Energy flow in a semi-infinite spatially dispersive absorbing dielectric*

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We consider energy flow in a semi-infinite spatially dispersive absorbing dielectric bounded by vacuum, on which light is incident from the vacuum, with the direction of propagation normal to the surface. While the total energy flux in the vacuum is given by its electromagnetic Poynting vector, the total energy flux in the crystal is given by the sum of the electromagnetic Poynting vector and a mechanical Poynting vector, which arises from the energy transported by the excitations in the médium. We consider two models, the first of which is a semi-infinite medium in the dielectric approximation, which consists of assuming that the nonlocal dielectric function of the semi-infinite crystal is that of the infinitely extended medium, so that the surface of the medium enters the theory only through the restriction of the coordinates normal to the surface to the half-space occupied by the medium. We show that this model fails to conserve energy in the sense that the surface acts as a source of energy, because for this model the mechanical Poynting vector is positive on the surface, while the electromagnetic Poynting vector is continuous across the surface. The second model considered includes the effects of a surface in a phenomenological way in the dielectric function. We find that for this model energy is conserved; that is, the surface acts neither as a source nor sink of energy. Finally, we find that for normal incidence, when the additional boundary condition for a given model of a spatially dispersive dielectric medium may be expressed in terms of the polarization $\vec{P}(z)$ associated with the dipole-active excitation in the medium as $[\alpha\vec{P}(z) + \beta\, d\vec{P}(z)/dz]_{z=0} = 0$, the coefficients α and β determine whether or not the surface is a source or sink of energy. The mechanical Poynting vector is proportional to $\mathrm{Im}(\alpha/\beta)$, so that when this quantity vanishes, the surface is neither a source nor sink of energy, but when it is nonzero, the surface is either a source or sink of energy, depending on the sign of the other constants entering into the expression for the mechanical Poynting vector.

I. INTRODUCTION

Considerable interest has arisen recently in the optical properties of bounded absorbing spatially dispersive dielectrics. Properties that have been studied include reflectivities at normal and non-normal incidence, the dispersion relation for surface polaritons, and the attenuated-total-reflection spectrum. However, energy flow in such systems has been little studied to date. Energy flow in unbounded, absorbing dielectric media, in which effects of spatial dispersion are neglected, has been studied in considerable detail by Loudon.[1] Recently, Maddox and Mills[2] have briefly considered this problem for an unbounded spatially dispersive dielectric, with the neglect of damping, and showed that the energy flux vector $\vec{S}$ in such a medium is the sum of the electromagnetic Poynting vector $\vec{S}_E = (c/4\pi)\vec{E}\times\vec{H}$ and a mechanical Poynting vector $\vec{S}_M$, which is the contribution to $\vec{S}$ from the energy transported by the excitations in the medium.

In this paper we extend the work of Loudon and of Maddox and Mills by considering energy flow in a system consisting of a semi-infinite spatially dispersive absorbing dielectric separated by a plane interface from the vacuum outside it. For simplicity, we consider only the case in which the energy flux is normal to the dielectric-vacuum interface.

The present work is prompted by the following considerations. In the existing calculations of the optical properties of bounded spatially dispersive absorbing media models of the nonlocal dielectric constant of varying complexity have been employed. Some of these models depend on the microscopic properties of the crystals studied,[3] while others are purely macroscopic in nature.[4] It is the latter class of models that concerns us in this note. Of particular interest is the model that assumes the dielectric approximation, because it is used frequently. The dielectric approximation consists of assuming translationally invariant dielectric functions all the way up to the boundary.

One of our purposes in this paper is to caution those who would depend on such a model for the prediction of the optical properties of interest about an important failure of that model. We find that, for electromagnetic radiation incident normally on the surface of a semi-infinite crystal, the dielectric-approximation model fails to conserve energy; that is, the surface acts as a source of energy. This is due to a discontinuous flux of energy across the boundary. This occurs because, at normal incidence the electromagnetic Poynting vector is continuous across the boundary, but the mechanical Poynting vector, which arises from the energy transported by the excitations in the medium, is discontinuous, since it is nonzero on the surface for this model.

As in the work of Loudon[1] and of Maddox and Mills,[2] the spatially dispersive and absorbing medium in our work will be described by a collection of damped noninteracting harmonic oscillators, driven by a macroscopic electric field. These oscillators represent the optical vibrations of a diatomic cubic polar crystal or, with a suitable redefinition of the coefficients in their equations of motion, the relative motion of the electron and hole constituting an exciton in an insulating crystal. The effects of spatial dispersion are incorporated in the equations of motion of the oscillators through the presence of terms containing spatial derivatives. In Sec. II we display the oscillator equations of motion used in the dielectric approximation for the determination of the dielectric constant of a semi-infinite medium. We also obtain the relation between the oscillator coordinates and the driving electric field, as well as expressions for the electric fields inside and outside the medium. In Sec. IV we derive the form of the energy conservation condition for this model, and show that the dielectric approximation leads to the surface being a source of energy.

In order to understand the reasons for this, we consider in Sec. III a more-general model of the dielectric medium in which the effects of a surface are taken into account explicitly. We show in Sec. IV that for this model the surface is neither a source nor sink of energy, since for this case the mechanical Poynting vector vanishes on the surface. In Sec. V, we consider the general conditions on a macroscopic model that the surface be neither a source nor sink of energy.

A rather general, but brief, discussion of the conditions under which the surface of a spatially dispersive dielectric medium is neither a source nor sink of energy has been given by Hopfield.[5] However, this discussion is incomplete, in our view, because Hopfield assumed that the energy flux in the dielectric medium is given by the electromagnetic Poynting vector, and it is now known that there is an additional contribution, which is given by the mechanical Poynting vector.

II. MODEL OF A SEMI-INFINITE MEDIUM IN THE DIELECTRIC APPROXIMATION

In this section, we consider a simple model for the dielectric constant of a semi-infinite homogeneous isotropic spatially dispersive medium that has been used by several authors.[4] It is assumed in this model that the dielectric function of the semi-infinite crystal is that of the infinitely extended medium up to and including the surface. In particular, this approximation, called the dielectric approximation, requires that the nonlocal dielectric function $\epsilon(\vec{x},\vec{x}';t-t')$ depend on the position coordinates $\vec{x}$ and $\vec{x}'$ only through their difference.

