma_\mu x - k_x\nu a_x). \tag{38}$$

The magnetic field in the region $|x| < a_x$ due to dipoles for all $\nu \neq 0$, is found using Eqs. (31) and (38) to be

$$H_y^{2\mathrm{D}} = \frac{-i2\beta m_y\sqrt{-\epsilon}}{a_y(1-\epsilon)}e^{-k_z^+(z+d)}e^{-ik_y y} \times \sum_{\mu=-\infty}^{\infty}\Gamma_\mu e^{-i(2\pi\mu/a_y)y}\sum_{\nu=1}^{\infty}e^{-i\Gamma_\mu\nu a_x} \times \cos(\Gamma_\mu x - k_x\nu a_x), \tag{39}$$

and here we are interested more specifically in the magnetic field at the location of the dipole,

$$H_y^{2\mathrm{D}}(0) = \frac{-i2\beta m_y\sqrt{-\epsilon}}{a_y(1-\epsilon)}e^{-2k_z^+ d} \times \sum_{\mu=-\infty}^{\infty}\Gamma_\mu\sum_{\nu=1}^{\infty}e^{-i\Gamma_\mu\nu a_x}\cos(k_x\nu a_x). \tag{40}$$

A straightforward application of Poisson's summation technique can again be used to simplify the sum over ν, yielding

$$\sum_{\nu=1}^{\infty}e^{-i\Gamma_\mu\nu a_x}\cos(k_x\nu a_x) = -1/2 - \sum_{\nu=-\infty}^{\infty}\frac{i\Gamma_\mu}{a_x\Gamma_{\mu\nu}^2}, \tag{41}$$

where $\Gamma_{\mu\nu} = \sqrt{\beta^2 - (2\pi\mu/a_y - k_y)^2 - (2\pi\nu/a_x - k_x)^2}$.

The contribution to the interaction constant due to all of the lines of dipoles excluding the line at $x = 0$ is defined as $C^{2\mathrm{D}} = H^{2\mathrm{D}}(0)/m_y$, which is

$$C^{2\mathrm{D}} = \frac{\sqrt{-\epsilon}}{(1-\epsilon)}e^{-2k_z^+ d} \times \left[\sum_{\mu=-\infty}^{\infty}\frac{i\beta\Gamma_\mu}{a_y} - \frac{2\beta}{a_x a_y}\sum_{\mu=-\infty}^{\infty}\sum_{\nu=-\infty}^{\infty}\frac{\Gamma_\mu^2}{\Gamma_{\mu\nu}^2}\right]. \tag{42}$$

The total interaction constant is finally

$$C = C^{0\mathrm{D}} + C^{1\mathrm{D}} + C^{2\mathrm{D}} = \frac{\sqrt{-\epsilon}}{(1-\epsilon)}e^{-2k_z^+ d} \times \left[\sum_{\mu=-\infty}^{\infty}\frac{i\beta\Gamma_\mu}{a_y} - \sum_{\mu\in U}\frac{i\beta\Gamma_\mu}{a_y} - \frac{2\beta}{a_x a_y}\sum_{\mu=-\infty}^{\infty}\sum_{\nu=-\infty}^{\infty}\frac{\Gamma_\mu^2}{\Gamma_{\mu\nu}^2}\right.$$

$$- \beta^3 \sum_{\mu=1}^{\infty} \frac{Y_1(\beta\mu a_y)}{\beta\mu a_y} \cos(k_y \mu a) \Bigg]$$

$$= \frac{\sqrt{-\epsilon}}{(1-\epsilon)} e^{-2k_z^+ d} \Bigg[\sum_{\mu \notin U} \frac{i\beta\Gamma_\mu}{a_y} - \frac{2\beta}{a_x a_y} \sum_{\mu=-\infty}^{\infty} \sum_{\nu=-\infty}^{\infty} \frac{\Gamma_\mu^2}{\Gamma_{\mu\nu}^2} - \beta^3 \sum_{\mu=1}^{\infty} \frac{Y_1(\beta\mu a_y)}{\beta\mu a_y} \cos(k_y \mu a) \Bigg]. \quad (43)$$

Notice that, in the limit of purely real permittivity, the contribution to the interaction constant from the 2D lattice in Eq. (42) contains a sum over all modes propagating away from each column of dipoles in constant x. This term serves to cancel out the imaginary term in Eq. (30) that corresponds to the power loss due to the modes propagating away from each column of dipoles. Provided that the permittivity is purely real, then the interaction constant C is purely *real*, meaning that there is no net loss by the dipoles to the surface plasmon. Conservation of energy and Poynting's theorem is thereby maintained by the lattice in a very roundabout way: Dipoles exert a force on themselves according to their own energy loss via the radiation reaction, but when placed in a lattice, the dipoles exert forces on each other that exactly cancel the radiation reaction force and replace it with a new force that corresponds to the radiation losses of the lattice as a whole. This is already known to be true for metamaterial lattices in free space [14], but here we have demonstrated this is also true when the dipoles are coupled to a metal film such that their Green's function is dominated by the surface plasmon mode.

VI. APPLICATIONS TO METAMATERIAL ABSORBERS

Although the main result in Eq. (43) is that there is no net alteration to the Q factor of a metasurface when it is coupled to a metal film that supports surface plasmons, the real part of the interaction constant predicts a resonance frequency shift, and the imaginary part predicts additional Ohmic losses due to absorption by surface plasmons. Furthermore, the expression for the interaction constant in Eq. (43) includes a series of singularities in the term,

$$\frac{2\beta}{a_x a_y} \sum_{\mu=-\infty}^{\infty} \sum_{\nu=-\infty}^{\infty} \frac{\Gamma_\mu^2}{\Gamma_{\mu\nu}^2}, \quad (44)$$

when $\Gamma_{\mu\nu} = 0$, which occur when $\beta = \sqrt{(2\pi\nu/a_x - k_x)^2 + (2\pi\mu/a_y - k_y)^2}$, where $\mu \in \mathbb{Z}$ and $\nu \in \mathbb{Z} \setminus \{0\}$. Since there is no singularity when $\nu = 0$, the lowest order singularity is therefore the case where $\mu = 0$ and $\nu = \pm 1$, and occurs when $\beta^2 = (2\pi/a_x \pm k_x)^2 + k_y^2$. Under normal incidence, Eq. (43) predicts that there will be additional resonance when $\beta = \sqrt{(2\pi\nu/a_x)^2 + (2\pi\mu/a_y)^2}$, the lowest order term of which is when $\beta = 2\pi/a_x$, i.e., when the period of the lattice is equal to the surface plasmon wavelength. We claim that these resonances are the Wood's anomalies of the film-coupled metasurface.

