Perturbation theory for anisotropic dielectric interfaces, and application to subpixel smoothing of discretized numerical methods

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We derive a correct first-order perturbation theory in electromagnetism for cases where an interface between two anisotropic dielectric materials is slightly shifted. Most previous perturbative methods give incorrect results for this case, even to lowest order, because of the complicated discontinuous boundary conditions on the electric field at such an interface. Our final expression is simply a surface integral, over the material interface, of the continuous field components from the unperturbed structure. The derivation is based on a "localized" coordinate-transformation technique, which avoids both the problem of field discontinuities and the challenge of constructing an explicit coordinate transformation by taking the limit in which the coordinate perturbation is infinitesimally localized around the boundary. Not only is our result potentially useful in evaluating boundary perturbations, e.g., from fabrication imperfections, in highly anisotropic media such as many metamaterials, but it also has a direct application in numerical electromagnetism. In particular, we show how it leads to a subpixel smoothing scheme to ameliorate staircasing effects in discretized simulations of anisotropic media, in such a way as to greatly reduce the numerical errors compared to other proposed smoothing schemes.

I. INTRODUCTION

In this paper, we present a technique to apply perturbative techniques to Maxwell's equations with anisotropic materials, in particular for the case where the position of an interface between two such materials is perturbed, generalizing an earlier result for isotropic materials [1]. In this case, the discontinuities of the fields at the interface cause many standard perturbative methods to fail, which is unfortunate because such methods are very useful for many problems in electromagnetism where one wishes to study the effect of small deviations from a given structure—not only do perturbative methods allow one to apply the computational efficiency of idealized problems to more realistic situations, but they may also offer greater analytical insight than brute-force numerical approaches. The corrected solution described in this paper should aid the study of interface perturbations, from surface roughness to fiber birefringence, in the context of anisotropic materials. Such materials have become increasingly important thanks to the discovery of "metamaterials," subwavelength composite structures that simulate homogeneous media with unusual properties such as negative refractive indices [2], and which may be strongly anisotropic in certain applications—for example, those involving spherical or cylindrical geometries [3] such as recent proposals for "invisibility" cloaks [4]. Furthermore, we have recently shown that interface-perturbation analyses benefit even purely brute-force computations, because they enable the design of subpixel smoothing techniques that greatly increase the accuracy (and may even increase the *order* of convergence) of discretized methods [5], which are normally degraded by discontinuous interfaces [6,7]. Here, we show that our corrected perturbation analysis provides similar benefits

for modeling anisotropic materials, where it yields a second-order accurate smoothing technique (correcting a previous heuristic proposal [6]).

There have been several previous approaches to rigorous treatment of interface perturbations in electromagnetism, where classic approaches for small $\Delta\varepsilon$ perturbations fail because of the field discontinuities [1,8–12]. One approach that was applied successfully to boundaries between isotropic materials is essentially to guess the correct form of the perturbation integral and then to prove *a posteriori* that it is correct [1]. For isotropic materials, where there is some guidance from effective-medium heuristics [13], this was practical, but the correct answer (below) appears to be much more difficult to guess for anisotropic materials. Another approach, which generalizes to the more difficult case of small surface "bumps" that are not locally flat, was to express the problem in terms of finding the polarizability of the perturbation and then connecting it back to the perturbation integral via the method of images [12]. For a locally flat perturbation between isotropic materials, this process can be carried out analytically to reproduce the previous result from Ref. [1], but it becomes rather complicated for anisotropic media. Third, one can transform the problem into a statement about the coordinate system to avoid problems of shifting field discontinuities, by finding a coordinate transformation that expresses the interface shift [10,11]. This approach, while powerful, has two shortcomings: first, finding an explicit coordinate transformation may be difficult for a complicated interface perturbation; and second, the resulting perturbation integrals are expressed in terms of the fields everywhere in space, not just at the boundaries. Intuitively, one expects that the effect of the perturbation should depend only on the field at the boundaries, as was found explicitly for the isotropic case [1,12]. In this paper, we derive precisely such an expression for the case of interfaces between anisotropic materials, by developing a general analytical technique for interface

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perturbations: we express the perturbation as a coordinate transformation, but using a coordinate transform *localized* around the perturbed interface, and take a limit in which this localization becomes narrower and narrower so that the choice of transform disappears from the final result.

In the following sections, we first formulate the problem of the effect of an interface perturbation more precisely, relate our formulation to other possibilities, and summarize our final result in the form of Eq. (3). We then derive quite generally how to formulate the problem of interface perturbations in terms of a localized coordinate transformation, and show how this allows us to express the perturbation-theory integral as a sum of contributions around individual *points* on the interface. Next, we apply this framework to the specific problem of a boundary between two anisotropic dielectric materials, and derive our final result. As a check, our perturbation theory is then validated against brute-force computations for a simple numerical example. Finally, we discuss the application of our perturbation result to subpixel smoothing of discretized numerical methods, and show that we obtain a smoothing technique that leads to much more accurate results at a given spatial resolution. In the Appendix, we provide a compact derivation and generalization of a useful result [14] relating coordinate transformations to changes in ε and μ.

II. PROBLEM FORMULATION

There are many ways to formulate perturbation techniques in electromagnetism. One common formulation, analogous to "time-independent perturbation theory" in quantum mechanics [15], is to express Maxwell's equations as a generalized Hermitian eigenproblem $\nabla \times \nabla \times \mathbf{E} = \omega^2 \varepsilon \mathbf{E}$ in the frequency ω and electric field $\mathbf{E}$ (or equivalent formulations in terms of the magnetic field $\mathbf{H}$) [16], and then to consider the first-order change $\Delta\omega$ in the frequency from a small change $\Delta\varepsilon$ in the dielectric function $\varepsilon(\mathbf{x})$ (assumed real and positive), which turns out to be [16]

$$\frac{\Delta\omega}{\omega} = -\frac{\int \mathbf{E}^* \cdot \Delta\varepsilon \mathbf{E} \, d^3\mathbf{x}}{2 \int \mathbf{E}^* \cdot \varepsilon \mathbf{E} \, d^3\mathbf{x}} + O(\Delta\varepsilon^2), \quad (1)$$

where $\mathbf{E}$ and ω are the electric field and eigenfrequency of the *unperturbed* structure ε, respectively, and $*$ denotes complex conjugation. The key part of this expression is the numerator of the right-hand side, which is what expresses the effect of the perturbation, and this same numerator appears in a nearly identical form for many different perturbation techniques. For example, one obtains a similar expression in: finding the perturbation $\Delta\beta$ in the propagation constant β of a waveguide mode [17]; the coupling coefficient $(\sim \int \mathbf{E}^* \cdot \Delta\varepsilon \mathbf{E}')$ between two modes $\mathbf{E}$ and $\mathbf{E}'$ in coupled-wave theory [18–20]; or the scattering current $\mathbf{J} \sim \Delta\varepsilon \mathbf{E}$ (and the scattered power $\sim \int \mathbf{J}^* \cdot \mathbf{E}$) in the "volume-current" method (equivalent to the first Born approximation) [12,21–23]. Equation (1) also corresponds to an *exact* result for the *derivative* of ω with respect to any parameter p of ε,
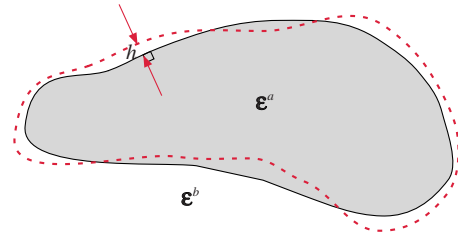

FIG. 1. (Color online) Schematic of an interface perturbation: the interface between two materials ϵ^a and ϵ^b (possibly anisotropic) is shifted by some small position-dependent displacement h.

since if we write $\Delta\varepsilon = \frac{\partial\varepsilon}{\partial p}\Delta p + O(\Delta p^2)$ we can divide both sides by Δp and take the limit $\Delta p \to 0$; this result is equivalent to the Hellmann-Feynman theorem of quantum mechanics [1,15]. In cases where the unperturbed ε is not real, corresponding to absorption or gain, or when one is considering "leaky modes," the eigenproblem typically becomes complex symmetric rather than Hermitian, and one obtains a similar formula but without the complex conjugation [24]. Therefore, any modification to the form of this numerator for the frequency-perturbation theory immediately leads to corresponding modified formulas in many other perturbative techniques, and it is sufficient for our purposes to consider frequency-perturbation theory only.