We assume that the surface of the semi-infinite crystal lies in the xy plane and that the crystal occupies the half-space $z\geqslant 0$. In order to derive the dielectric function, we begin with the equations of motion for the infinitely extended crystal, which we assume to be the same as the equations of motion for the semi-infinite crystal in the region $z\geqslant 0$. We consider a diatomic cubic crystal in which the macroscopic electric field $\vec{E}$ in it couples with the long-wavelength optical displacements of the ions. We write the equations of motion in terms of the relative displacement $\vec{\xi}$, defined by

$$\vec{\xi}=\sqrt{\mu}\,[\vec{u}(+)-\vec{u}(-)]\,, \tag{2.1}$$

where $\vec{u}(+)$ and $\vec{u}(-)$ are the actual displacements of the positive and negative sublattices and μ is their reduced mass. The equations of motion for the semi-infinite crystal for $z\geqslant 0$, in the presence of spatial dispersion are assumed to be

$$\frac{e_T^*}{\sqrt{\mu}}\,\vec{E}=\frac{d^2\vec{\xi}}{dt^2}+\gamma\frac{d\vec{\xi}}{dt}+\omega_T^2\vec{\xi}-D\nabla^2\vec{\xi}\,. \tag{2.2}$$

Here e_T^* is the transverse effective charge, ω_T is the transverse optical frequency for the mode of interest, γ is a phenomenological damping constant, and D is a phenomenological parameter that describes the amount of spatial dispersion and is determined by the curvature of the dispersion relation for the mode of interest.

We assume an oscillatory dependence of the electric field $\vec{E}$ and of the relative displacement $\vec{\xi}$ on the spatial variables parallel to the surface, i.e., in the xy plane, and on the time. That is, we assume

$$\vec{\xi}(\vec{x},t)=\vec{\xi}(z)\,e^{i\vec{k}_{\parallel}\cdot\vec{x}_{\parallel}-i\omega t}\,, \tag{2.3a}$$

$$\vec{E}(\vec{x},t)=\vec{E}(z)\,e^{i\vec{k}_{\parallel}\cdot\vec{x}_{\parallel}-i\omega t}\,. \tag{2.3b}$$

With this assumption, Eq. (2.2) may be written in the form

$$-\frac{e_T^*}{\sqrt{\mu}\,D}\,\vec{E}(z)=\left(\frac{d^2}{dz^2}+\Gamma^2\right)\vec{\xi}(z)\,, \tag{2.4a}$$

where

$$\Gamma=[(-1/D)(\omega_T^2-\omega^2-i\omega\gamma+Dk_{\parallel}^2)]^{1/2}\,. \tag{2.4b}$$

We solve Eq. (2.4a) using Green's-function technique. That is, we introduce a Green's function $G_\alpha(z,z')$ by the equation

$$\left(\frac{d^2}{dz^2}+\Gamma^2\right)G_\alpha(z,z')=\delta(z-z')\,, \tag{2.5a}$$

whose solution is

$$G_\alpha(z,z') = \frac{e^{i\Gamma|z-z'|}}{2i\Gamma} . \tag{2.5b}$$

In terms of this function we obtain

$$\xi_\alpha(z) = \left(\frac{-e_T^*}{\sqrt{\mu}D}\right)\int_0^\infty G_\alpha(z,z')E_\alpha(z')\,dz' . \tag{2.5c}$$

Since the polarization in the crystal is given by

$$\vec{P}(z) = \frac{e_T^*}{\sqrt{\mu}}\,\vec{\xi}(z) + \chi_\infty \vec{E}(z) , \tag{2.6a}$$

where χ_∞ is the background dielectric susceptibility, and the total dielectric susceptibility is defined by the relation

$$\vec{P}(z) = \int_0^\infty dz'\,\chi(\vec{k}_\parallel,\omega;z,z')\vec{E}(z') \tag{2.6b}$$

for an isotropic dielectric, we may write the dielectric constant for the medium in the form

$$\epsilon(\vec{k}_\parallel\omega;zz') = \epsilon_\infty\delta(z-z') + \frac{\epsilon_\infty\Omega_p^2}{(-2i\Gamma)D}e^{i\Gamma|z-z'|} , \tag{2.7a}$$

where

$$\epsilon_\infty = 1 + 4\pi\chi_\infty \tag{2.7b}$$

and

$$\Omega_p^2 = 4\pi(e_T^*)^2/\epsilon_\infty\mu v_a . \tag{2.7c}$$

Using this result, we may solve for the electric and magnetic fields in the crystal ($z \geq 0$) and in the vacuum below the crystal ($z<0$). For simplicity in what follows, we will assume that light is incident on the crystal from below and propagates along the positive z direction (i.e., normal to the surface).

At normal incidence, the problem of solving Maxwell's equations reduces to solving the equation

$$\frac{-d^2}{dz^2}E(z) = \frac{\omega^2}{c^2}D(z) = \frac{\omega^2}{c^2}\int_0^\infty \epsilon(\omega;z-z')E(z')\,dz' \tag{2.8}$$

subject to the requirements that the tangential components of the electric and magnetic fields be continuous across the plane $z=0$. Here $\epsilon(\omega;z-z')$ is given by Eq. (2.7a), where $\epsilon(\omega;z-z') = \epsilon(\vec{0}\omega;z-z')$ and Γ is given by Eq. (2.4b) with $k=0$. Also, without loss of generality, we assume that the electric field and relative displacement for normal incidence of light are parallel to the x axis, and, for convenience, we drop the subscripts. Equation (2.8), when written out explicitly for this model, becomes

$$\left(\frac{d^2}{dz^2} + \epsilon_\infty\frac{\omega^2}{c^2}\right)E(z) + \epsilon_\infty\frac{\omega^2}{c^2}\frac{\Omega_p^2}{D}\frac{1}{(-2i\Gamma)} \times \int_0^\infty dz'\,e^{i\Gamma|z-z'|}E(z') = 0 . \tag{2.9}$$

To solve this equation we employ the method of Ref. 4c of operating on both sides of Eq. (2.9) with the operator

$$\mathcal{O} = \frac{d^2}{dz^2} + \Gamma^2 \tag{2.10a}$$

in order to convert this integro-differential equation to a differential equation, which is given by

$$\left(\frac{d^2}{dz^2} + \Gamma^2\right)\left(\frac{d^2}{dz^2} + \epsilon_\infty\frac{\omega^2}{c^2}\right)E(z) = \frac{\omega^2}{c^2}\epsilon_\infty\frac{\Omega_p^2}{D}E(z) . \tag{2.10b}$$

We seek a solution of this equation in the form

$$E(z) = e^{i\zeta z} . \tag{2.11}$$

Substitution of this expression into Eq. (2.10b) yields the following quartic equation for ζ:

$$(\zeta^2 - \Gamma^2)\left(\zeta^2 - \epsilon_\infty\frac{\omega^2}{c^2}\right) - \frac{\omega^2}{c^2}\epsilon_\infty\frac{\Omega_p^2}{D} = 0 . \tag{2.12}$$

Since Eq. (2.12) is quadratic in ζ^2, two of the four roots ζ_j of this equation are the negatives of the other two. In writing an expression for the total electric field in the crystal, we require that the field goes to zero as $z\to\infty$. Thus, we superpose the two solutions corresponding to ζ_1 and ζ_2, the two roots with positive imaginary parts

$$E(z) = \sum_{j=1}^{2} E_j e^{i\zeta_j z}, \quad z>0 . \tag{2.13}$$

This expression must also satisfy the original integro-differential equation (2.9). If we use the result that

$$\int_0^\infty dz'\,e^{i\Gamma|z-z'|}e^{i\zeta_j z'} = \frac{e^{i\zeta_j z}(2i\Gamma)}{i(\zeta_j^2-\Gamma^2)} - \frac{e^{i\Gamma z}}{i(\zeta_j-\Gamma)}, \tag{2.14}$$

we find that the expression given by Eq. (2.13) satisfies Eq. (2.9) provided that the coefficients E_1 and E_2 are related by

$$\sum_{j=1}^{2}\left(\frac{E_j}{\zeta_j-\Gamma}\right) = 0 . \tag{2.15}$$

This relation is called the additional boundary condition.