As an example of application of the theory, we consider a metamaterial surface consisting of nanopatches that are placed a small distance h away from a silver film, with a lattice constant of a, as shown in Fig. 2. The gap region between the nanopatch and the metal film is known to support a set of cavity modes, which couple to the incident magnetic field and scatter as a magnetic dipole [4]. The excitation of the cavity modes due to the incident field can be found using a form of temporal coupled mode theory, and the magnetic polarizability of the nanopatch is found from the amplitude of the magnetic dipole moment of the scattered field from the cavity. The magnetic polarizability of the nanopatch antenna given in [5] is

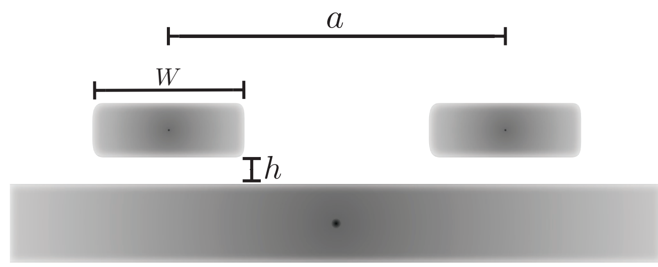

FIG. 2. Illustration of the film-coupled metasurface of optical patch antennas. Each patch is a cuboid of width W and height H that is lifted off the film by a distance h.

$$\alpha = \frac{8hc^2 \cos^2[\sin(\theta)kW/2]}{\omega_0^2 - \omega^2 + i\omega_0^2/Q}, \quad (45)$$

where W is the width of the nanopatch and θ is the angle of the incident magnetic field. Expressions for ω_0 and Q can be found in [4,5]. The reflection coefficient of the entire flim-coupled nanopatch metasurface system is [5]

$$r = r_{\rm TM} + \frac{-ik(1-r_{\rm TM})^2}{2a^2\cos(\theta)}\alpha, \quad (46)$$

where $r_{\rm TM}$ is the fresnel reflection coefficient of the bare metal film under TM polarization.

In Ref. [5], all interactions between the nanopatches through surface plasmons or evanescent radiation modes were neglected, and only the loss due to propagating radiation modes was taken into account by a choice of Q that included the radiation loss of the metasurface. However, since the nanopatch antennas scatter as magnetic dipoles and are placed very close to the surface of the metal film, they will couple through surface plasmons. Neglecting the evanescent radiation mode interaction and assuming the remaining coupling is primarily mediated through surface plasmon modes, the effective polarizability of the dipoles will become

$$\alpha_{\rm eff} = \frac{\alpha}{1 - C\alpha}, \quad (47)$$

where C is the interaction constant in Eq. (43). The interaction constant is calculated using the measured Johnson and Christy data for the dielectric constant of silver [32]. The magnetic dipole that is generated by the film-coupled nanopatch is created by an effective magnetic surface current that lies on the boundary of the gap region between the nanopatch and the metal film. Since the size of this gap is typically extremely subwavelength (∼5 nm), we take $d = 0$ in the calculation of C, which places the magnetic dipole exactly adjacent to the metal film.

The new, corrected reflection coefficient with the surface plasmon interaction taken into account will now be

$$r = r_{\mathrm{TM}} + \frac{-ik(1-r_{\mathrm{TM}})^2}{2a^2\cos(\theta)}\alpha_{\mathrm{eff}}, \tag{48}$$

which is plotted alongside Eq. (46) in Fig. 3 and compared with simulation results. The particular system presented in Fig. 3 is for a periodic array of cubic patches illuminated under normal incidence with a width W of 80 nm, and separated from a metal film by a distance of $h = 5$ nm. Since the coupling coefficient is able to perfectly account for the resonance frequency shift and predict nearly all other features of the reflection spectrum, the coupling between nanopatches must be dominated by surface plasmon interactions, and the evanescent and propagating radiation modes play nearly no effect, aside from the propagating radiation modes determining the radiation Q factor.

Returning to Eq. (14), we note that the imaginary part of the interaction constant of the lattice is a measure of the loss rate of each magnetic dipole to surface plasmons. Every dipole in the lattice may be thought of as emitting surface plasmons into the metal film at a certain rate, which is proportional to the radiation reaction force due to the surface plasmon coupling, or $C^{0\mathrm{D}}$, in Eq. (21). The surface plasmons are then either re-absorbed by another dipole, which is proportional to the sum $C^{1\mathrm{D}} + C^{2\mathrm{D}}$, or dissipate into Ohmic losses. The imaginary part of the interaction constant given in Eq. (43), which is due to the surface plasmon interaction between the dipoles, is therefore a measure of the loss rate of any particular dipole in the lattice to surface plasmons, minus the reabsorption rate. The imaginary part of C is then the overall rate of loss of the lattice to surface plasmons that are eventually dissipated in Ohmic losses rather than reabsorbed by the dipoles in the lattice, which we refer to as the Ohmic loss rate due to surface plasmons, or

$$\Gamma_{\mathrm{spp}} = \omega_0/Q_{\mathrm{spp}} = \omega_0 A \,\mathrm{Im}\{C\}. \tag{49}$$

The constant A is the amplitude of the dipole's Lorentzian response, as in Eq. (12). We compare the Ohmic loss rate to surface plasmons with the radiative loss rate of the dipoles, which was found in [4] to be

$$\Gamma_{\mathrm{rad}} = \omega_0/Q_{\mathrm{rad}} = \omega_0 A \frac{2k|1-r_{\mathrm{TM}}|^2}{a^2}, \tag{50}$$

for a periodic metasurface of dipoles coupled to a metal film with lattice constant a. The ratio $\Gamma_{\mathrm{spp}}/\Gamma_{\mathrm{rad}}$ is plotted in Fig. 4 as a function of the lattice constant for fixed wavelength, for a metal film with $\epsilon = -15(1 + i\delta)$, where δ is the loss tangent. Surprisingly, the surface plasmon losses are below or on the order of a few percent of the total loss rate, until it approaches the Wood's anomaly at $a/\lambda = k/\beta \approx 0.97$. At that point, the losses are by far dominated by the surface plasmon losses since the field becomes dominated by standing waves between the dipoles.