As we showed in Ref. [1], Eq. (1) is not valid when $\Delta\varepsilon$ is due to a small change in the position of a boundary between two dielectric materials (except in the limit of low dielectric contrast), but a simple correction is possible. In particular, let us consider situations like the one shown in Fig. 1, where the dielectric boundary between two materials ε^a and ε^b is shifted by some small displacement h (which may be a function of position). Directly applying Eq. (1), with $\Delta\varepsilon = \pm(\varepsilon^a - \varepsilon^b)$ in the regions where the material has changed, gives an incorrect result, and in particular $\Delta\omega/h$ (which should ideally go to the exact derivative $d\omega/dh$) is incorrect even for $h \to 0$. The problem turns out to be not so much that $\Delta\varepsilon$ is not small, but rather that $\mathbf{E}$ is discontinuous at the boundary, and the standard method in the limit $h \to 0$ leads to an ill-defined surface integral of $\mathbf{E}$ over the interfaces. For *isotropic* materials, corresponding to *scalar* $\varepsilon^{a,b}$, the correct numerator turns out to be, instead, the following surface integral over the boundary [1]:

$$\int \mathbf{E}^* \cdot \Delta\varepsilon \mathbf{E} \, d^3\mathbf{x}$$

$$\to \int \int \left[(\varepsilon^a - \varepsilon^b)|\mathbf{E}_\parallel|^2 - \left(\frac{1}{\varepsilon^a} - \frac{1}{\varepsilon^b}\right)|D_\perp|^2 \right] \mathbf{h} \cdot d\mathbf{A}, \quad (2)$$

where $\mathbf{E}_\parallel$ and $D_\perp$ are the (continuous) components of $\mathbf{E}$ and $\mathbf{D} = \varepsilon\mathbf{E}$ parallel and perpendicular to the boundary, respectively, $d\mathbf{A}$ points toward ε^b, and $\mathbf{h}$ is the displacement of the interface from ε^a toward ε^b.

In this paper, we will generalize Eq. (2) to handle the case where the two materials are *anisotropic*, corresponding to arbitrary 3×3 tensors $\boldsymbol{\varepsilon}^a$ and $\boldsymbol{\varepsilon}^b$ (assumed Hermitian and

positive definite to obtain a well-behaved Hermitian eigen-problem). In the generalized case, it is convenient to define a local coordinate frame (x_1, x_2, x_3) at each point on the surface, where the x_1 direction is orthogonal to the surface and the (x_2, x_3) directions are parallel. We also define a continuous field "vector" $\mathbf{F} = (D_1, E_2, E_3)$ so that $F_1 = D_\perp$ and $\mathbf{F}_{2,3} = \mathbf{E}_\parallel$. As derived below, the resulting numerator of Eq. (1), generalizing Eq. (2), is

$$\int\int \mathbf{F}^* \cdot [\boldsymbol{\tau}(\varepsilon^a) - \boldsymbol{\tau}(\varepsilon^b)]\mathbf{F}\mathbf{h} \cdot d\mathbf{A}, \qquad (3)$$

where $\boldsymbol{\tau}(\boldsymbol{\varepsilon})$ is the 3×3 matrix

$$\boldsymbol{\tau}(\boldsymbol{\varepsilon}) = \begin{pmatrix} -\dfrac{1}{\varepsilon_{11}} & \dfrac{\varepsilon_{12}}{\varepsilon_{11}} & \dfrac{\varepsilon_{13}}{\varepsilon_{11}} \\[2ex] \dfrac{\varepsilon_{21}}{\varepsilon_{11}} & \varepsilon_{22} - \dfrac{\varepsilon_{21}\varepsilon_{12}}{\varepsilon_{11}} & \varepsilon_{23} - \dfrac{\varepsilon_{21}\varepsilon_{13}}{\varepsilon_{11}} \\[2ex] \dfrac{\varepsilon_{31}}{\varepsilon_{11}} & \varepsilon_{32} - \dfrac{\varepsilon_{31}\varepsilon_{12}}{\varepsilon_{11}} & \varepsilon_{33} - \dfrac{\varepsilon_{31}\varepsilon_{13}}{\varepsilon_{11}} \end{pmatrix}, \qquad (4)$$

which reduces to Eq. (2) when $\boldsymbol{\varepsilon}$ is a scalar multiple ε of the identity matrix. (Our assumption that ε is positive definite guarantees that $\varepsilon_{11} > 0$.)

We should note an important restriction: Eqs. (2) and (3) require that the radius of curvature of the interface be much larger than $h = |\mathbf{h}|$, except possibly on a set of measure zero (such as at isolated corners or edges). Otherwise, more complicated methods must be employed [12]. For example, one cannot apply the above equations to the case of a hemispherical "bump" of radius h on the unperturbed surface, in which case the lowest-order perturbation is $\Delta\omega \sim O(h^3)$ and requires a small numerical computation of the polarizability of the hemisphere [12].

III. LOCAL COORDINATE PERTURBATIONS

The difficulty with applying the standard perturbation-theory result (1) to a boundary perturbation is that, instead of a *small* $\Delta\varepsilon$ with *fixed* boundary conditions on the fields (to lowest order), we have a *large* $\Delta\varepsilon$ over a small region in which the field boundary discontinuities have *shifted*. However, we can transform one problem into the other: we construct a coordinate transformation that maps the new boundary location back onto the old boundary, so that in the new coordinates the boundary conditions are unaltered, while there is a small change in the differential operators due to the coordinate shift. In expressing the problem in this fashion, we will present two key techniques. First, we employ a result from [14], generalized in the Appendix to anisotropic materials, which expresses an arbitrary coordinate transform as a change $\Delta\varepsilon$ and $\Delta\boldsymbol{\mu}$ in the permittivity and permeability tensors, which allows us to directly apply Eq. (1). Second, unlike Refs. [10,11], we do not wish to explicitly construct any coordinate transformation, since this may become very complicated for an arbitrary perturbation in an arbitrary-shaped boundary. Instead, we express the boundary shift in terms of a local coordinate transform, which only "nudges" the coordinates near the perturbed boundary, and in the limit where

the region of this coordinate perturbation becomes arbitrarily small we will recover the coordinate-independent surface integrals (2) and (3).

A. Coordinate perturbations

Suppose that in a certain coordinate system $\mathbf{x}$ we have electric field $\mathbf{E}(\mathbf{x}, t)$, magnetic field $\mathbf{H}(\mathbf{x}, t)$, dielectric tensor $\boldsymbol{\varepsilon}(\mathbf{x})$, and relative magnetic permeability tensor $\boldsymbol{\mu}(\mathbf{x})$, satisfying the Euclidean Maxwell equations. Now, we transform to some new coordinates $\mathbf{x}'(\mathbf{x})$, with a 3×3 Jacobian matrix $\mathcal{J}$ defined by $\mathcal{J}_{ij} = \frac{\partial x_i'}{\partial x_j}$. In the new coordinates, the fields can still be written as the solution of the Euclidean Maxwell equations if the following transformations are made in addition to the change of coordinates:

$$\mathbf{E}' = (\mathcal{J}^T)^{-1}\mathbf{E}, \qquad (5)$$

$$\mathbf{H}' = (\mathcal{J}^T)^{-1}\mathbf{H}, \qquad (6)$$

$$\boldsymbol{\varepsilon}' = \frac{\mathcal{J}\boldsymbol{\varepsilon}\mathcal{J}^T}{\det \mathcal{J}}, \qquad (7)$$

$$\boldsymbol{\mu} = \frac{\mathcal{J}\boldsymbol{\mu}\mathcal{J}^T}{\det \mathcal{J}}, \qquad (8)$$

where $\mathcal{J}^T$ denotes the transpose. This result is derived in the Appendix, generalized from the result for scalar ε and μ from Ref. [14].