We now turn to a determination of the electric field in the vacuum below the crystal, $z<0$. With the assumption of normal incidence, the electric field in the vacuum may be written

$$E(z)=e^{i(\omega/c)z}+Re^{-i(\omega/c)z}, \quad z<0. \tag{2.16}$$

The first term describes the incident wave, and the second describes the reflected wave.

We must now match the solutions (2.13) and (2.16) across the plane at $z=0$. For an isotropic crystal at normal incidence, this requires that the tangential components of the electric and magnetic fields are continuous across the boundary, which reduces to the requirement that $E(z)$ and $dE(z)/dz$ be continuous across the boundary. These conditions may be written explicitly as

$$1+R=E_1+E_2, \tag{2.17a}$$

$$(\omega/c)(1-R)=\zeta_1E_1+\zeta_2E_2. \tag{2.17b}$$

Thus, from Eqs. (2.15) and (2.17), we determine E_1, E_2, and R to be

$$E_1=2(\zeta_1-\Gamma)/(\zeta_1-\zeta_2)(1+\eta), \tag{2.18a}$$

$$E_2=-2(\zeta_2-\Gamma)/(\zeta_1-\zeta_2)(1+\eta), \tag{2.18b}$$

$$R=(1-\eta)/(1+\eta), \tag{2.18c}$$

where

$$\eta=(c/\omega)(\zeta_1+\zeta_2-\Gamma). \tag{2.18d}$$

In addition, we find the expression for the relative displacement $\xi(z)$ from Eqs. (2.5b), (2.5c), and (2.13)–(2.15) to be

$$\xi(z)=\left(\frac{-e_T^*}{D\sqrt{\mu}}\right)\sum_{j=1}^{2}\frac{E_je^{i\zeta_jz}}{(\zeta_j^2-\Gamma^2)}, \quad z\geqslant 0, \tag{2.19}$$

where E_1 and E_2 are given by Eqs. (2.18a) and (2.18b).

III. MORE-GENERAL MODEL

In Sec. II, the equations of motion for the system [Eq. (2.2)] contained no information about the presence of a surface at $z=0$, other than the restriction of the range of applicability of the equations to the upper half-space. In the present section, we include the effects of a surface in a phenomenological manner by beginning the analysis with a Lagrangian density subject to a dissipative force, assuming that the Lagrangian density and the dissipative force are nonzero only in the upper half-plane ($z\geq 0$). Then, given these assumptions, we derive the equations of motion for the system. For the model under consideration, we assume that the Lagrangian density for the system is given by

$$\mathcal{L}=\sqrt{\mu}\left[\frac{1}{2}\left(\frac{d\vec{\xi}}{dt}\right)^2-\tfrac{1}{2}\vec{\xi}^2-\Theta(z)\tfrac{1}{2}D\sum_{\mu\nu}\left(\frac{\partial\xi_\mu}{\partial x_\nu}\right)^2+\frac{e_T^*}{\sqrt{\mu}}\vec{\xi}\cdot\vec{\mathrm{E}}-\Theta(z)\sum_{\lambda\mu\nu}C_{\lambda\mu\nu}\xi_\lambda\frac{\partial\xi_\mu}{\partial x_\nu}\right], \tag{3.1a}$$

where $\Theta(z)$ is the Heaviside unit step function. We further assume that the system is subject to a dissipative force, which may be derived from Rayleigh's dissipation function for this system, given by

$$\mathfrak{F}=\tfrac{1}{2}\sqrt{\mu}\,\gamma\left(\frac{d\vec{\xi}}{dt}\right)^2. \tag{3.1b}$$

By the use of the general form of Lagrange's equation of motion in the presence of this dissipative function

$$\frac{-\partial\mathfrak{F}}{\partial(d\xi_\alpha/dt)}+\frac{\partial\mathcal{L}}{\partial\xi_\alpha}-\frac{d}{dt}\frac{\partial\mathcal{L}}{\partial(d\xi_\alpha/dt)}-\sum_\nu\frac{d}{dx_\nu}\frac{\partial\mathcal{L}}{\partial(\partial\xi_\alpha/\partial x_\nu)}=0, \tag{3.2}$$

we may obtain the equations of motion for the model system, and from these proceed to calculate the dielectric constant, the electric fields, and the displacement vector $\vec{\xi}$. All the quantities appearing in Eq. (3.1), except the $C_{\lambda\mu\nu}$, are the same as those defined in Sec. II. The $C_{\lambda\mu\nu}$ are additional constants related to the spatial dispersion present in the crystal. The equations of motion for this model may thus be written

$$\left(\frac{e_T^*}{\sqrt{\mu}}\right)E_\alpha=\frac{d^2\xi_\alpha}{dt^2}+\gamma\frac{d\xi_\alpha}{dt}+\omega_T^2\xi_\alpha-\Theta(z)D\nabla^2\xi_\alpha+\Theta(z)\sum_{\mu\nu}(C_{\alpha\mu\nu}-C_{\mu\alpha\nu})\frac{\partial\xi_\mu}{\partial x_\nu}-\delta(z)\left(\sum_\mu C_{\mu\alpha z}\xi_\mu+D\frac{\partial\xi_\alpha}{\partial z}\right). \tag{3.3}$$

We assume that the $C_{\lambda\mu\nu}$ are symmetric in the first two indices λ and μ, and from consideration of the symmetry of the semi-infinite crystal, we find that the only nonzero components of $C_{\lambda\mu\nu}$ appearing in the equations of motion are those of the form $C_{\alpha\alpha z}$ ($\alpha=x,y,z$). For simplicity, we assume that these are given by

$$C_{\alpha\alpha z}=-\alpha\omega_T^2, \tag{3.4}$$

independent of α. The simplified form of the equations of motion thus becomes

$$\left(\frac{e_T^*}{\sqrt{\mu}}\right)\vec{\mathrm{E}}=\frac{d^2\vec{\xi}}{dt^2}+\gamma\frac{d\vec{\xi}}{dt}+\omega_T^2\vec{\xi}-D\nabla^2\vec{\xi}+\delta(z)\left(\alpha\omega_T^2\vec{\xi}-D\frac{\partial\vec{\xi}}{\partial z}\right), \quad z\geq 0. \tag{3.5}$$