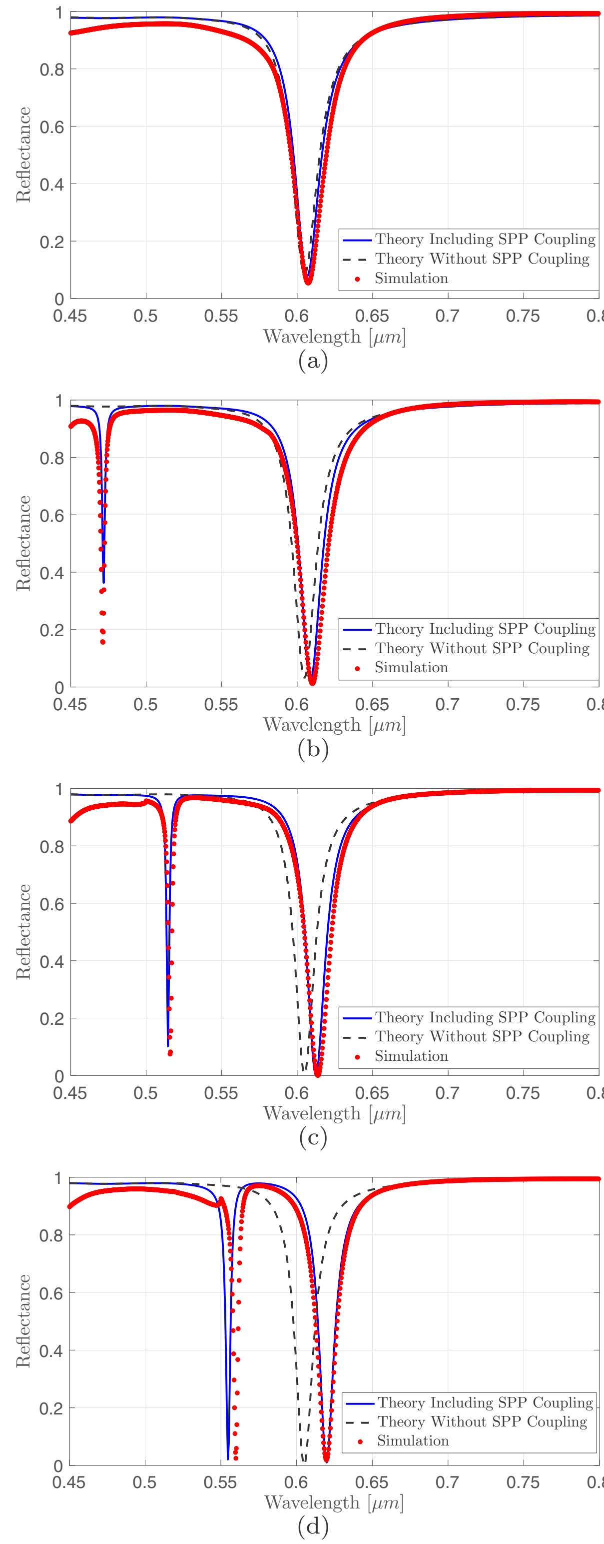

FIG. 3. Comparison of reflection coefficient including surface plasmon coupling (blue line) and excluding surface plasmon coupling (green line) with full-wave simulation results (dots) for nanopatches with a pitch of (a) 400 nm, (b) 450 nm, (c) 500 nm, and (d) 550 nm.

VII. CONCLUSION

When a metasurface is tightly coupled to a metal film, the Green's function of the dipoles is perturbed, which changes how the lattice is homogenized. The dipoles that compose the lattice are now able to both couple into bound surface plasmon modes as well as radiation modes. We have demonstrated that conservation of energy is upheld by the lattice in the sense that every surface plasmon that is emitted into the lattice is reabsorbed by the lattice, in the limit that the metal

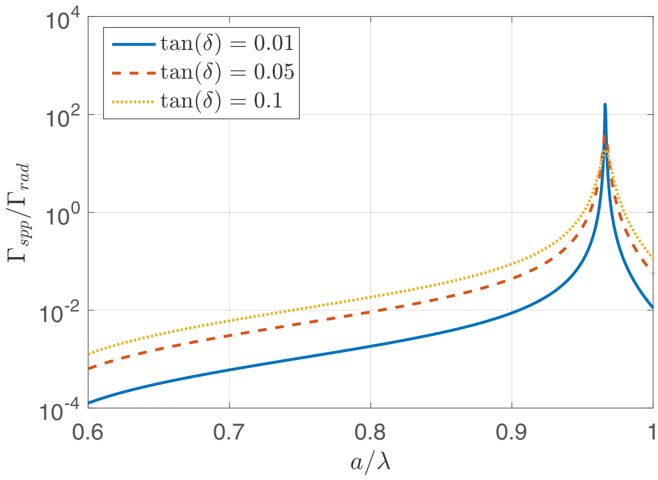

FIG. 4. Ratio of the losses of the metasurface to surface plasmons relative to the radiative loss rate, when coupled to a metal film with $\epsilon = -15(1 + i\delta)$. The metasurface is assumed to be placed infinitely close to the metal film (i.e., $d = 0$).

exhibits zero Ohmic losses. In addition, the expressions for the interaction constant derived here allow the change in the frequency response of the metasurface to be computed as it is brought closer to the metal film. Higher order diffraction modes due to the surface plasmon interaction are explained, and a means is provided to directly calculating the overall loss rate of the metasurface to surface plasmons that are eventually dissipated in the metal film.

ACKNOWLEDGMENTS

This work was supported by the Air Force Office of Scientific Research (AFOSR, Grant No. FA9550-12-1-0491).

APPENDIX A: UNCONJUGATED COUPLED MODE THEORY FOR FREE-SPACE MODES IN A CYLINDRICAL HANKEL BASIS

Coupled mode theory is a method to find solutions to Maxwell's equations,

$$\nabla \times \mathbf{E} = -i\omega\mu_0\mathbf{H} - i\omega\mu_0\mathbf{M}, \tag{A1}$$

$$\nabla \times \mathbf{H} = i\omega\epsilon_0\mathbf{E} + i\omega\mathbf{P}, \tag{A2}$$

by expanding the field in a sum of modes,

$$\mathbf{E} = \sum_{\mu\nu} A_{\mu\nu}\mathbf{E}_{\mu\nu}, \tag{A3a}$$

$$\mathbf{H} = \sum_{\mu\nu} A_{\mu\nu}\mathbf{H}_{\mu\nu}, \tag{A3b}$$

where the modes are themselves solutions of Maxwell's equations:

$$\nabla \times \mathbf{E}_{\mu\nu} = -i\omega\mu_0\mathbf{H}_{\mu\nu} - i\omega\mu_0\mathbf{M}_{\mu\nu}, \tag{A4}$$

$$\nabla \times \mathbf{H}_{\mu\nu} = i\omega\epsilon_0\epsilon\mathbf{E}_{\mu\nu} + i\omega\mathbf{P}_{\mu\nu}. \tag{A5}$$

Here, we are viewing the solution to Maxwell's equations as the actual fields distributed everywhere in the system, with **P** and **M** representing the actual electric and magnetic polarizations of each of the metamaterial elements. This problem will be solved by expanding the fields in an eigenmode basis, which is given by the cylindrical waveguide modes. We will consider these modes in a Hankel function basis, where the modes are all propagating waves. The details of these modes and their derivation are given in the appendix. However, there are two important properties of these modes that must first be noted before deriving the coupled mode theory equations.