Now, suppose the coordinate change is "small," meaning that $\mathcal{J} = \mathbf{1} + \Delta\mathcal{J}$, where the eigenvalues of $\Delta\mathcal{J}(\mathbf{x})$ are everywhere $O(\delta)$ for some small parameter δ. Then $\Delta\boldsymbol{\varepsilon}(\mathbf{x}') = \boldsymbol{\varepsilon}'(\mathbf{x}') - \boldsymbol{\varepsilon}[\mathbf{x}(\mathbf{x}')] = O(\delta)$ and similarly $\Delta\boldsymbol{\mu} = O(\delta)$. Therefore, the solutions of Maxwell's equations will be *nearly* those of $\boldsymbol{\varepsilon}$ and $\boldsymbol{\mu}$ merely translated to the new coordinate locations, and the difference due to $\Delta\boldsymbol{\varepsilon}$ and $\Delta\boldsymbol{\mu}$ can be accounted for, to $O(\delta^2)$, by first-order perturbation theory. That is, generalizing Eq. (1) to the case of anisotropic media with both $\boldsymbol{\varepsilon}$ and $\boldsymbol{\mu}$, one finds by elementary perturbation theory for the generalized eigenproblem

$$\frac{\Delta\omega}{\omega_0} = -\frac{\int (\mathbf{E}_0^* \cdot \Delta\boldsymbol{\varepsilon}\mathbf{E}_0 + \mathbf{H}_0^* \cdot \Delta\boldsymbol{\mu}\mathbf{H}_0)d^3\mathbf{x}'}{\int (\mathbf{E}_0^* \cdot \boldsymbol{\varepsilon}\mathbf{E}_0 + \mathbf{H}_0^* \cdot \boldsymbol{\mu}\mathbf{H}_0)d^3\mathbf{x}'} + O(\delta^2)$$

$$= -\frac{\int (\mathbf{E}_0^* \cdot \Delta\boldsymbol{\varepsilon}\mathbf{E}_0 + \mathbf{H}_0^* \cdot \Delta\boldsymbol{\mu}\mathbf{H}_0)d^3\mathbf{x}'}{2\int \mathbf{E}_0^* \cdot \boldsymbol{\varepsilon}\mathbf{E}_0 d^3\mathbf{x}'} + O(\delta^2), \quad (9)$$

where the 0 subscripts denote the solution for the unperturbed system, given by $\boldsymbol{\varepsilon}[\mathbf{x}(\mathbf{x}')]$ and $\boldsymbol{\mu}[\mathbf{x}(\mathbf{x}')]$, i.e., $\boldsymbol{\varepsilon}$ and $\boldsymbol{\mu}$ simply translated into the $\mathbf{x}'$ coordinates without transforming by the Jacobian factors.

B. Interface-localized coordinate transforms

Suppose that we have an unperturbed interface between two materials $\boldsymbol{\varepsilon}^a$ and $\boldsymbol{\varepsilon}^b$ that forms a surface S_0 (i.e., the

points $\mathbf{x}_0 \in S_0$), and we perturb it to a new interface S by a small perpendicular shift $\mathbf{h}(\mathbf{x})$ as depicted schematically in Fig. 1. In order to investigate this boundary shift, we will perform a coordinate transform $\mathbf{x}'(\mathbf{x})$ that shifts S to $S' = S_0$. That is, in our new coordinates, the interface has not been perturbed, but the materials have changed by the Jacobian factors as described in the previous section. Moreover, we will construct our coordinate transform so that it is *localized* to the interface, i.e., so that $\mathbf{x}' = \mathbf{x}$ far from S_0. In particular, we write

$$\mathbf{x}' = \mathbf{x} - \mathbf{h}(\mathbf{x})L(\mathbf{x}), \qquad (10)$$

where $L(\mathbf{x}) \in [0,1]$ is some differentiable localized function, equal to unity on the interface $[L(S) = 1]$ and identically zero outside some small radius $R/2$ neighborhood of the interface (the *support* of L lies within this neighborhood), chosen so that $|\nabla L| = O(1/R)$. Equation (10) is constructed so that $\mathbf{x} \in S$ implies $\mathbf{x}' \in S' = S_0$, causing the new interface S to be mapped to S_0 as desired. Thus, $\mathbf{h}(\mathbf{x})$ for $\mathbf{x} \in S$ must be the perpendicular displacement from S_0 to S. For $\mathbf{x} \notin S$, $\mathbf{h}(\mathbf{x})$ should be some differentiable, slowly varying function (except possibly at isolated surface kinks and discontinuities). The precise functions L and $\mathbf{h}$ will turn out to be irrelevant to our final answer (3), so we need not construct them explicitly.

We will take $|\mathbf{h}| = h \ll 1$ to be the small parameter of our perturbation theory, and will concern ourselves with obtaining the correct first-order $\Delta\omega$ in the limit $h \to 0$. We will also eventually take the limit $R \to 0$, but will still require $h \ll R$ in order to ensure, as will become apparent below, that the Jacobian factor of the coordinate transformation remains close to unity. (That is, we let h go to zero faster than R.) Finally, in order to have $\mathbf{h}(\mathbf{x})$ be sufficiently slowly varying that we can neglect its derivatives compared to the derivatives of $L(\mathbf{x})$, below, it will be important to require that the radius of curvature of S_0 and S be much larger than h, except possibly at isolated points; otherwise, more complicated perturbative methods are required [12].

C. Point-localized coordinate transforms

The coordinate transformation (10) representing our boundary perturbation is localized around the perturbed interface, but it is convenient to go one step further: we will represent the coordinate transform as a summation of coordinate transformations localized around individual points on the interface, by exploiting the concept of a *partition of unity* from topology [25], reviewed below.

Consider the support of the function $L(\mathbf{x})$ from above. This support is covered by the open set of spherical radius R neighborhoods of every point on the surface, and that covering must admit a locally finite subcovering $\{U^{(\alpha)}\}$; that is, a subset of neighborhoods $\{U^{(\alpha)}\}$ such that every point on the surface intersects finitely many neighborhoods $U^{(\alpha)}$, and the union of the $U^{(\alpha)}$ covers the support of L. There must also exist a partition of unity $\{\phi^{(\alpha)}\}$: a set of differentiable functions $\phi^{(\alpha)}(\mathbf{x}) \in [0,1]$ with support $\subseteq U^{(\alpha)}$, such that $\Sigma_\alpha \phi^{(\alpha)}(\mathbf{x}) = 1$ everywhere in the support of L. We can then write

$$L(\mathbf{x}) = \left(\sum_\alpha \phi^{(\alpha)}(\mathbf{x}) \right) L(\mathbf{x}) = \sum_\alpha K^{(\alpha)}(\mathbf{x}), \qquad (11)$$

where each $K^{(\alpha)}(\mathbf{x}) = \phi^{(\alpha)}(\mathbf{x})L(\mathbf{x}) \in [0,1]$ is a differentiable function localized to a small radius R neighborhood $U^{(\alpha)}$ of a single point on the interface. The Jacobian $\mathcal{J}$ of the coordinate transformation (10) can then be written in the form

$$\mathcal{J} = 1 + \sum_\alpha \Delta\mathcal{J}^{(\alpha)}, \qquad (12)$$

where

$$\Delta\mathcal{J}_{ij}^{(\alpha)} = -\frac{\partial}{\partial x_j}[h_i(\mathbf{x})K^{(\alpha)}(\mathbf{x})] \qquad (13)$$

has support $\subseteq U^{(\alpha)}$.