We assume that the temporal and spatial dependences of the electric field $\vec{E}$ and of the relative displacement $\vec{\xi}$ are those given by Eqs. (2.3). Thus, the problem of solving the equations of motion (3.5) reduces to the problem of solving the equation

$$-\left(\frac{e_T^*}{D\sqrt{\mu}}\right)\vec{E}(z)=\left(\frac{d^2}{dz^2}+\Gamma^2\right)\vec{\xi}(z) - \frac{\delta(z)}{D}\left(a\omega_T^2\vec{\xi}(z)-D\frac{\partial\vec{\xi}}{\partial z}\right), \quad (3.6)$$

where Γ is given by Eq. (2.4b). Using the Green's-function technique, we find that the $\xi_\alpha(z)$ are given in terms of the $E_\alpha(z)$ by the relation (2.5c), provided that Eq. (2.5a) is solved subject to the following boundary condition at $z=0$:

$$\left(a\omega_T^2\xi_\alpha(z)-D\frac{\partial\xi_\alpha}{\partial z}\right)_{z=0}=0. \quad (3.7)$$

In this way, we find that the Green's function $G_\alpha(z,z')$ is given by

$$G_\alpha(z,z')=\frac{1}{2i\Gamma}\left(e^{i\Gamma|z-z'|}+Qe^{i\Gamma(z+z')}\right), \quad (3.8a)$$

where

$$Q=(iD-a\omega_T^2)/(iD+a\omega_T^2). \quad (3.8b)$$

Now, by the use of Eqs. (2.5c), (2.6a), and (2.6b), we obtain an expression for the dielectric constant in the medium

$$\epsilon(k_\parallel\omega;zz')=\epsilon_\infty\delta(z-z')+[\epsilon_\infty\Omega_p^2/(-2i\Gamma)D] \times\left(e^{i\Gamma|z-z'|}+Qe^{i\Gamma(z+z')}\right). \quad (3.9)$$

We now follow the methods outlined in Sec. II in order to obtain the electric and magnetic fields in the crystal ($z\ge 0$) at normal incidence to the crystal surface. We thus wish to solve Eq. (2.8) with $\epsilon(\omega;zz')=\epsilon(\vec{0}\omega;zz')$ given by Eq. (3.9), and where Γ is given by Eq. (2.4b) with $\vec{k}_\parallel=0$. As in Sec. II, we assume that the electric field and relative displacement for normal incidence of light are parallel to the x axis, and we again drop the subscripts. With this, we may write Eq. (2.8) explicitly as

$$\left(\frac{d^2}{dz^2}+\epsilon_\infty\frac{\omega^2}{c^2}\right)E(z)+\epsilon_\infty\frac{\omega^2}{c^2}\frac{\Omega_p^2}{D}\frac{1}{-2i\Gamma}\int_0^\infty dz'\left(e^{i\Gamma|z-z'|}+Qe^{i\Gamma(z+z')}\right)E(z')=0. \quad (3.10)$$

When we act on Eq. (3.10) with the operator $\mathcal{O}$ defined by Eq. (2.10a), we obtain the differential equation (2.10b). Thus, the analysis of Sec. II follows in this case, and we obtain the form of the electric field in the crystal given by Eq. (2.13). This expression must now satisfy the original integro-differential equation (3.10). We now use Eq. (2.15), together with the relation

$$\int_0^\infty dz'\,e^{i\zeta_j z'}e^{i\Gamma(z+z')}=\frac{-e^{i\Gamma z}}{i(\zeta_j+\Gamma)} \quad (3.11)$$

to obtain the condition on E_1 and E_2 so that Eq. (2.12) will be a solution of Eq. (3.10):

$$\sum_{j=1}^{2}E_j\left(\frac{\zeta_j+\beta}{\zeta_j^2-\Gamma^2}\right)=0, \quad (3.12a)$$

where

$$\beta=i(a\omega_T^2/D). \quad (3.12b)$$

Next we solve the two equations given by Eq. (3.12a) together with the two Maxwell boundary conditions [Eqs. (2.17)] in order to obtain expressions for E_1, E_2, and R, which appear in the solutions for the electric fields in the crystal and vacuum, Eqs. (2.13) and (2.16). In this way we obtain

$$E_1=\frac{2(\zeta_1^2-\Gamma^2)(\zeta_2+\beta)}{(\zeta_1-\zeta_2)(\zeta_1\zeta_2+\Gamma^2)(1+\eta)}, \quad (3.13a)$$

$$E_2=\frac{-2(\zeta_2^2-\Gamma^2)(\zeta_1+\beta)}{(\zeta_1-\zeta_2)(\zeta_1\zeta_2+\Gamma^2)(1+\eta)}, \quad (3.13b)$$

$$R=\frac{1-\eta}{1+\eta}+\frac{2\beta(\zeta_1+\zeta_2)}{(\zeta_1\zeta_2+\Gamma^2)(1+\eta)}, \quad (3.13c)$$

where

$$\eta=\frac{c}{\omega}\beta+\frac{\zeta_1+\zeta_2}{\zeta_1\zeta_2+\Gamma^2}\times\left(\beta\left[1+\frac{c}{\omega}(\zeta_1-\zeta_2)\right]+\frac{c}{\omega}\zeta_1\zeta_2\right). \quad (3.13d)$$

In addition, we find that, in the determination of $\xi(z)$ in terms of $E(z)$, the evaluation of Eq. (2.5c), together with Eqs. (2.13), (2.14), (3.11), and (3.12), exactly yields the form of Eq. (2.19), where in this case E_1 and E_2 are given by Eqs. (3.13a) and (3.13b).

IV. POYNTING'S THEOREM

In this section, we derive Poynting's theorem in the presence of damping and spatial dispersion, for a semi-infinite crystal in the upper half-space ($z\ge 0$) and vacuum in the lower half-space ($z<0$). The starting point for our analysis is Maxwell's equations, from which we will obtain the energy-conservation condition. The equations of interest are

$$\nabla\times\vec{E}=\left(\frac{-1}{c}\right)\frac{\partial\vec{B}}{\partial t},\quad \nabla\times\vec{H}=\left(\frac{4\pi}{c}\right)\vec{J}+\left(\frac{1}{c}\right)\frac{\partial\vec{D}}{\partial t}. \quad (4.1a)$$

We assume nonmagnetic media, so that $\vec{B}=\vec{H}$, and that no external charges or currents are present. We combine these two equations, together with the identity from vector analysis,

$$\nabla\cdot(\vec{E}\times\vec{H})=\vec{H}\cdot(\nabla\times\vec{E})-\vec{E}\cdot(\nabla\times\vec{H}),\qquad(4.1b)$$

and the relation connecting the electric displacement vector $\vec{D}$ to the polarization $\vec{P}$,

$$\vec{D}=\vec{E}+4\pi\vec{P},\qquad(4.1c)$$

to obtain the following relation:

$$\left(\frac{c}{4\pi}\right)\nabla\cdot(\vec{E}\times\vec{H})=\left(\frac{-1}{4\pi}\right)\left(\vec{E}\cdot\frac{d\vec{E}}{dt}+\vec{H}\cdot\frac{d\vec{H}}{dt}\right)-\vec{E}\cdot\frac{d\vec{P}}{dt}.\qquad(4.2)$$