First, it ought to be noted that the cylindrical Hankel functions are *not* source-free solutions to Maxwell's equations. Normally, coupled mode theory is developed using a basis of source-free solutions of Maxwell's equations (i.e., $\mathbf{P}_\nu = \mathbf{M}_\nu = 0$), which are therefore eigenmodes of Maxwell's equations. This is the assumption that was used in Refs. [29,30] when deriving the coupling of sources to Hankel cylindrical modes. However, the cylindrical Hankel basis that we are considering is not a set of source-free solutions to Maxwell's equations, since each of those modes imply the existence of of a point source at the origin. For example, the source implied by the fundamental TM mode may be found by using the integral form of Maxwell's equations,

$$i\omega\int_S \mathbf{P}^{\pm}_{\mu\nu}\cdot d\mathbf{a} = \int_{\partial S}\mathbf{H}^{\pm}_{\mu\nu}\cdot d\mathbf{l} - i\omega\epsilon_0\epsilon\int_S \mathbf{E}^{\pm}_{\mu\nu}\cdot d\mathbf{a}, \tag{A6}$$

where the + sign corresponds to solutions that are outgoing waves and the − sign corresponds to solutions that are incoming waves. The surface S may be chosen to be a small disk oriented in the $\hat{\mathbf{z}}$ direction with any arbitrary radius. If the TE and TM modes with $\nu = 0$ (see Appendix B) are used in Eq. (A6), then the right-hand side evaluates to

$$i\omega\int_S \mathbf{P}^{\pm}_{\mu 0}\cdot d\mathbf{a} = \frac{\mp 4\epsilon(z)Z_\mu(z)}{\beta_\mu Z_0}, \tag{A7}$$

which is independent of the radius of the disk. Clearly, $\mathbf{P}^{\pm}_{\mu\nu}$ cannot be zero everywhere. Moreover, since the right-hand side is entirely independent of the radius of the disk of integration, the integral on the left must also be independent of the disk of integration. The argument $\mathbf{P}^{\pm}_{\mu\nu}$ must either go as $1/r$, or else have a delta-function form in the radial coordinate. Since the Hankel functions are known to be source-free solutions when $r \neq 0$, $\mathbf{P}^{\pm}_{\mu\nu}$ must have a delta-function form. Hence, we have

$$\mathbf{P}^{\mathrm{TM}\pm}_{\mu 0} = \hat{\mathbf{z}}\frac{\pm i4\epsilon_0\epsilon(z)Z_\mu(z)}{\beta_\mu k}\frac{\delta(r)}{2\pi r}, \tag{A8a}$$

$$\mathbf{M}^{\mathrm{TM}\pm}_{\mu 0} = 0, \tag{A8b}$$

$$\mathbf{P}^{\mathrm{TE}\pm}_{\mu 0} = 0, \tag{A8c}$$

$$\mathbf{M}^{\mathrm{TE}\pm}_{\mu 0} = \hat{\mathbf{z}}\frac{\pm i4Z_\mu(z)}{\beta_\mu k}\frac{\delta(r)}{2\pi r}. \tag{A8d}$$

However, as shall be seen, there will be no need to exactly evaluate all of the electric and magnetic polarizations for each of the modes. This task will be particularly difficult when evaluating the sources corresponding to modes with $\nu \geqslant 1$, since there is no obvious way to define a surface such that the integral converges.

However, making some simple observations about the properties that these sources must have will provide a way forward. The absorbed power for each solution is given by Poynting's theorem as

$$P_{\text{abs}}^{\pm} = \text{Re}\left\{\int \mathbf{J}\cdot\mathbf{E}dV\right\} = -\omega\text{Im}\left\{\int \mathbf{P}_{\mu\nu}^{\pm}\cdot\mathbf{E}_{\mu\nu}^{\pm}dV\right\}. \quad \text{(A9)}$$

The outgoing and incoming wave solutions to Maxwell's equations must be related to each other such that $P_{\text{abs}}^{-} = -P_{\text{abs}}^{+}$. This absorbed power must also be finite, and so the phase of $\mathbf{P}_{\mu\nu}^{\pm}$ must be such that $\text{Im}\{\mathbf{P}_{\mu\nu}^{\pm}\cdot\mathbf{E}_{\mu\nu}^{\pm}\}$ only involves the $J_\nu(\beta_\mu r)$ portion of the Bessel function, which implies that

$$\text{Im}\{\mathbf{P}_{\mu\nu}^{+}\cdot\mathbf{E}_{\mu\nu}^{-}\} = \text{Im}\{\mathbf{P}_{\mu\nu}^{+}\cdot\mathbf{E}_{\mu\nu}^{+}\} = -\text{Im}\{\mathbf{P}_{\mu\nu}^{-}\cdot\mathbf{E}_{\mu\nu}^{-}\}. \quad \text{(A10)}$$

Therefore it follows that $\mathbf{P}_{\mu\nu}^{-} = -\mathbf{P}_{\mu\nu}^{+}$. An extension of the argument to include magnetic currents will also show that $\mathbf{M}_{\mu\nu}^{-} = -\mathbf{M}_{\mu\nu}^{+}$, and these conclusions are consistent with Eqs. (A8a)–(A8d).

The second important point to make note of regarding the cylindrical Hankel basis used here is the orthogonality property,

$$\int(\mathbf{E}_{\mu\nu}^{+}\times\mathbf{H}_{\rho\sigma}^{-} - \mathbf{E}_{\rho\sigma}^{-}\times\mathbf{H}_{\mu\nu}^{+})\cdot d\mathbf{a} = \frac{4L(1+\delta_{\nu0})}{Z_0 k}\delta_{\rho\mu}\delta_{\sigma\nu}, \quad \text{(A11)}$$

where the integration is carried out over the surface of a cylinder of any radius aligned along the z axis. This orthogonality relationship can be derived directly using the expressions for the modes given in Appendix B, which was also shown in [29], although with a different normalization. The choice of normalization that yields Eq. (A11) is given in Appendix B, where the constant L is defined in Eqs. (B7a) and (B7b) and has units of length. This particular choice of normalization leaves the electric field of the modes as dimensionless, the magnetic field with units of inverse impedance, and therefore the inner product of the modes has units of area times inverse impedance.

Coupled mode theory is derived using Lorentz reciprocity, and the unconjugated form of Lorentz reciprocity states that, for two solutions to Maxwell's equations $\{\mathbf{E}_1,\mathbf{H}_1,\mathbf{P}_1,\mathbf{M}_1\}$ and $\{\mathbf{E}_2,\mathbf{H}_2,\mathbf{P}_2,\mathbf{M}_2\}$,

$$\begin{aligned}&\nabla\cdot(\mathbf{E}_1\times\mathbf{H}_2 - \mathbf{E}_2\times\mathbf{H}_1)\\&\quad = i\omega(\mathbf{P}_1\cdot\mathbf{E}_2 - \mu_0\mathbf{M}_1\cdot\mathbf{H}_2 - \mathbf{P}_2\cdot\mathbf{E}_1 + \mu_0\mathbf{M}_2\cdot\mathbf{H}_1).\end{aligned} \quad \text{(A12)}$$