The key advantage of this construction arises if we look at $\Delta\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}' - \boldsymbol{\varepsilon}$ from Eq. (7). Assuming $\Delta\mathcal{J}$ is small and we are computing $\Delta\boldsymbol{\varepsilon}$ to first order, then we can write $\Delta\boldsymbol{\varepsilon} = \Sigma_\alpha \Delta\boldsymbol{\varepsilon}^{(\alpha)}$ as a sum of contributions from each $\Delta\mathcal{J}^{(\alpha)}$ individually, and similarly for $\Delta\boldsymbol{\mu}$. Therefore, when computing the first-order perturbation $\Delta\omega$ from Eq. (9), we can write $\Delta\omega = \Sigma_\alpha \Delta\omega^{(\alpha)}$ as a sum of contributions $\Delta\omega^{(\alpha)}$ analyzed in each point neighborhood separately. This removes the need to deal with the complex shape of the entire boundary at once, and is the procedure that we adopt in the following section.

IV. PERTURBATION THEORY DERIVATION

In the previous section, we established several important preliminary results that allow us to express a boundary perturbation, via coordinate transformation, as a sum of localized material perturbations $\Delta\boldsymbol{\varepsilon}^{(\alpha)}$ and $\Delta\boldsymbol{\mu}^{(\alpha)}$ around individual points of the boundary. We will now explicitly evaluate those contributions, taking the limit as the perturbation $h \to 0$ and the coordinate distortion radius $R \to 0$ to obtain our coordinate-independent final result, Eq. (3).

We therefore restrict our attention to a single neighborhood $U^{(\alpha)}$ and the contribution from the corresponding term $K^{(\alpha)}$ in the coordinate transformation. In this small neighborhood of radius R, we can take $\mathbf{h}(\mathbf{x}) \approx \mathbf{h}^{(\alpha)}$ to be a constant to lowest order in R. In this case, the interface is locally flat, and we can choose a local coordinate frame (x_1, x_2, x_3) so that x_1 is the direction perpendicular to the interface at $x_1 = 0$, with $x_1 < 0$ corresponding to $\boldsymbol{\varepsilon}^a$ and $x_1 > 0$ corresponding to $\boldsymbol{\varepsilon}^b$, as shown in Fig. 2. In this coordinate frame $\mathbf{h}^{(\alpha)} = (h^{(\alpha)}, 0, 0)$, the Jacobian contribution $\Delta\mathcal{J}^{(\alpha)}$ simplifies to

$$\Delta\mathcal{J}_{ij}^{(\alpha)} = -\delta_{i1}h^{(\alpha)}K_j^{(\alpha)} + O(h^{(\alpha)}R), \qquad (14)$$

where δ_{i1} is the Kronecker delta and $K_j^{(\alpha)}$ denotes $\partial K^{(\alpha)}/\partial x_j$. Since $R \gg |\mathbf{h}|$ by assumption and $K^{(\alpha)} \in [0,1]$ is a smooth localized function with support of radius R, $K^{(\alpha)}$ can be constructed so that $h^{(\alpha)}K_j^{(\alpha)} = O(h/R)$, i.e., so that the derivatives are small. This will make $\mathcal{J}$ close to unity and allow us to use the perturbation Eq. (9).

We must now construct $\Delta\boldsymbol{\varepsilon}^{(\alpha)}$ to first order. Since $\mathcal{J} = 1 + \Sigma_\alpha \Delta\mathcal{J}^{(\alpha)}$, we obtain
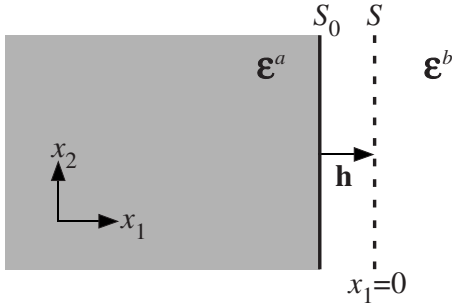
FIG. 2. Schematic of an interface perturbation as in Fig. 1, magnifying a small portion of the interface where the surface is locally flat. A local coordinate frame (x_1, x_2, x_3) is chosen so that x_1 is perpendicular to the surface, and so that $x_1 = 0$ denotes the location of the perturbed surface S (shifted perpendicularly by $\mathbf{h}$ from the original surface S_0).

$$\frac{1}{\det \mathcal{J}} = 1 + \sum_\alpha h^{(\alpha)} K_1^{(\alpha)} + O(h^2) + O(hR). \quad (15)$$

Combined with Eq. (13), we can now evaluate Eq. (7) for $\boldsymbol{\varepsilon}'$, to lowest order, to obtain $\Delta \boldsymbol{\varepsilon} = \sum_\alpha \Delta \boldsymbol{\varepsilon}^{(\alpha)} + O(h^2) + O(hR)$, with

$$\Delta \varepsilon_{ij}^{(\alpha)} = \left(\varepsilon_{ij} K_1^{(\alpha)} - \sum_k K_k^{(\alpha)} (\delta_{i1} \varepsilon_{kj} + \delta_{j1} \varepsilon_{ik}) \right) h^{(\alpha)}. \quad (16)$$

This will contribute to (9) via the integral

$$I^{(\alpha)} = \int_{U^{(\alpha)}} \mathbf{E}^* \cdot \Delta \boldsymbol{\varepsilon}^{(\alpha)} \mathbf{E} \, d^3\mathbf{x}, \quad (17)$$

where we have dropped the 0 subscript from the unperturbed field $\mathbf{E}$ for simplicity. In order to simplify this integral, we will write $\mathbf{E} = (E_1, E_2, E_3)$ in terms of $\mathbf{F} = (D_1, E_2, E_3)$, since $\mathbf{F}$ is continuous whereas E_1 is not. Solving for E_1 in $\mathbf{D} = \boldsymbol{\varepsilon}\mathbf{E}$ yields $E_1 = \frac{1}{\varepsilon_{11}}(D_1 - \varepsilon_{12}E_2 - \varepsilon_{13}E_3)$, and thus $\mathbf{E} = \mathcal{F}\mathbf{F}$ where

$$\mathcal{F}(\boldsymbol{\varepsilon}) = \begin{pmatrix} \frac{1}{\varepsilon_{11}} & -\frac{\varepsilon_{12}}{\varepsilon_{11}} & -\frac{\varepsilon_{13}}{\varepsilon_{11}} \\ & 1 & \\ & & 1 \end{pmatrix}. \quad (18)$$

Because $\mathbf{F}$ is continuous, we can write $\mathbf{F}(\mathbf{x}) = \mathbf{F}^{(\alpha)} + O(R)$, where the $O(R)$ term is a higher-order contribution to $I^{(\alpha)}$ that can be dropped and the $\mathbf{F}^{(\alpha)}$ is a constant that can be pulled out of the integral. Therefore, we are left with

$$I^{(\alpha)} = \mathbf{F}^{(\alpha)*} \cdot \left(\int_{U^{(\alpha)}} \mathcal{F}^\dagger \Delta \boldsymbol{\varepsilon}^{(\alpha)} \mathcal{F} \, d^3\mathbf{x} \right) \mathbf{F}^{(\alpha)} + O(hR), \quad (19)$$

where $\mathcal{F}^\dagger$ is the conjugate transpose. This integral now simplifies a great deal, because the only nonconstant terms are from the $K_j^{(\alpha)}$ and the step-function $\Theta(x_1)$ dependence of $\varepsilon(\mathbf{x})$. In particular, the integrals over the $K_2^{(\alpha)}$ and $K_3^{(\alpha)}$ terms vanish, because along the x_2 and x_3 directions, respectively, they are integrals of the derivatives of a function $K^{(\alpha)}$ that vanishes at the end points. We are left with the $K_1^{(\alpha)}$ terms, which yield the integrand