We now specialize to the case of a diatomic cubic crystal, where the polarization $\vec{P}(z)$ is given by Eq. (2.6a), with $\vec{\xi}(z)$ defined by Eq. (2.1). We now introduce the electromagnetic Poynting vector

$$\vec{S}_E=\left(\frac{c}{4\pi}\right)(\vec{E}\times\vec{H})\qquad(4.3a)$$

and the electromagnetic energy density

$$U_E=\left(\frac{1}{8\pi}\right)(\epsilon_\infty\vec{E}^2+\vec{H}^2)\qquad(4.3b)$$

in order to write Eq. (4.2) in a simplified form

$$\nabla\cdot\vec{S}_E+\frac{d}{dt}U_E+\left(\frac{1}{v_a}\right)\left(\frac{e_T^*}{\sqrt{\mu}}\right)\left(\vec{E}\cdot\frac{d\vec{\xi}}{dt}\right)=0.\qquad(4.4)$$

It is now desirable to write the term proportional to $\vec{E}\cdot d\vec{\xi}/dt$ in a form similar to that of the other two terms in Eq. (4.4) by defining a Poynting vector and an energy density that arise from the mechanical vibrations in a crystal in the presence of spatial dispersion. In order to complete this task, we need an expression for $\vec{E}$ in terms of $\vec{\xi}$ from the equations of motion of the crystal, which are model dependent. Therefore, in what follows, we consider the two different models described in Secs. II and III.

A. Poynting's theorem for a model of a semi-infinite medium in the dielectric approximation

We use Eq. (2.2) of Sec. II in order to write $\vec{E}\cdot d\vec{\xi}/dt$ as a function of $\vec{\xi}$ alone. Thus, we have

$$\vec{E}\cdot\frac{d\vec{\xi}}{dt}=\left(\frac{\sqrt{\mu}}{e_T^*}\right)\left(\frac{d^2\vec{\xi}}{dt^2}+\gamma\frac{d\vec{\xi}}{dt}+\omega_T^2\vec{\xi}-D\nabla^2\vec{\xi}\right)\cdot\frac{d\vec{\xi}}{dt}.\qquad(4.5)$$

We note that this is equivalent to the following form, in which we have written some of the terms as a total time derivative:

$$\vec{E}\cdot\frac{d\vec{\xi}}{dt}=\left(\frac{\sqrt{\mu}}{e_T^*}\right)\left\{\frac{d}{dt}\left[\left(\frac{d\vec{\xi}}{dt}\right)^2+\omega_T^2\vec{\xi}^2+D(\nabla\vec{\xi})^2\right]-D\left[(\nabla^2\vec{\xi})\cdot\frac{d\vec{\xi}}{dt}+\nabla\vec{\xi}\cdot\nabla\frac{d\vec{\xi}}{dt}\right]+\gamma\left(\frac{d\vec{\xi}}{dt}\right)^2\right\}.\qquad(4.6)$$

We now introduce what we will call the mechanical Poynting vector, which is nonzero only in the crystal, ($z\geq 0$), and which is given by the relation:

$$\vec{S}_M=-\frac{D}{v_a}\sum_\beta\hat{x}_\beta\Theta(z)\frac{d\vec{\xi}}{dt}\cdot\nabla\left(\frac{\partial\vec{\xi}}{\partial x_\beta}\right),\qquad(4.7)$$

where $\hat{x}_\beta$ is a unit vector along the β Cartesian axis. Therefore, the divergence of the mechanical Poynting vector is given by

$$\nabla\cdot\vec{S}_M=-\frac{D}{v_a}(\nabla^2\vec{\xi})\cdot\frac{d\vec{\xi}}{dt}-\frac{D}{v_a}\nabla\vec{\xi}\cdot\nabla\frac{d\vec{\xi}}{dt}-\frac{D}{v_a}\delta(z)\frac{d\vec{\xi}}{dt}\cdot\left(\frac{\partial\vec{\xi}}{\partial z}\right).\qquad(4.8)$$

If we define a mechanical-energy density

$$U_M=\frac{1}{2v_a}\left[\left(\frac{d\vec{\xi}}{dt}\right)^2+\omega_T^2\vec{\xi}^2+D(\nabla\vec{\xi})^2\right],\qquad(4.9)$$

then we may write Eq. (4.4) in the following simple form:

$$\nabla\cdot(\vec{S}_E+\vec{S}_M)+\frac{d}{dt}(U_E+U_M)=-\frac{\gamma}{v_a}\left(\frac{d\vec{\xi}}{dt}\right)^2-\frac{D}{v_a}\delta(z)\frac{d\vec{\xi}}{dt}\cdot\left(\frac{\partial\vec{\xi}}{\partial z}\right);\qquad(4.10)$$

or, if we take the time average of both sides of the equation, then

$$\nabla\cdot(\langle\vec{S}_E\rangle+\langle\vec{S}_M\rangle)=-\frac{\gamma}{v_a}\left\langle\left(\frac{d\vec{\xi}}{dt}\right)^2\right\rangle-\frac{D}{v_a}\delta(z)\left\langle\frac{d\vec{\xi}}{dt}\cdot\left(\frac{\partial\vec{\xi}}{\partial z}\right)\right\rangle.\qquad(4.11)$$

If we now specialize to the case of normal incidence, so that the components of $\vec{E}$ and $\vec{\xi}$ normal to the surface vanish, we may write the time averages of the electromagnetic and mechanical Poynting vectors in terms of the complex forms of the electric fields by the use of Eqs. (2.19), (4.3a), and (4.7). Thus, we have

$$\langle\vec{S}_E\rangle=\hat{z}\left(\frac{c}{8\pi}\right)\left(\frac{c}{\omega}\right)\mathrm{Re}\left[\left(\sum_{j=1}^{2}E_je^{i\zeta_jz}\right)\times\left(\sum_{j=1}^{2}\zeta_j^*E_j^*e^{-i\zeta_j^*z}\right)\right]\Theta(z)+\hat{z}\left(\frac{c}{8\pi}\right)(1-|R|^2)\Theta(-z),\qquad(4.12a)$$

$$\langle\vec{S}_M\rangle=\hat{z}\left(\frac{\omega}{2D}\right)\left(\frac{\epsilon_\infty\Omega_p^2}{4\pi}\right)\mathrm{Re}\left[\left(\sum_{j=1}^{2}\frac{E_je^{i\zeta_jz}}{\zeta_j^2-\Gamma^2}\right)\times\left(\sum_{j=1}^{2}\frac{\zeta_j^*E_j^*e^{-i\zeta_j^*z}}{\zeta_j^{*2}-\Gamma^{*2}}\right)\right]\Theta(z),\qquad(4.12b)$$

where E_1, E_2, and R are given by Eqs. (2.18).