First, we will derive the Rayleigh-Carson reciprocity theorem from Eq. (A12) by requiring $\{\mathbf{E},\mathbf{H},\mathbf{P},\mathbf{M}\}$ to be the particular solution to Maxwell's equations that we are seeking, and $\{\mathbf{E}_2,\mathbf{H}_2,\mathbf{P}_2,\mathbf{M}_2\} = \{\mathbf{E}_{\mu\nu}^{+},\mathbf{H}_{\mu\nu}^{+},\mathbf{P}_{\mu\nu}^{+},\mathbf{M}_{\mu\nu}^{+}\}$, and taking the volume integral of Eq. (A12) over all space. This yields

$$\begin{aligned}&\int(\mathbf{E}\times\mathbf{H}_{\mu\nu}^{+} - \mathbf{E}_{\mu\nu}^{+}\times\mathbf{H})\cdot d\mathbf{a}\\&\quad = i\omega\int(\mathbf{P}\cdot\mathbf{E}_{\mu\nu}^{+} - \mu_0\mathbf{M}\cdot\mathbf{H}_{\mu\nu}^{+}\\&\qquad - \mathbf{P}_{\mu\nu}^{+}\cdot\mathbf{E} + \mu_0\mathbf{M}_{\mu\nu}^{+}\cdot\mathbf{H})dV.\end{aligned} \quad \text{(A13)}$$

If the sources $\mathbf{P}$ and $\mathbf{M}$ do not extend to infinity so that all of the modes that compose $\mathbf{E}$ and $\mathbf{H}$ at infinity are outgoing waves, then the orthogonality relationship in Eq. (A11) will guarantee that the surface integral will vanish. The result is the Rayleigh-Carson reciprocity theorem,

$$\begin{aligned}&\int(\mathbf{P}\cdot\mathbf{E}_{\mu\nu}^{+} - \mu_0\mathbf{M}\cdot\mathbf{H}_{\mu\nu}^{+})dV\\&\quad = \int(\mathbf{P}_{\mu\nu}^{+}\cdot\mathbf{E} - \mu_0\mathbf{M}_{\mu\nu}^{+}\cdot\mathbf{H})dV.\end{aligned} \quad \text{(A14)}$$

Now, let $\{\mathbf{E},\mathbf{H},\mathbf{P},\mathbf{M}\}$ remain as the solution to Maxwell's equations that we are seeking, but set $\{\mathbf{E}_2,\mathbf{H}_2,\mathbf{P}_2,\mathbf{M}_2\} = \{\mathbf{E}_{\mu\nu}^{-},\mathbf{H}_{\mu\nu}^{-},\mathbf{P}_{\mu\nu}^{-},\mathbf{M}_{\mu\nu}^{-}\}$. The electric and magnetic fields $\mathbf{E}$ and $\mathbf{H}$ may moreover be expanded using Eqs. (A3a) and (A3b). Using Eqs. (A3a) and (A3b) in Eq. (A12) and taking the volume integral of both sides, and applying the orthogonality condition in Eq. (A11) yields

$$\begin{aligned}A_{\mu\nu} = \frac{ik^2}{4L\epsilon_0(1+\delta_{\nu0})}&\int(\mathbf{P}\cdot\mathbf{E}_{\mu\nu}^{-} - \mu_0\mathbf{M}\cdot\mathbf{H}_{\mu\nu}^{-}\\&- \mathbf{P}_{\mu\nu}^{-}\cdot\mathbf{E} + \mu_0\mathbf{M}_{\mu\nu}^{-}\cdot\mathbf{H})dV.\end{aligned} \quad \text{(A15)}$$

Using the particular property of the cylindrical Hankel sources that $\mathbf{P}_{\mu\nu}^{-} = -\mathbf{P}_{\mu\nu}^{+}$ and $\mathbf{M}_{\mu\nu}^{-} = -\mathbf{M}_{\mu\nu}^{+}$, and applying Eq. (A14), we obtain

$$\begin{aligned}A_{\mu\nu} = \frac{ik^2}{4L\epsilon_0(1+\delta_{\nu0})}&\int\mathbf{P}\cdot(\mathbf{E}_{\mu\nu}^{+} + \mathbf{E}_{\mu\nu}^{-})\\&- \mu_0\mathbf{M}\cdot(\mathbf{H}_{\mu\nu}^{+} + \mathbf{H}_{\mu\nu}^{-})dV.\end{aligned} \quad \text{(A16)}$$

The result in Eq. (A16) allows the calculation of the coupling of a dipole to cylindrical Hankel functions, because the singularity at the origin is canceled in the sum of incoming and outgoing waves.

As an example of the new coupled mode theory equation Eq. (A16), consider an electric dipole placed at position $(x,y,z) = (0,0,d)$, with dipole moment $\mathbf{p} = p_z\hat{\mathbf{z}}$. The coupling to the surface plasmon is calculated using the quantity,

$$E_{\nu z}^{\text{TM}+} + E_{\nu z}^{\text{TM}-} = 2n_{\text{sp}}Z(z)\cos(\nu\theta)J_\nu(\beta r), \quad \text{(A17a)}$$

$$E_{\nu z}^{\text{TE}+} + E_{\nu z}^{\text{TE}-} = 0, \quad \text{(A17b)}$$

where $n_{\text{sp}} = \beta/k$, and the index μ has been removed since there is only one bound mode ($\mu = 0$), which corresponds to the surface plasmon. The mode amplitudes excited by this source are, then,

$$A_\nu^{\text{TM}c} = \frac{p_z\beta^2 Z_0}{4L}Z^{\text{TM}}(d)\delta_{\nu0}, \quad \text{(A18a)}$$

$$A_\nu^{\text{TM}s} = 0, \quad \text{(A18b)}$$

$$A_\nu^{\text{TE}c} = 0, \quad \text{(A18c)}$$

$$A_\nu^{\text{TE}s} = 0. \quad \text{(A18d)}$$

The z component of the electric field emitted by this source is therefore

$$E_z = \frac{p_z}{\epsilon_0}\frac{i\beta^5\sqrt{-\epsilon}}{2k^2(1-\epsilon)}e^{-k_z^{+}(z+d)}H_0^{(2)}(\beta r). \quad \text{(A19)}$$

The power dissipated into the surface plasmon by this dipole is given by $P_{\rm sp} = (\omega/2){\rm Im}\{\mathbf{p}^* \cdot \mathbf{E}\}$, which is

$$P_{\rm sp} = \omega \frac{|p_z|^2}{\epsilon_0} \frac{\beta^5\sqrt{-\epsilon}}{4k^2(1-\epsilon)} e^{-2k_z^+ d}. \tag{A20}$$

The result in Eq. (A20) agrees with Eq. (3.21) in [33] for the power emitted into the surface plasmon. Alternatively, we can consider an electric dipole placed parallel to the surface. A similar calculation using these same methods will also yield the same result as Eq. (3.21) in [33] for the horizontal electric dipole.