$$\mathcal{F}^\dagger \begin{pmatrix} -\varepsilon_{11} & & \\ & \varepsilon_{22} & \varepsilon_{23} \\ & \varepsilon_{32} & \varepsilon_{33} \end{pmatrix} \mathcal{F} K_1^{(\alpha)} h^{(\alpha)}$$
$$= \boldsymbol{\tau}(\boldsymbol{\varepsilon}) K_1^{(\alpha)} h^{(\alpha)} = \{\boldsymbol{\tau}(\boldsymbol{\varepsilon}^a) + [\boldsymbol{\tau}(\boldsymbol{\varepsilon}^b) - \boldsymbol{\tau}(\boldsymbol{\varepsilon}^a)]\Theta(x_1)\} K_1^{(\alpha)} h^{(\alpha)}, \quad (20)$$

where the product of the three matrices gives precisely the matrix $\boldsymbol{\tau}(\boldsymbol{\varepsilon})$ defined in Eq. (4), using the assumption that $\boldsymbol{\varepsilon}$ is Hermitian ($\boldsymbol{\varepsilon}^\dagger = \boldsymbol{\varepsilon}$). When Eq. (20) is integrated by parts in the x_1 direction, we obtain the integral of $K^{(\alpha)}$ multiplied by a delta function $\delta(x_1)$ from the derivative of $\Theta(x_1)$, producing

$$\int \int [\boldsymbol{\tau}(\boldsymbol{\varepsilon}^a) - \boldsymbol{\tau}(\boldsymbol{\varepsilon}^b)] K^{(\alpha)}(0, x_2, x_3) h^{(\alpha)} dx_2 dx_3. \quad (21)$$

When this is summed over α to obtain the total perturbation integral, however, $\sum_\alpha K^{(\alpha)}(0, x_2, x_3) = L(0, x_2, x_3) = 1$ by construction (since $L = 1$ on the interface). Thus, we obtain the surface integral of Eq. (3), as desired, where $h^{(\alpha)} dx_2 dx_3 = \mathbf{h} \cdot d\mathbf{A}$.

The analysis of the $\Delta \boldsymbol{\mu}^{(\alpha)}$ term proceeds identically, although here the continuous field components are (B_1, H_2, H_3), but in this case it yields zero if $\boldsymbol{\mu}^a = \boldsymbol{\mu}^b$ (as in the common case of nonmagnetic materials where $\boldsymbol{\mu}$ is identically 1).

V. NUMERICAL VALIDATION

To check the correctness of the perturbative analysis above, we performed the following numerical computation. We solve the full-vector Maxwell eigenproblem numerically, for inhomogeneous anisotropic dielectric structures, by iterative Rayleigh-quotient minimization in a plane-wave basis, using a freely available software package [6]. Given an arbitrary structure, we can then evaluate the derivative of the eigenfrequency for a shifting interface, both by the perturbation Eq. (3) and by numerical differentiation of the eigenfrequencies (here, differentiating a cubic-spline interpolation).

In particular, we considered a two-dimensional photonic crystal [16] consisting of a square lattice (lattice constant a) of $0.4a \times 0.2a$ dielectric blocks of a material $\boldsymbol{\varepsilon}^a$ surrounded by $\boldsymbol{\varepsilon}^b$, with Gaussian bumps on one side (inset of Fig. 3). Here, $\boldsymbol{\varepsilon}^a$ and $\boldsymbol{\varepsilon}^b$ are chosen to be random, symmetric, positive-definite matrices with eigenvalues ranging from 2 to 12 for $\boldsymbol{\varepsilon}^a$ and from 1 to 5 for $\boldsymbol{\varepsilon}^b$. On the right side of each block (along one of the $0.4a$ edges) is a Gaussian bump of height $h(y) = he^{-y^2/2w^2}$, with a width $w = 0.1a$ and amplitude h (where $h < 0$ denotes an indentation). We then computed the lowest eigenvalue $\omega(A)$ and eigenfields $\mathbf{E}$ for a set of h values $h/a \in [-0.17, +0.17]$, at a Bloch wave vector $\mathbf{k} = (0, 0, 0.5)2\pi/a$ (leading to modes with a vacuum wavelength $\lambda \sim 3a$). Given these data, we then compared the derivative $d\omega/dh$ as computed by the perturbation Eq. (3) compared to the derivative of a cubic-spline fit of the frequency data. This was repeated for six different random $\boldsymbol{\varepsilon}^a$ and $\boldsymbol{\varepsilon}^b$. The results, shown in Fig. 3, demonstrate that the perturbation formula indeed predicts the exact slope h as expected (with tiny discrepancies, due to the finite resolution, too small to see on this graph).
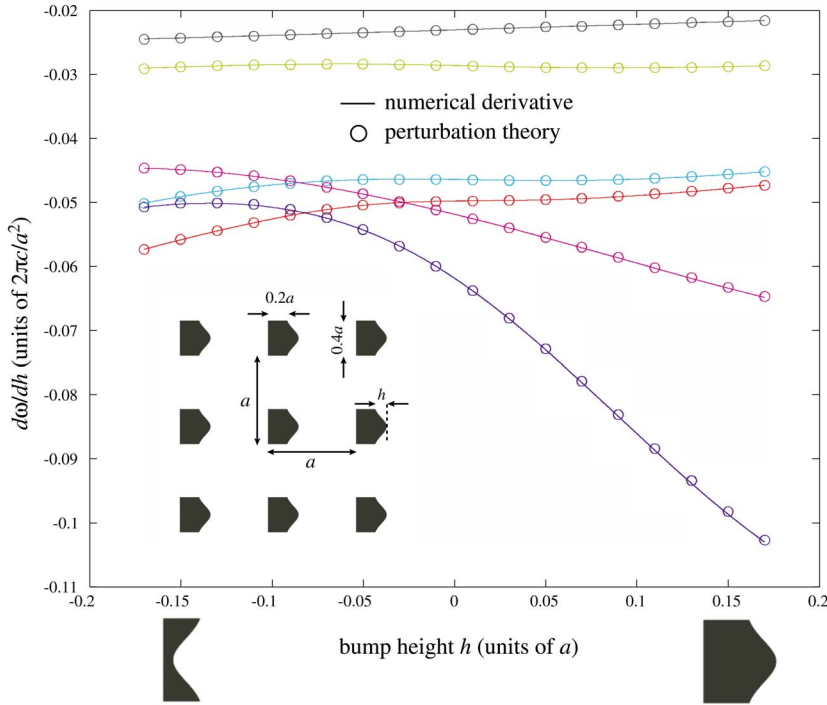
FIG. 3. (Color online) Numerical validation of perturbation-theory formula, applied to compute the derivative $d\omega/dh$ for a Gaussian "bump" of height h on a square lattice (period a) of anisotropic-ϵ rectangles (inset) with an eigenfrequency ω (corresponding to $\lambda \sim 3a$). Positive (negative) h indicate bumps (indentations) (see lower right and left insets for $h = \pm 0.15a$), respectively. Solid lines are numerical differentiation of the eigenfrequency, and dots are from perturbation theory. The different lines correspond to different random dielectric tensors ϵ^a and ϵ^b.