The electromagnetic Poynting vector $\vec{S}_E$ is continuous across the surface of the crystal at $z=0$. This is assured by the Maxwell boundary conditions of conservation of tangential components of $\vec{E}$ and $\vec{H}$ across the boundary, as we see by rewriting the quantity $(1-|R|^2)$ in terms of E_1 and E_2 with the help of Eqs. (2.17):

$$\begin{aligned} 1-|R|^2 &= \mathrm{Re}[(1+R)(1-R^*)] \\ &= (c/\omega)\,\mathrm{Re}[(E_1+E_2)(\zeta_1^* E_1^* + \zeta_2^* E_2^*)]. \end{aligned} \tag{4.12c}$$

On the other hand, the mechanical Poynting vector $\vec{S}_M$ is discontinuous at $z=0$, since its value is nonzero at $z=0$. In order to see why this is true, we rewrite the condition (2.16) in terms of $\xi(z)$. This yields the relation, for $z=0$:

$$\left(i\Gamma\xi(z) + \frac{d\xi(z)}{dz}\right)_{z=0} = 0. \tag{4.13}$$

We write the time average of $[d\xi(z)/dt]\,[d\xi(z)/dz]$ at the plane $z=0$ as

$$\begin{aligned} \left\langle \frac{d\xi(z)}{dt}\,\frac{d\xi(z)}{dz}\right\rangle_{z=0} &= \tfrac{1}{2}\,\mathrm{Re}\left(-i\omega\xi(z)\,\frac{d\xi^*(z)}{dz}\right)_{z=0} \\ &= \frac{i\omega}{4}\left[\xi(z)\left(\frac{d\xi^*(z)}{dz} - i\Gamma^*\xi^*(z)\right) - \xi^*(z)\left(\frac{d\xi(z)}{dz} + i\Gamma\xi(z)\right) + i\Gamma^*|\xi(z)|^2 + i\Gamma|\xi(z)|^2\right]_{z=0} . \end{aligned} \tag{4.14a}$$

We see that since the first two terms of Eq. (4.14a) satisfy the condition (4.13), we may write

$$\left\langle \frac{d\xi(z)}{dt}\,\frac{d\xi(z)}{dz}\right\rangle_{z=0} = \frac{-\omega}{2}\,\mathrm{Re}(\Gamma)|\xi(0)|^2, \tag{4.14b}$$

so that the value of the mechanical Poynting vector at the surface becomes

$$\langle \vec{S}_M\rangle|_{z=0} = \hat{z}(\tfrac{1}{2}\omega)(D/v_a)\,\mathrm{Re}(\Gamma)|\xi(0)|^2, \tag{4.15}$$

which is nonzero whenever $\mathrm{Re}(\Gamma)$ is nonzero, since $\xi(0)$ is nonzero for this model. This is because, if $\xi(0)=0$, by Eq. (4.13), $[d\xi(z)/dz]_{z=0}=0$, which violates Eq. (2.19), since E_1 and E_2 are not both zero. In much of the existing literature on spatial dispersion, the additional boundary condition, Eq. (4.13) is expressed in terms of the polarization $\vec{P}_M(z)$ associated with the dipole-active excitation in the medium, or the "mechanical" polarization, where

$$\vec{P}_M(z) = (e_T^*/\sqrt{\mu})\vec{\xi}(z). \tag{4.16a}$$

Therefore, for comparison with other work on spatial dispersion, we rewrite Eq. (4.13) as

$$\left(i\Gamma\vec{P}_M(z) + \frac{d\vec{P}_M(z)}{dz}\right)_{z=0} = 0, \tag{4.16b}$$

where for this case of normal incidence, $\vec{P}_M(z)$ lies along the x axis.

The equality (4.11) may be easily verified by using Eqs. (4.12) if one notes the following identities, which are obtained from Eq. (2.12), and where we let $\zeta_j = n_j + i\kappa_j$:

$$\left[-(2n_j\kappa_j)\left(\frac{c}{8\pi}\right)\left(\frac{c}{\omega}\right) - \frac{\omega}{2D}\,\frac{\epsilon_\infty}{4\pi}\,\Omega_p^2\,\frac{2n_j\kappa_j}{|\zeta_j^2-\Gamma^2|^2} + \frac{\gamma\omega^2}{2D^2}\,\frac{\epsilon_\infty}{4\pi}\,\Omega_p^2\,\frac{1}{|\zeta_j^2-\Gamma^2|^2}\right] = 0, \tag{4.17a}$$

$$\left(\frac{i}{2}\right)\left(\frac{c}{\omega}\right)\left(\frac{c}{8\pi}\right)(\zeta_1^2 - \zeta_2^{*2}) + \left(\frac{i}{2}\right)\left(\frac{\omega}{2D}\right)\frac{\epsilon_\infty}{4\pi}\,\Omega_p^2\,\frac{\zeta_1^2-\zeta_2^{*2}}{(\zeta_1^2-\Gamma^2)(\zeta_2^{*2}-\Gamma^{*2})} + \frac{\gamma\omega^2}{2D^2}\,\frac{\epsilon_\infty}{4\pi}\,\Omega_p^2\,\frac{1}{(\zeta_1^2-\Gamma^2)(\zeta_2^{*2}-\Gamma^{*2})} = 0. \tag{4.17b}$$

That is, the divergences of the electrical and mechanical Poynting vectors, or the left-hand side of Eq. (4.11), combine to give the term proportional to γ and the δ-function term on the right-hand side. The term proportional to γ, which is negative, gives the amount of radiation absorbed by the medium per unit time. The δ-function term indicates that the surface of the crystal serves as a source or sink of energy. If the coefficient of the δ function is negative (the same sign as the absorption term), then the surface is a sink of energy, or the surface absorbs energy. If the coefficient is positive, then the surface is a source of energy. In the present case, in the presence of damping, this term is always positive, and the surface acts as a source of energy. In the absence of damping, this quantity vanishes for a range of frequency, with the result that for these frequencies the surface acts neither as a source nor sink of energy, but it is nonzero and positive for all other frequencies, where the surface acts as a source of energy.