APPENDIX B: SOLUTIONS TO MAXWELL'S EQUATIONS IN CYLINDRICAL COORDINATES

We want to find the solutions to Maxwell's equations in cylindrical coordinates. This kind of expansion has been done before, and the results in Ref. [29] are summarized here. We start with the z component of the electric and magnetic fields, which must follow the Helmholtz equation,

$$(\nabla^2 + \epsilon k^2)\begin{Bmatrix} E_z \\ H_z \end{Bmatrix} = 0, \tag{B1}$$

where $k = \omega/c$ is defined as the free-space wave number. By splitting the Laplacian operator into normal and planar components, expressing it in cylindrical coordinates, and then using the curl equations, one can express all of the components of the electric and magnetic fields solely in terms of derivatives of the z components [28,29]:

$$\begin{aligned} E_r &= \frac{1}{\beta^2}\left[\frac{\partial^2 E_z}{\partial z \partial r} - \frac{ikZ_0}{r}\frac{\partial H_z}{\partial \theta}\right], \\ E_\theta &= \frac{1}{\beta^2}\left[\frac{1}{r}\frac{\partial^2 E_z}{\partial \theta \partial z} + ikZ_0\frac{\partial H_z}{\partial r}\right], \\ H_r &= \frac{1}{\beta^2}\left[\frac{ik\epsilon}{Z_0 r}\frac{\partial E_z}{\partial \theta} + \frac{\partial^2 H_z}{\partial r \partial z}\right], \\ H_\theta &= \frac{1}{\beta^2}\left[\frac{-ik\epsilon}{Z_0}\frac{\partial E_z}{\partial r} + \frac{1}{r}\frac{\partial^2 H_z}{\partial \theta \partial z}\right]. \end{aligned} \tag{B2}$$

We define TE waves as those where $E_z = 0$, and TM waves as those where $H_z = 0$. Using these definitions, we perform separation of variables on the z component of the field:

$$E_z(r,\theta,z) = R_{\mu\nu}(r)\Theta_\nu(\theta)Z_\mu(z). \tag{B3}$$

This provides the solution for TM modes. TM modes are found by assuming

$$H_z(r,\theta,z) = R_{\mu\nu}(r)\Theta_\nu(\theta)Z_\mu(z). \tag{B4}$$

Plugging these expressions into (B1) one at a time, with the Laplacian expressed in cylindrical coordinates, we can separate the variables as

$$\frac{d^2 Z_\mu}{dz^2} + k^2\epsilon(z)Z_\mu = \beta_\mu^2 Z_\mu, \tag{B5a}$$

$$\frac{d^2\Theta_\nu}{d\theta^2} = -\nu^2\Theta_\nu, \tag{B5b}$$

$$r\frac{d}{dr}\left(r\frac{dR_\nu}{dr}\right) + [(\beta_\mu r)^2 - \nu^2]R_\nu = 0, \tag{B5c}$$

where the variables β_μ and ν are constants of separation. The $\Theta_\nu(\theta)$ and $Z_\mu(z)$ functions must be indexed by mode numbers ν and μ, respectively, since we assume here that the boundary conditions are applied in the z and θ coordinates, which turns Eqs. (B5a) and (B5b) into an eigenvalue problem with β_μ^2 and ν^2 as eigenvalues. The r coordinate is assumed to have no boundary conditions, so $R_{\mu\nu}(r)$ inherits its mode numbers from the $\Theta_\nu(\theta)$ and $Z_\mu(z)$ functions through the separation of variables process.

The solutions to Eq. (B5b) are given immediately as

$$\Theta_\nu(\theta) = e^{i\nu\theta}, \tag{B6}$$

and since the expression for $\Theta_\nu(\theta)$ must be 2π periodic, ν must be an integer.

The boundary conditions corresponding to the z coordinate will yield an eigenvalue problem for $Z_\mu(z)$, with β_μ^2 as the eigenvalue. The boundary conditions themselves will come from substituting $Z_\mu(z)$ into (B2), and requiring that the fields either decay to zero at infinity (which yields the surface plasmon guided solution), or satisfy the radiation condition at infinity (which yields the radiation modes).

The $Z_\mu(z)$ functions that correspond to bound modes can be normalized so that

$$\int_{-\infty}^{\infty} \epsilon(z)\big[Z_\mu^{TM}(z)\big]^2 dz = L, \tag{B7a}$$

$$\int_{-\infty}^{\infty} \big[Z_\mu^{TE}(z)\big]^2 dz = L, \tag{B7b}$$

for bound (SPP) modes, where L is an arbitrary normalization constant with units of length. This particular normalization needs to be used in order for the orthogonality relationship given in Eq. (A11) to have the same normalization for TM and TE modes, and ensures that the $Z_\mu(z)$ functions will be dimensionless.

In the particular example of the interface between a dielectric and a metal film, there is only one TM bound mode, which is the SPP. In this case, the z dependence is given by

$$Z^{\rm TM}(z) = \begin{cases} \frac{k_z^-}{k}\sqrt{\frac{2k_z^+ L}{1-\epsilon}}e^{-k_z^+ z} & z \geqslant 0 \\ \frac{-k_z^+}{k}\sqrt{\frac{2k_z^+ L}{1-\epsilon}}e^{k_z^- z} & z \leqslant 0, \end{cases} \tag{B8}$$

where $k_z^+ = ik/\sqrt{\epsilon+1}$, and $k_z^- = -i\epsilon k/\sqrt{\epsilon+1}$, and the eigenvalue that corresponds to this solution is $\beta = k\sqrt{\epsilon/(\epsilon+1)}$.

The solutions for the $R_\nu(r)$ equation are the Hankel functions $H_\nu^{(2)}(\beta_\mu r)$ for outgoing waves and $H_\nu^{(1)}(\beta_\mu r)$ for incoming waves (assuming an $e^{i\omega t}$ time dependence). Putting all of this together and substituting into (B2), we have an expansion for the TM modes in terms of the *cylindrical Bessel functions*,

$$E_{\mu\nu z}^{\rm TM} = n_\mu H_\nu^{(2)}(\beta_\mu r)e^{i\nu\theta}Z_\mu^{\rm TM}(z), \tag{B9a}$$

$$E_{\mu\nu r}^{\rm TM} = \frac{1}{k}\frac{\partial}{\partial(\beta_\mu r)}H_\nu^{(2)}(\beta_\mu r)e^{i\nu\theta}\frac{dZ_\mu^{\rm TM}(z)}{dz}, \tag{B9b}$$

$$E_{\mu\nu\theta}^{\rm TM} = \frac{i\nu}{k}\frac{H_\nu^{(2)}(\beta_\mu r)}{\beta_\mu r}e^{i\nu\theta}\frac{dZ_\mu^{\rm TM}(z)}{dz}, \tag{B9c}$$

$$H^{\rm TM}_{\mu\nu z} = 0, \tag{B9d}$$

$$H^{\rm TM}_{\mu\nu r} = \frac{-\nu\epsilon}{Z_0}\frac{H^{(2)}_\nu(\beta_\mu r)}{\beta_\mu r}e^{i\nu\theta}Z^{\rm TM}_\mu(z), \tag{B9e}$$

$$H^{\rm TM}_{\mu\nu\theta} = \frac{-i\epsilon}{Z_0}\frac{\partial}{\partial(\beta_\mu r)}H^{(2)}_\nu(\beta_\mu r)e^{i\nu\theta}Z^{\rm TM}_\mu(z), \tag{B9f}$$