VI. APPLICATION TO SUBPIXEL SMOOTHING

In any numerical method involving the solution of the full-vector Maxwell's equations on a discrete grid or its equivalent, such as the plane-wave method above [6] or the finite-difference time-domain (FDTD) method [26], discontinuities in the dielectric function ε (and the corresponding field discontinuities) generally degrade the accuracy of the method, typically reducing it to only linear convergence with resolution [6,7]. Unfortunately, a piecewise-continuous ε is the most common experimental situation, so a technique to improve the accuracy (without switching to an entirely different computational method) is desirable. One simple approach that has been proposed by several authors is to *smooth* the dielectric function, or equivalently to set the ε of each pixel to be some average of ε within the pixel, rather than merely sampling ε in a staircase fashion [5,6,13,27–31]. Unfortunately, this smoothing itself changes the structure, and therefore introduces errors. We analyzed this situation in a recent paper for the FDTD method [5], and showed that the problem is closely related to perturbation theory: one desires a smoothing of ε that has zero first-order effect, to minimize the error introduced by smoothing and so that the underlying second-order accuracy can potentially be preserved. At an interface between two isotropic dielectric materials, the first-order perturbation is given by Eq. (2), and this leads to an *anisotropic* smoothing: one averages ε^{-1} for field components perpendicular to the interface, and averages ε for field components parallel to the interface, a result that was previously proposed heuristically by several authors [6,13,29].

In this section, we generalize that result to interfaces between anisotropic materials, and illustrate numerically that it leads to dramatic improvements in both the absolute magnitude and the convergence rate of the discretization error. In the anisotropic-interface case, a heuristic subpixel smoothing scheme was previously proposed [6], but we now show that this method was suboptimal: although it is better than other smoothing schemes, it does not set the first-order perturbation to zero and therefore does not minimize the error or permit the possibility of second-order accuracy. Specifically, as discussed more explicitly below, a second-order smoothing is obtained by averaging $\tau(\varepsilon)$ and then inverting $\tau(\varepsilon)$ to obtain the smoothed "effective" dielectric tensor. Because this scheme is analytically guaranteed to eliminate the first-order error otherwise introduced by smoothing, we expect it to generally lead to the smallest numerical error compared to competing smoothing schemes, and there is the hope that the overall convergence rate may be quadratic with resolution.

First, let us analyze how perturbation theory leads to a smoothing scheme. Suppose that we smooth the underlying dielectric tensor $\varepsilon(\mathbf{x})$ into some locally averaged tensor $\overline{\varepsilon}(\mathbf{x})$, by some method to be determined below. This involves a change $\Delta\varepsilon = \overline{\varepsilon} - \varepsilon$, which is likely to be large near points where ε is discontinuous (and, conversely, is zero well inside regions where ε is constant). In particular, suppose that we employ a smoothing radius (defined more precisely below) proportional to the spatial resolution Δx of our numerical method, so that $\Delta\varepsilon$ is zero [or at most $O(\Delta x^2)$] except within a distance $\sim\Delta x$ of discontinuous interfaces. To evaluate the effect of this large perturbation near an interface, we must employ an equivalent reformulation of Eq. (3):

$$\Delta\omega \sim \int \mathbf{F}^* \cdot \Delta\boldsymbol{\tau}\mathbf{F} \, d^3\mathbf{x},$$

where $\Delta\boldsymbol{\tau} = \boldsymbol{\tau}(\overline{\boldsymbol{\varepsilon}}) - \boldsymbol{\tau}(\boldsymbol{\varepsilon})$. It is sufficient to look at the perturbation in ω, since (as we remarked in Sec. II) the same integral appears in the perturbation theory for many other

quantities (such as scattered power, etc.). If we let x_1 denote the (local) coordinate orthogonal to the boundary, then the x_1 integral is simply proportional to $\sim\int\Delta\boldsymbol{\tau}\,dx_1+O(\Delta x^2)$: since **F** is continuous and $\Delta\boldsymbol{\tau}=0$ except near the interface, we can pull **F** out of the x_1 integral to lowest order. That means, in order to make the first-order perturbation zero for all fields **F**, it is sufficient to have $\int\Delta\boldsymbol{\tau}\,dx_1=0$. This is achieved by averaging $\boldsymbol{\tau}$ as follows.

The most straightforward interpretation of smoothing would be to convolve ε with some localized kernel $s(\mathbf{x})$, where $\int s(\mathbf{x})d^3\mathbf{x}=1$ and $s(\mathbf{x})=0$ for $|\mathbf{x}|$ greater than some smoothing radius (the support radius) proportional to the resolution $\sim\Delta x$. That is, $\overline{\boldsymbol{\varepsilon}}(\mathbf{x})=\boldsymbol{\varepsilon}*s=\int\boldsymbol{\varepsilon}(\mathbf{y})s(\mathbf{x}-\mathbf{y})d^3\mathbf{y}$. For example, the simplest subpixel smoothing, simply computing the average of $\boldsymbol{\varepsilon}$ over each pixel, corresponds to $s=1$ inside a pixel at the origin and $s=0$ elsewhere. However, this will not lead to the desired $\int\Delta\boldsymbol{\tau}=0$ to obtain second-order accuracy. Instead, we employ

$$\overline{\boldsymbol{\varepsilon}}(\mathbf{x})=\boldsymbol{\tau}^{-1}[\boldsymbol{\tau}(\boldsymbol{\varepsilon})*s]=\boldsymbol{\tau}^{-1}\left(\int\boldsymbol{\tau}[\boldsymbol{\varepsilon}(\mathbf{y})]s(\mathbf{x}-\mathbf{y})d^3\mathbf{y}\right),$$
(22)

where $\boldsymbol{\tau}^{-1}$ is the inverse of the $\boldsymbol{\tau}(\boldsymbol{\varepsilon})$ mapping, given by

$$\boldsymbol{\tau}^{-1}(\boldsymbol{\tau})=\begin{pmatrix} -\dfrac{1}{\tau_{11}} & -\dfrac{\tau_{12}}{\tau_{11}} & -\dfrac{\tau_{13}}{\tau_{11}} \\ -\dfrac{\tau_{21}}{\tau_{11}} & \tau_{22}-\dfrac{\tau_{21}\tau_{12}}{\tau_{11}} & \tau_{23}-\dfrac{\tau_{21}\tau_{13}}{\tau_{11}} \\ -\dfrac{\tau_{31}}{\tau_{11}} & \tau_{32}-\dfrac{\tau_{31}\tau_{12}}{\tau_{11}} & \tau_{33}-\dfrac{\tau_{31}\tau_{13}}{\tau_{11}} \end{pmatrix}.$$
(23)

The reason why Eq. (22) works, regardless of the smoothing kernel $s(\mathbf{x})$, is that

$$\int\Delta\boldsymbol{\tau}\,d^3\mathbf{x}=\int d^3\mathbf{x}\left(\int\boldsymbol{\tau}[\boldsymbol{\varepsilon}(\mathbf{y})]s(\mathbf{x}-\mathbf{y})d^3\mathbf{y}-\boldsymbol{\varepsilon}(\mathbf{x})\right)$$

$$=\int d^3\mathbf{y}\,\boldsymbol{\tau}[\boldsymbol{\varepsilon}(\mathbf{y})]\left(\int s(\mathbf{x}-\mathbf{y})d^3\mathbf{y}-1\right)=0.$$
(24)

This guarantees that the integral of $\Delta\boldsymbol{\tau}$ is zero over all space, but above we required what appears to be a stronger condition, that the local, interface-perpendicular integral $\int\Delta\boldsymbol{\tau}\,dx_1$ be zero (at least to first order). However, in a small region where the interface is locally flat (to first order in the smoothing radius), $\Delta\boldsymbol{\tau}$ must be a function of x_1 only by translational symmetry, and therefore (24) implies that $\int\Delta\boldsymbol{\tau}\,dx_1=0$ by itself. Although the above convolution formulas may look complicated, for the simplest smoothing kernel $s(\mathbf{x})$ the procedure is quite simple: in each pixel, average $\boldsymbol{\tau}(\boldsymbol{\varepsilon})$ in the pixel and then apply $\boldsymbol{\tau}^{-1}$ to the result. (This is no more difficult to apply than the procedure implemented in Ref. [6], for example.)