In order to understand more clearly the consequences of the delta function term, it is useful to consider the flux of energy through planes parallel to the surface of the crystal, both in the vacuum and the crystal, in the absence of damping (i.e., for $\gamma = 0$). The flux of electromagnetic radiation through any plane in the vacuum parallel to the crystal surface is the same constant value given by

$$\langle \vec{\mathcal{S}}_E \rangle_{z \le 0} = \hat{z}(c/8\pi)(1 - |R|^2) = \langle \vec{\mathcal{S}}_E \rangle_{z=0}, \tag{4.18a}$$

as can be seen from Eqs. (4.12a) and (4.12c). The total flux through a plane in the crystal at $z = l$, however, is given by the sum of the contributions of the electrical and mechanical Poynting vectors, Eqs. (4.12a) and (4.12b). In the absence of damping, this quantity simplifies greatly. This is because, in the absence of damping, a given root ζ_j of Eq. (2.12) is either purely real or purely imaginary, so that either κ_j or n_j vanishes, respectively. Therefore, Eq. (4.17a) is identically satisfied and, since $\zeta_1^2 \ne \zeta_2^2$, Eq. (4.17b) becomes

$$\frac{c^2}{8\pi\omega} + \left(\frac{\omega}{2D}\right)\left(\frac{\epsilon_\infty \Omega_p^2}{4\pi}\right)\frac{1}{(\zeta_1^2 - \Gamma^2)(\zeta_2^{*2} - \Gamma^{*2})} = 0. \tag{4.18b}$$

This relation requires that all the terms in the sum of the two Poynting vectors that are proportional to $E_1 E_2^*$ and $E_1^* E_2$ must cancel. To see this, we consider the electromagnetic and mechanical Poynting vectors separately. We add and subtract the values of these quantities at the surface and make use of Eq. (4.18b) in order to rewrite Eqs. (4.12). The separate electromagnetic and mechanical energy fluxes through a plane at $z = l$ thus become

$$\begin{aligned}\langle \vec{\mathcal{S}}_E \rangle_{z=l} = \langle \vec{\mathcal{S}}_E \rangle_{z=0} &+ \hat{z}(c^2/8\pi\omega)[n_1|E_1|^2(e^{-2\kappa_1 l} - 1) \\ &+ n_2|E_2|^2(e^{-2\kappa_2 l} - 1)] + \vec{\mathcal{S}}_{12}(l),\end{aligned} \tag{4.19a}$$

$$\begin{aligned}\langle \vec{\mathcal{S}}_M \rangle_{z=l} = \langle \vec{\mathcal{S}}_M \rangle_{z=0} &+ \hat{z}\left(\frac{\omega}{2D}\right)\left(\frac{\epsilon_\infty \Omega_p^2}{4\pi}\right)\left(\frac{n_1|E_1|^2(e^{-2\kappa_1 l} - 1)}{|\zeta_1^2 - \Gamma^2|^2}\right. \\ &\left. + \frac{n_2|E_2|^2 e^{-2\kappa_2 l}}{|\zeta_2^2 - \Gamma^2|^2}\right) - \vec{\mathcal{S}}_{12}(l),\end{aligned} \tag{4.19b}$$

where

$$\vec{\mathcal{S}}_{12}(l) = \hat{z}(c^2/8\pi\omega)\mathrm{Re}[(\zeta_1 + \zeta_2^*)E_1 E_2^*(e^{i(\zeta_1 - \zeta_2^*)l} - 1)]. \tag{4.19c}$$

Since $\zeta_j = n_j + i\kappa_j$ is either purely real or purely imaginary (i.e., either n_j or $\kappa_j = 0$) in the absence of damping, the terms in these expressions that are proportional to $n_1(e^{-2\kappa_1 l} - 1)$ or to $n_2(e^{-2\kappa_2 l} - 1)$ vanish identically, and we are left with the expressions

$$\langle \vec{\mathcal{S}}_E \rangle_{z=l} = \langle \vec{\mathcal{S}}_E \rangle_{z=0} + \vec{\mathcal{S}}_{12}(l), \tag{4.20a}$$

$$\langle \vec{\mathcal{S}}_M \rangle_{z=l} = \langle \vec{\mathcal{S}}_M \rangle_{z=0} - \vec{\mathcal{S}}_{12}(l), \tag{4.20b}$$

where $\vec{\mathcal{S}}_{12}(l)$ is given by Eq. (4.19c). Therefore, although separately the electromagnetic and mechanical Poynting vectors depend on l, the z coordinate of the plane through which the flux is considered, the total flux, the sum of Eqs. (4.20a) and (4.20b), is independent of the position of the plane and is the same as the sum evaluated at $z = 0$. That is,

$$\langle \vec{\mathcal{S}}_E \rangle_{z=l} + \langle \vec{\mathcal{S}}_M \rangle_{z=l} = \langle \vec{\mathcal{S}}_E \rangle_{z=0} + \langle \vec{\mathcal{S}}_M \rangle_{z=0}. \tag{4.21}$$

Thus, we see that the flux in the crystal is larger than that in the vacuum by exactly the value of the mechanical Poynting vector evaluated at the surface, whose magnitude is identical to the value of the coefficient of the delta function term in the expression for Poynting's theorem equation (4.11). In the absence of damping for $D > 0$, this quantity vanishes for $\omega < \omega_T$, but is positive for $\omega > \omega_T$ [see Eqs. (4.15) and (2.4b)]. For $D < 0$, these inequalities are reversed. However, in the presence of damping, the case of greater interest, this quantity is positive for all ω, regardless of the sign of D.

B. Poynting's theorem for a more-general model

The derivation of Poynting's theorem for the more-general model that was discussed in Sec. III proceeds in the same way as the analysis of Sec. IV A, except that in this case the equations of motion contain additional terms proportional to $\delta(z)$. The definition of a mechanical Poynting vector for this case is identical to that given by Eq. (4.7). However, the mechanical energy for this system is defined by

$$U_M = \frac{1}{2v_a}\left[\left(\frac{d\vec{\xi}}{dt}\right)^2 + \omega_T^2 \vec{\xi}^2 + D(\nabla \vec{\xi})^2 + a\omega_T^2 \vec{\xi}^2 \delta(z)\right]. \tag{4.22}$$

The energy conservation condition, the analog to Eq. (4.10), thus becomes

$$\nabla \cdot (\vec{\mathcal{S}}_E + \vec{\mathcal{S}}_M) + \frac{d}{dt}(U_E + U_M) = -\frac{\gamma}{v_a}\left(\frac{d\vec{\xi}}{dt}\right)^2, \tag{4.23a}$$

or, after taking the time average of both sides, we have

$$\nabla\cdot(\langle\vec{\mathrm{S}}_E\rangle+\langle\vec{\mathrm{S}}_M\rangle)=-\frac{\gamma}{v_a}\left\langle\left(\frac{d\vec{\xi}}{dt}\right)^2\right\rangle. \tag{4.23b}$$

The forms of the electromagnetic and mechanical Poynting vectors for this model are given by Eqs. (4.12), where E_1, E_2, and R are given by Eqs. (3.13). Here, as for the model described in Sec. IV A, the electromagnetic Poynting vector is continuous across the boundary at $z=0$. However, unlike that model, the mechanical Poynting vector here is continuous across the surface at $z=0$, that is, it vanishes on the surface of the crystal. In order to demonstrate this, we consider the condition given by Eq. (3.7) in order to rewrite the time average of $[d\xi(z)/dt][d\xi(z)/dz]$ at $z=0$:

$$\left\langle\frac{d\xi(z)}{dt}\,\frac{d\xi(z)}{dz}\right\rangle_{z=0}=\tfrac{1}{2}\,\mathrm{Re}\left(-i\omega\xi(z)\frac{d\xi^*(z)}{dz}\right)_{z=0}$$

$$=\frac{i\omega}{4}\left[\xi(z)\left(\frac{d\xi^*(z)}{dz}-\frac{a\omega_T^2}{D}\xi^*(z)\right)-\xi^*(z)\left(\frac{d\xi(z)}{dz}-\frac{a\omega_T^2}{D}\xi(z)\right)\right]_{z=0}. \tag{4.24a}$$