and the TE modes,

$$E^{\rm TE}_{\mu\nu z} = 0, \tag{B10a}$$

$$E^{\rm TE}_{\mu\nu r} = \nu\frac{H^{(2)}_\nu(\beta_\mu r)}{\beta_\mu r}e^{i\nu\theta}Z^{\rm TE}_\mu(z), \tag{B10b}$$

$$E^{\rm TE}_{\mu\nu\theta} = i\frac{\partial}{\partial(\beta_\mu r)}H^{(2)}_\nu(\beta_\mu r)e^{i\nu\theta}Z^{\rm TE}_\mu(z), \tag{B10c}$$

$$H^{\rm TE}_{\mu\nu z} = \frac{n_\mu}{Z_0}H^{(2)}_\nu(\beta_\mu r)e^{i\nu\theta}Z^{\rm TE}_\mu(z), \tag{B10d}$$

$$H^{\rm TE}_{\mu\nu r} = \frac{1}{Z_0 k}\frac{\partial}{\partial(\beta_\mu r)}H^{(2)}_\nu(\beta_\mu r)e^{i\nu\theta}\frac{dZ^{\rm TE}_\mu(z)}{dz}, \tag{B10e}$$

$$H^{\rm TE}_{\mu\nu\theta} = \frac{i\nu}{Z_0 k}\frac{H^{(2)}_\nu(\beta_\mu r)}{\beta_\mu r}e^{i\nu\theta}\frac{dZ^{\rm TE}_\mu(z)}{dz}. \tag{B10f}$$

Note that the electric field of the eigenmodes has been normalized here to be dimensionless, and the magnetic field has units of inverse impedance. The modes have also been normalized by a factor of $n_\mu = \beta_\mu/k$ in order for both the TE and TM modes to obey the same orthogonality relationship in Eq. (A11).

It is useful to express the modes in a $\{\sin(\nu\theta), \cos(\nu\theta)\}$ basis instead of the complex exponential basis. In that basis, the TM modes are given by

$$E^{\rm TMc}_{\mu\nu z} = n_\mu H^{(2)}_\nu(\beta_\mu r)\cos(\nu\theta)Z^{\rm TM}_\mu(z), \tag{B11a}$$

$$E^{\rm TMc}_{\mu\nu r} = \frac{1}{k}\frac{\partial}{\partial(\beta_\mu r)}H^{(2)}_\nu(\beta_\mu r)\cos(\nu\theta)\frac{dZ^{\rm TM}_\mu(z)}{dz}, \tag{B11b}$$

$$E^{\rm TMc}_{\mu\nu\theta} = \frac{-\nu}{k}\frac{H^{(2)}_\nu(\beta_\mu r)}{\beta_\mu r}\sin(\nu\theta)\frac{dZ^{\rm TM}_\mu(z)}{dz}, \tag{B11c}$$

$$H^{\rm TMc}_{\mu\nu z} = 0, \tag{B11d}$$

$$H^{\rm TMc}_{\mu\nu r} = \frac{-i\nu\epsilon}{Z_0}\frac{H^{(2)}_\nu(\beta_\mu r)}{\beta_\mu r}\sin(\nu\theta)Z^{\rm TM}_\mu(z), \tag{B11e}$$

$$H^{\rm TMc}_{\mu\nu\theta} = \frac{-i\epsilon}{Z_0}\frac{\partial}{\partial(\beta_\mu r)}H^{(2)}_\nu(\beta_\mu r)\cos(\nu\theta)Z^{\rm TM}_\mu(z), \tag{B11f}$$

$$E^{\rm TMs}_{\mu\nu z} = n_\mu H^{(2)}_\nu(\beta_\mu r)\sin(\nu\theta)Z^{\rm TM}_\mu(z), \tag{B12a}$$

$$E^{\rm TMs}_{\mu\nu r} = \frac{1}{k}\frac{\partial}{\partial(\beta_\mu r)}H^{(2)}_\nu(\beta_\mu r)\sin(\nu\theta)\frac{dZ^{\rm TM}_\mu(z)}{dz}, \tag{B12b}$$

$$E^{\rm TMs}_{\mu\nu\theta} = \frac{-i\nu}{k}\frac{H^{(2)}_\nu(\beta_\mu r)}{\beta_\mu r}\cos(\nu\theta)\frac{dZ^{\rm TM}_\mu(z)}{dz}, \tag{B12c}$$

$$H^{\rm TMs}_{\mu\nu z} = 0, \tag{B12d}$$

$$H^{\rm TMs}_{\mu\nu r} = \frac{i\nu\epsilon}{Z_0}\frac{H^{(2)}_\nu(\beta_\mu r)}{\beta_\mu r}\cos(\nu\theta)Z^{\rm TM}_\mu(z), \tag{B12e}$$

$$H^{\rm TMs}_{\mu\nu\theta} = \frac{-i\epsilon}{Z_0}\frac{\partial}{\partial(\beta_\mu r)}H^{(2)}_\nu(\beta_\mu r)\sin(\nu\theta)Z^{\rm TM}_\mu(z). \tag{B12f}$$

The TE modes in the $\{\sin(\nu\theta), \cos(\nu\theta)\}$ basis are

$$E^{\rm TEc}_{\mu\nu z} = 0, \tag{B13a}$$

$$E^{\rm TEc}_{\mu\nu r} = -\nu\frac{H^{(2)}_\nu(\beta_\mu r)}{\beta_\mu r}\sin(\theta)Z^{\rm TE}_\mu(z), \tag{B13b}$$

$$E^{\rm TEc}_{\mu\nu\theta} = -\frac{\partial}{\partial(\beta_\mu r)}H^{(2)}_\nu(\beta_\mu r)\cos(\theta)Z^{\rm TE}_\mu(z), \tag{B13c}$$

$$H^{\rm TEc}_{\mu\nu z} = \frac{in_\mu}{Z_0}H^{(2)}_\nu(\beta_\mu r)\cos(\theta)Z^{\rm TE}_\mu(z), \tag{B13d}$$

$$H^{\rm TEc}_{\mu\nu r} = \frac{i}{Z_0 k}\frac{\partial}{\partial(\beta_\mu r)}H^{(2)}_\nu(\beta_\mu r)\cos(\theta)\frac{dZ^{\rm TE}_\mu(z)}{dz}, \tag{B13e}$$

$$H^{\rm TEc}_{\mu\nu\theta} = \frac{-i\nu}{Z_0 k}\frac{H^{(2)}_\nu(\beta_\mu r)}{\beta_\mu r}\sin(\theta)\frac{dZ^{\rm TE}_\mu(z)}{dz}, \tag{B13f}$$

$$E^{\rm TEs}_{\mu\nu z} = 0, \tag{B14a}$$

$$E^{\rm TEs}_{\mu\nu r} = \nu\frac{H^{(2)}_\nu(\beta_\mu r)}{\beta_\mu r}\cos(\theta)Z^{\rm TE}_\mu(z), \tag{B14b}$$

$$E^{\rm TEs}_{\mu\nu\theta} = -\frac{\partial}{\partial(\beta_\mu r)}H^{(2)}_\nu(\beta_\mu r)\sin(\theta)Z^{\rm TE}_\mu(z), \tag{B14c}$$

$$H^{\rm TEs}_{\mu\nu z} = \frac{in_\mu}{Z_0}H^{(2)}_\nu(\beta_\mu r)\sin(\theta)Z^{\rm TE}_\mu(z), \tag{B14d}$$

$$H^{\rm TEs}_{\mu\nu r} = \frac{i}{Z_0 k}\frac{\partial}{\partial(\beta_\mu r)}H^{(2)}_\nu(\beta_\mu r)\sin(\theta)\frac{dZ^{\rm TE}_\mu(z)}{dz}, \tag{B14e}$$

$$H^{\rm TEs}_{\mu\nu\theta} = \frac{i\nu}{Z_0 k}\frac{H^{(2)}_\nu(\beta_\mu r)}{\beta_\mu r}\cos(\theta)\frac{dZ^{\rm TE}_\mu(z)}{dz}. \tag{B14f}$$