Strictly speaking, the use of this smoothing does not guarantee second-order accuracy, even if the underlying numerical method is nominally second-order accurate or better. For one thing, although we have canceled the first-order error

due to smoothing, it may be that the next-order correction is not second order. Precisely, this situation occurs if one has a structure with sharp dielectric corners, edges, or cusps, as discussed in Ref. [1]: in this case, smoothing leads to a convergence rate between first order (which would be obtained with no smoothing) and second order, with the exponent determined by the nature of the field singularity that occurs at the corner.

A. Numerical smoothing validation

As a simple illustration of the efficacy of the subpixel smoothing we propose in Eq. (22), let us consider a two-dimensional example problem: a square lattice (period a) of ellipses made of $\boldsymbol{\varepsilon}^a$ surrounded by $\boldsymbol{\varepsilon}^b$, where we will find the lowest-ω Bloch eigenmode. As above, we choose the dielectric tensors to be random positive-definite symmetric matrices with random eigenvalues in [2,12] for $\boldsymbol{\varepsilon}^a$ and in [1,5] for $\boldsymbol{\varepsilon}^b$, and the ellipses are oriented at an arbitrary angle, at an arbitrary Bloch wave vector $\mathbf{k}a/2\pi=(0.1,0.2,0.3)$, to avoid fortuitous symmetry effects. (The vacuum wavelength λ corresponding to the eigenfrequency ω is $\lambda=5.03a$.) For each resolution Δx, we assign an $\overline{\boldsymbol{\varepsilon}}$ to each pixel by computing $\boldsymbol{\tau}^{-1}$ of the average of $\boldsymbol{\tau}(\boldsymbol{\varepsilon})$ within that pixel. Then, we compute the relative error $\Delta\omega/\omega$ (compared to a calculation at a much higher resolution) as a function of resolution. For comparison, we also consider four other smoothing techniques: no smoothing, averaging $\boldsymbol{\varepsilon}$ in each pixel [28], averaging $\boldsymbol{\varepsilon}^{-1}$ in each pixel, and a heuristic anisotropic averaging proposed by Ref. [6] in analogy to the scalar case. The results are shown in Fig. 4, based on the same plane-wave method as above [6], and show that the smoothing technique clearly leads to the lowest errors $\Delta\omega/\omega$. Also, whereas the other methods yield clearly first-order convergence, the method seems to exhibit roughly second-order convergence. The no-smoothing case has extremely erratic errors, as is typical for staircasing phenomena.

In Fig. 5, we also show results from a similar calculation in three dimensions (3D). Here, we look at the lowest eigenmode of a cubic lattice (period a) of 3D ellipsoids (oriented at a random angle) made of $\boldsymbol{\varepsilon}^a$ surrounded by $\boldsymbol{\varepsilon}^b$, both random positive-definite symmetric matrices as above. The frequency ω, at an arbitrarily chosen wave vector $\mathbf{k}a/2\pi=(0.4,0.3,0.1)$, corresponds to a vacuum wavelength $\lambda=3.14a$. Again, this method almost always has the lowest error by a wide margin, especially if the unpredictable dips of the no-smoothing case are excluded, and is the only one to exhibit (apparently) better than linear convergence.

Our previous heuristic proposal from Ref. [6], while better than the other smoothing schemes (and less erratic than no smoothing), is clearly inferior to this method. Previously, we had observed what seemed to have been quadratic convergence from the heuristic scheme [6], but this result seems to have been fortuitous—as we demonstrated recently, even non-second-order schemes can sometimes appear to have second-order convergence over some range of resolutions for a particular geometry [5]. The key distinction of this scheme that lends us greater confidence in it than one or two examples can convey is that it is no longer heuristic. This
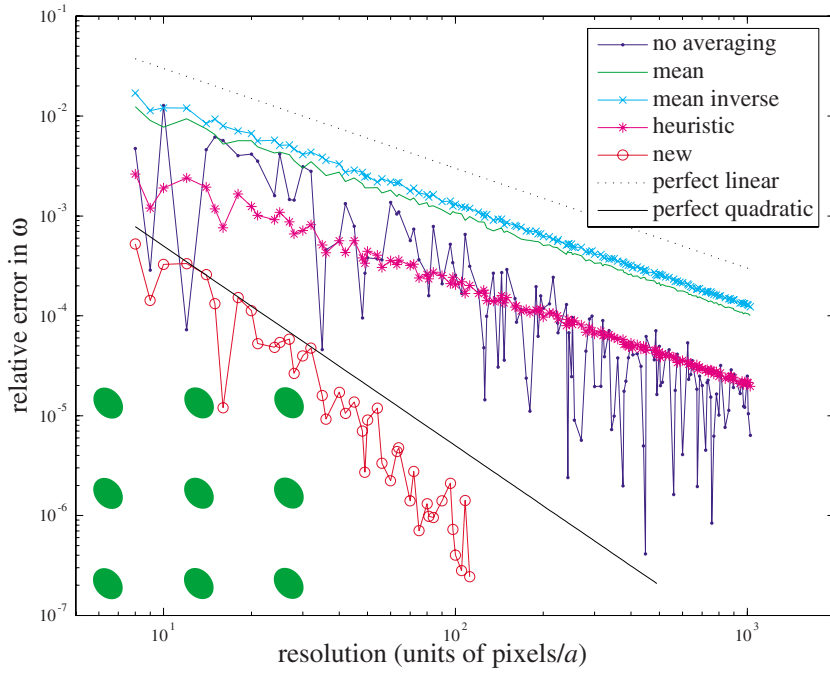
FIG. 4. (Color online) Relative error $\Delta\omega/\omega$ for an eigenmode calculation with a square lattice (period a) of 2D anisotropic ellipses (green inset), versus spatial resolution, for a variety of subpixel smoothing techniques. Straight lines for perfect linear (black dashed) and perfect quadratic (black solid) convergence are shown for reference.

smoothing scheme is based on a clear analytical criterion—setting the first-order perturbative effect of the smoothing to zero—which explains why it should be an accurate choice in a wide variety of circumstances.

VII. CONCLUDING REMARKS

We have shown how to correctly treat lowest-order perturbations to a boundary between two anisotropic materials, a problem for which previous approaches were stymied by the complicated discontinuous boundary conditions on the electric field. This result immediately led to an improved subpixel smoothing scheme for discretized numerical methods—we demonstrated it for a plane-wave method, but we expect that it will similarly be applicable to other methods, e.g., FDTD methods [5]. The same result can also be applied to constructing an effective-medium theory for subwavelength multilayer films of anisotropic materials. Moreover, in the process of deriving our perturbative result, we developed a local coordinate-transform approach that may be useful in treating many other types of interface perturbations, because it circumvents the difficulty of shifting discontinuities without requiring one to construct an explicit coordinate transformation.
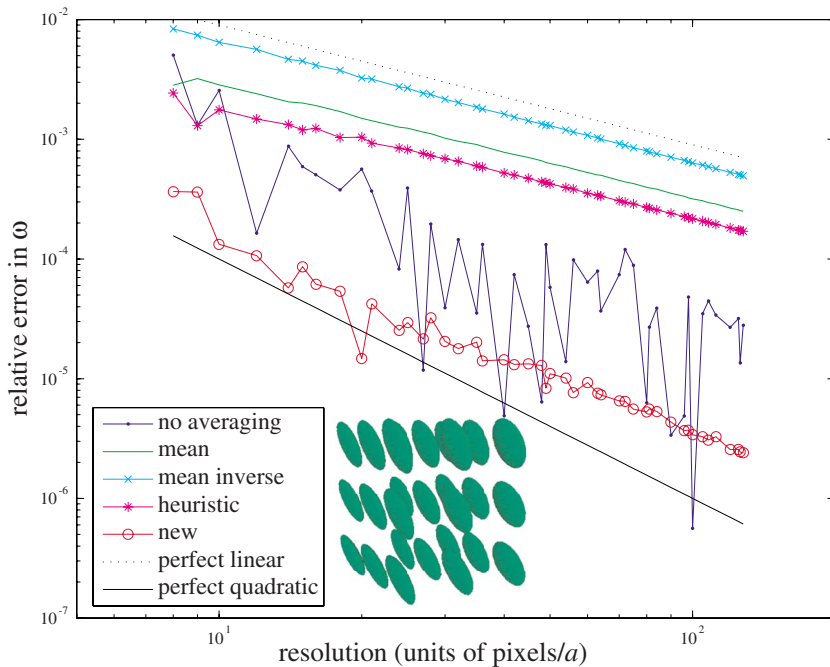

FIG. 5. (Color online) Relative error $\Delta\omega/\omega$ for an eigenmode calculation with cubic lattice (period a) of 3D anisotropic ellipsoids (green inset), versus spatial resolution, for a variety of subpixel smoothing techniques. Straight lines for perfect linear (black dashed) and perfect quadratic (black solid) convergence are shown for reference.