Since the condition (3.7) requires this quantity to vanish, we have

$$\langle\vec{\mathrm{S}}_M\rangle_{z=0}=0. \tag{4.24b}$$

The equality in Eq. (4.23b) may be verified, as in Sec. IV A, through the use of the equalities given by Eqs. (4.17). Also, the flux through planes parallel to the crystal surface in the crystal and the vacuum may be calculated as in Sec. IV A, with the same general results obtained, that is, those of Eqs. (4.18a), (4.20), and (4.21). However, the important difference here is that the mechanical Poynting vector vanishes on the surface, so the total flux in the crystal is the same as that in the vacuum, and the surface is neither a source nor sink of energy. We note that although the mechanical Poynting vector vanishes on the surface in this case, its value inside the crystal is nonzero, as can be seen from Eq. (4.20b). Here, as in Sec. IV A, for comparison with the existing literature on spatial dispersion, we rewrite the additional boundary condition (3.7) in terms of the "mechanical" polarization as

$$\left(a\omega_T^2\vec{\mathrm{P}}(z)-D\frac{\partial\vec{\mathrm{P}}}{\partial z}\right)_{z=0}=0. \tag{4.25}$$

V. CONCLUSIONS

In the preceding sections, we have discussed energy flow at normal incidence on the bases of two simple models for a semi-infinite isotropic spatially dispersive dielectric in the presence of damping. One of these, namely, the dielectric approximation model, has been widely used recently in the study of the optical properties of such crystals. As we have seen, this model, in which the effects of the surface are not properly taken into account, leads to a situation in which the surface acts as a source of energy. Clearly, care must be exercised in employing a model with such properties for the investigation of the optical properties of spatially dispersive bounded media.

The condition that we have obtained for normal incidence reflectivity in order that the surface not be a source or sink of energy, namely, that the mechanical Poynting vector vanish on the surface, is actually a much more general result than one might think on the basis of the two specific models considered here. For normal incidence the Maxwell boundary conditions of conservation of the tangential components of $\vec{\mathrm{E}}$ and $\vec{\mathrm{H}}$ across the surface of the crystal demand that the electromagnetic Poynting vector $\vec{\mathrm{S}}_E$ be continuous across the surface. Therefore, in order that the divergence of the total flux not contain a δ-function term describing an emission or absorption of energy by the surface, the total flux $\vec{\mathrm{S}}_E+\vec{\mathrm{S}}_M$ must be continuous across the surface. This can only happen if the mechanical Poynting vector $\vec{\mathrm{S}}_M$ vanishes on the surface, since it vanishes identically in the vacuum.

In view of these findings, it is desirable to know under what conditions a given microscopic model of a bounded spatially dispersive medium will not have a source or sink of energy at the surface. This question can readily be answered when the additional boundary condition expressed in terms of $\vec{\xi}$, may be expressed generally as

$$\left(\alpha\vec{\xi}+\beta\frac{d\vec{\xi}}{dz}\right)_{z=0}=0, \tag{5.1}$$

where α and β are both complex. For the models we have considered here, Eqs. (4.13) and (3.7) are the analogous conditions. As in Secs. IV A and IV B, we may express this Eq. (5.1) in terms of the "mechanical" polarization in the medium for comparison with existing theories on spatial dispersion. Thus, condition (5.1) becomes, in analogy to Eqs. (4.16) and (4.25),

$$\left(\alpha\vec{\mathrm{P}}+\beta\frac{d\vec{\mathrm{P}}}{dz}\right)_{z=0}=0. \tag{5.2}$$

In the following, we will work with Eq. (5.1) rather than (5.2), but the conclusions that we make concerning the coefficients α and β apply, obviously, to both equations. Since for normal incidence the mechanical Poynting vector at the surface of the medium is directly proportional to the quantity

$$\left\langle \frac{d\xi}{dt}\frac{d\xi}{dz}\right\rangle_{z=0},$$

it is this expression that we study.

Obviously, if either $\xi(0)$ or $[d\xi(z)/dz]_{z=0}$ vanish, then this quantity is zero, and so is the mechanical Poynting vector on the surface. In fact, the boundary condition $\xi(0)=0$ was the one introduced by Pekar,[6] so that for this boundary condition the surface is neither a source nor sink of energy.

If, alternatively, we consider the case in which α and β, $\xi(0)$ and $[d\xi(z)/dz]_{z=0}$ are nonzero, we have

$$\left\langle \frac{d\xi}{dt}\frac{d\xi}{dz}\right\rangle_{z=0} = -\frac{i\omega}{2}\left(\xi\frac{d\xi^*}{dz} - \xi^*\frac{d\xi}{dz}\right)_{z=0}$$

$$= -\frac{i\omega}{2}\left[\frac{\xi}{\beta^*}\left(\beta^*\frac{d\xi^*}{dz} + \alpha^*\xi^*\right) - \frac{\xi^*}{\beta}\left(\beta\frac{d\xi}{dz} + \alpha\xi\right)\right.$$

$$\left. - \frac{\alpha^*}{\beta^*}|\xi|^2 + \frac{\alpha}{\beta}|\xi|^2\right]_{z=0}. \qquad (5.3)$$

Since the first two terms in this equation vanish by the condition (5.1), the mechanical Poynting vector at $z=0$ becomes

$$\langle \vec{S}_E\rangle_{z=0} = -\frac{D}{v_a}\left\langle \frac{d\xi}{dt}\frac{d\xi}{dz}\right\rangle_{z=0}$$

$$= \frac{i\omega}{2}\left(\frac{D}{v_a}\right)\mathrm{Im}\left(\frac{\alpha}{\beta}\right)|\xi(0)|^2, \qquad (5.4)$$

so that for $\xi(0)\neq 0$, this expression vanishes only if the imaginary part of α/β vanishes. Thus, if α and β in Eq. (5.1) or (5.2) are complex, the surface is a source or sink of energy. It is a source if $iD\,\mathrm{Im}(\alpha/\beta)$ is positive and a sink if this quantity is negative. If α and β are real, then the surface is neither a source nor sink of energy. For the dielectric approximation model, $\alpha = i\Gamma$ and $\beta = 1$, according to Eq. (4.13), so that the mechanical Poynting vector does not vanish at $z=0$, as was shown in Sec. IV. However, for the more-general model considered in Secs. III and IV B, $\alpha = a\omega_T^2$ and $\beta = -D$, so that α and β are both real and the mechanical Poynting vector vanishes at $z=0$, as was also shown in Sec. IV.

The property of the dielectric approximation model exposed here, viz., that it gives rise to a source of energy at the vacuum-medium interface, should be kept in mind in all subsequent applications of this model to the study of optical properties of bounded media.

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