[1] C. M. Watts, X. Liu, and W. J. Padilla, Metamaterial electromagnetic wave absorbers, Adv. Mater. **24**, OP98 (2012).

[2] G. M. Akselrod, J. Huang, T. B. Hoang, P. T. Bowen, L. Su, D. R. Smith, and M. H. Mikkelsen, Large-area metasurface perfect absorbers from visible to near-infrared, Adv. Mater. **27**, 8028 (2015).

[3] C. Ciraci, J. Britt Lassiter, A. Moreau, and D. R. Smith, Quasi-analytic study of scattering from optical plasmonic patch antennas, J. Appl. Phys. **114**, 163108 (2013).

[4] P. T. Bowen and D. R. Smith, Coupled-mode theory for film-coupled plasmonic nanocubes, Phys. Rev. B **90**, 195402 (2014).

[5] P. T. Bowen, A. Baron, and D. R. Smith, Theory of patch-antenna metamaterial perfect absorbers, Phys. Rev. A **93**, 063849 (2016).

[6] H. Lorentz, *Collected Papers*, Vol. 1 (Martinus Nijhoff, The Hague, 1936), p. 1.

[7] G. de Haas-Lorentz, H. Lorentz, and J. Auer, *H. A. LORENTZ: Impressions of His Life and Work* (North-Holland, Amsterdam, 1957).

[8] J. V. Kranendonk and J. Sipe, V foundations of the macroscopic electromagnetic theory of dielectric media, in *Progress in Optics*, edited by E. Wolf (Elsevier, Amsterdam, 1977), pp. 245–350.

[9] P. P. Ewald, Zur begründung der kristalloptik, Ann. Phys. **354**, 1 (1916).

[10] V. E. Madelung, Das elektrische feld in systemen von regelmäßig angeordneten punktladungen, Phys. Z. **19**, 524 (1918).

[11] H. Hoek, Algemeene theorie der optische activiteit van isotrope media, Dissertation, Rijksuniversiteit te Leiden, 1939.

[12] S. R. De Groot, The Maxwell equations, *Studies in Statistical Mechanics*, Vol. 4 (North-Holland, Amsterdam, 1969).

[13] J. Sipe and J. Van Kranendonk, Macroscopic electromagnetic theory of resonant dielectrics, Phys. Rev. A **9**, 1806 (1974).

[14] P. A. Belov and C. R. Simovski, Homogenization of electromagnetic crystals formed by uniaxial resonant scatterers, Phys. Rev. E **72**, 026615 (2005).

[15] M. Marino, A. Carati, and L. Galgani, Classical light dispersion theory in a regular lattice, Ann. Phys. **322**, 799 (2007).

[16] N. Landy and D. R. Smith, Two-dimensional metamaterial device design in the discrete dipole approximation, J. Appl. Phys. **116**, 044906 (2014).

[17] P. T. Bowen, T. Driscoll, N. B. Kundtz, and D. R. Smith, Using a discrete dipole approximation to predict complete scattering of complicated metamaterials, New J. Phys. **14**, 033038 (2012).

[18] A. I. Dimitriadis, D. L. Sounas, N. V. Kantartzis, C. Caloz, and T. D. Tsiboukis, Surface susceptibility bianisotropic matrix model for periodic metasurfaces of uniaxially mono-anisotropic scatterers under oblique TE-wave incidence, IEEE Trans. Antennas Propag. **60**, 5753 (2012).

[19] T. D. Karamanos *et al.*, Polarizability matrix extraction of a bianisotropic metamaterial from the scattering parameters of normally incident plane waves, Adv. Electromagn. **1**, 64 (2012).

[20] G. M. Akselrod, C. Argyropoulos, T. B. Hoang, C. Ciracì, C. Fang, J. Huang, D. R. Smith, and M. H. Mikkelsen, Probing the mechanisms of large purcell enhancement in plasmonic nanoantennas, Nat. Photon. **8**, 835 (2014).

[21] T. B. Hoang, G. M. Akselrod, and M. H. Mikkelsen, Ultrafast room-temperature single photon emission from quantum dots coupled to plasmonic nanocavities, Nano Lett. **16**, 270 (2016).

[22] L. Rosenfeld, *Theory of Electrons*, Vol. 1 (North-Holland, Amsterdam, 1951).

[23] W. C. Chew, Some observations on the spatial and eigenfunction representations of dyadic Green's functions [electromagnetic theory], IEEE Trans. Antennas Propag. **37**, 1322 (1989).

[24] D. J. Griffiths, Hyperfine splitting in the ground state of hydrogen, Am. J. Phys. **50**, 698 (1982).

[25] A. D. Yaghjian, Electric dyadic Green's functions in the source region, Proc. IEEE **68**, 248 (1980).

[26] L. Novotny and B. Hecht, *Principles of Nano-optics* (Cambridge University Press, Cambridge, 2012).

[27] R. E. Collin, *Field Theory of Guided Waves*, IEEE/OUP Series on Electromagnetic Wave Theory (IEEE Press, New York, 1991), published under the sponsorship of the IEEE Antennas and Propagation Society.

[28] A. W. Snyder and J. Love, *Optical Waveguide Theory* (Springer Science & Business Media, Berlin/Heidelberg, 2012).

[29] C. Wu, T. Makino, J. Glinski, R. Maciejko, and S. I. Najafi, Self-consistent coupled-wave theory for circular gratings on planar dielectric waveguides, J. Lightwave Technol. **9**, 1264 (1991).

[30] J. Yang, J.-P. Hugonin, and P. Lalanne, Near-to-far field transformations for radiative and guided waves, ACS Photonics **3**, 395 (2016).

[31] F. Oberhettinger, *Fourier Transforms of Distributions and Their Inverses: A Collection of Tables*, Vol. 16 (Academic Press, Cambridge, 2014).

[32] P. B. Johnson and R. W. Christy, Optical constants of the noble metals, Phys. Rev. B **6**, 4370 (1972).

[33] G. W. Ford and W. H. Weber, Electromagnetic interactions of molecules with metal surfaces, Phys. Rep. **113**, 195 (1984).