APPENDIX: COORDINATE TRANSFORMATION OF MAXWELL'S EQUATIONS

As discussed in Sec. III A above, any differentiable coordinate transformation of Maxwell's equations can be recast as merely a transformation of ε and μ, with the same solutions **E** and **H** only multiplied by a matrix in addition to the coordinate change [14]. This result has been exploited by Pendry *et al.* to obtain a number of beautiful analytical results from cylindrical superlenses [3] to invisibility cloaks [4]. It (and related ideas) can be used to derive coupled-mode expressions for bending loss in optical waveguides [17,19]. A similar result has also been employed to design perfectly-matched layers (PMLs), via a *complex* coordinate stretching, to truncate numerical grids [32]. It is likely that there are many other applications, as well as equivalent derivations, that we are not aware of. Here, we review the proof in a compact form, generalized to arbitrary anisotropic media. (Most previous derivations seem to have been for isotropic media in at least one coordinate frame [14], or for coordinate transformations with purely diagonal Jacobians $\mathcal{J}$ where $\mathcal{J}_{ii}$ depends only on x_i [32], or for constant affine coordinate transforms [33].)

We begin with the usual Maxwell's equations for Euclidean space (in natural units):

$$\nabla \times \mathbf{H} = \varepsilon \frac{\partial \mathbf{E}}{\partial t} + \mathbf{J}, \tag{A1}$$

$$\nabla \times \mathbf{E} = -\mu \frac{\partial \mathbf{H}}{\partial t}, \tag{A2}$$

$$\nabla \cdot (\varepsilon \mathbf{E}) = \rho, \tag{A3}$$

$$\nabla \cdot (\mu \mathbf{H}) = 0, \tag{A4}$$

where **J** and ρ are the usual free current and charge densities, respectively. We will proceed in index notation, employing the Einstein convention whereby repeated indices are summed over. Ampère's law, Eq. (A1), is now expressed as

$$\partial_a H_b \epsilon_{abc} = \varepsilon_{cd} \frac{\partial E_d}{\partial t} + J_c, \tag{A5}$$

where ϵ_{abc} is the usual Levi-Città permutation tensor and $\partial_a = \partial/\partial x_a$. Under a coordinate change $\mathbf{x} \mapsto \mathbf{x}'$, if we let $\mathcal{J}_{ab} = \frac{\partial x'_a}{\partial x'_b}$ be the (nonsingular) Jacobian matrix associated with the coordinate transform (which may be a function of $\mathbf{x}$), we have

$$\partial_a = \mathcal{J}_{ba} \partial'_b. \tag{A6}$$

Furthermore, as in Eqs. (5) and (6), let

$$E_a = \mathcal{J}_{ba} E'_b, \tag{A7}$$

$$H_a = \mathcal{J}_{ba} H'_b. \tag{A8}$$

Hence, Eq. (A5) becomes

$$\mathcal{J}_{ia} \partial'_i \mathcal{J}_{jb} H'_j \epsilon_{abc} = \varepsilon_{cd} \mathcal{J}_{ld} \frac{\partial E'_l}{\partial t} + J_c. \tag{A9}$$

Here, the $\mathcal{J}_{ia} \partial'_i = \partial_a$ derivative falls on both the $\mathcal{J}_{jb}$ and H'_j terms, but we can eliminate the former thanks to the ϵ_{abc}: $\partial_a \mathcal{J}_{jb} \epsilon_{abc} = 0$ because $\partial_a \mathcal{J}_{jb} = \partial_b \mathcal{J}_{ja}$. Then, again multiplying both sides by the Jacobian $\mathcal{J}_{kc}$, we obtain

$$\mathcal{J}_{kc} \mathcal{J}_{jb} \mathcal{J}_{ia} \partial'_i H'_j \epsilon_{abc} = \mathcal{J}_{kc} \varepsilon_{cd} \mathcal{J}_{ld} \frac{\partial E'_l}{\partial t} + \mathcal{J}_{kc} J_c. \tag{A10}$$

Noting that $\mathcal{J}_{ia} \mathcal{J}_{jb} \mathcal{J}_{kc} \epsilon_{abc} = \epsilon_{ijk} \det \mathcal{J}$ by definition of the determinant, we finally have

$$\partial'_i H'_j \epsilon_{ijk} = \frac{1}{\det \mathcal{J}} \mathcal{J}_{kc} \varepsilon_{cd} \mathcal{J}_{ld} \frac{\partial E'_l}{\partial t} + \frac{\mathcal{J}_{kc} J_c}{\det \mathcal{J}} \tag{A11}$$

or, back in vector notation,

$$\nabla' \times \mathbf{H}' = \frac{\mathcal{J} \varepsilon \mathcal{J}^T}{\det \mathcal{J}} \frac{\partial \mathbf{E}'}{\partial t} + \mathbf{J}', \tag{A12}$$

where $\mathbf{J}' = \mathcal{J} \mathbf{J} / \det \mathcal{J}$. Thus, we see that we can interpret Ampère's law in arbitrary coordinates as the usual equation in Euclidean coordinates, as long as we replace the materials, etc., by Eqs. (5)–(7). By an identical argument, we obtain

$$\nabla' \times \mathbf{E}' = -\frac{\mathcal{J} \mu \mathcal{J}^T}{\det \mathcal{J}} \frac{\partial \mathbf{H}'}{\partial t}, \tag{A13}$$

which yields the corresponding transformation (8) for μ.

The transformation of the remaining divergence equations into equivalent forms in the new coordinates is also straightforward. Gauss's law, Eq. (A3), becomes

$$\rho = \partial_a \varepsilon_{ab} E_b = \mathcal{J}_{ia} \partial'_i \varepsilon_{ab} \mathcal{J}_{jb} E'_j = \mathcal{J}_{ia} \partial'_i (\det \mathcal{J}) \mathcal{J}^{-1}_{ak} \varepsilon'_{kj} E'_j$$
$$= (\det \mathcal{J}) \partial'_i \varepsilon'_{ij} E'_j + (\partial_a \mathcal{J}^{-1}_{ak} \det \mathcal{J}) \varepsilon'_{kj} E'_j = (\det \mathcal{J}) \partial'_i \varepsilon'_{ij} E'_j, \tag{A14}$$

which gives $\nabla' \cdot (\varepsilon' \mathbf{E}') = \rho'$ for $\rho' = \rho / \det \mathcal{J}$, and similarly for Eq. (A4). Here, we have used the fact that

$$\partial_a \mathcal{J}^{-1}_{ak} \det \mathcal{J} = \partial_a \epsilon_{anm} \epsilon_{kij} \mathcal{J}_{in} \mathcal{J}_{jm} / 2 = 0, \tag{A15}$$

from the cofactor formula for the matrix inverse, and recalling that $\partial_a \mathcal{J}_{jb} \epsilon_{abc} = 0$ from above. In particular, note that $\rho = 0 \Leftrightarrow \rho' = 0$ and $\mathbf{J} = 0 \Leftrightarrow \mathbf{J}' = 0$, so a nonsingular coordinate transformation preserves the absence (or presence) of sources.

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