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Electrodynamics of elastic pyroelectrics

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We formulate an *ab initio* long-wavelength Lagrangian theory of electrodynamics of elastic pyroelectrics. A consistent set of constitutive relations and equations of motion of both the matter and electromagnetic field are derived. The theory applies to pyroelectrics, dielectrics, and piezoelectrics of any symmetry, any degree of anisotropy, any level of structural complexity, and any order of nonlinearity. All long-wavelength modes of mechanical motion of the crystal, which include the center-of-mass motion and an arbitrary number of internal motions, are considered. Discussions of the equations of motion, the conservation laws, the stress tensor, the boundary conditions, and the meaning of the natural state of the crystal are presented. In particular, we show that total angular momentum is conserved even though the properly defined total stress tensor is not symmetric.

I. INTRODUCTION

Recently we developed an *ab initio* Lagrangian theory of electrodynamics in elastic dielectrics.[1] The theory applies to crystals having any symmetry and degree of anisotropy, having any number of particles (ions and electrons) per unit cell, and having nonlinearities of any order in their constitutive relations. The theory, which applies to wavelengths long compared to unit-cell dimensions, is well suited to the study of interactions of electromagnetic and acoustic waves in crystals.

Application of the theory to the photoelastic interaction[2] led to the prediction that the independent elastic variable relevant to this interaction was the displacement gradient (the sum of the strain plus rotation), not the strain as long believed. This prediction was amply verified.[3] Application of the general theory to acoustically induced optical harmonic generation[4] demonstrated the usefulness of the theory in predicting indirect contributions to the over-all effect. Three two-step and two three-step indirect contributions, each wave-vector dependent, were found in addition to the direct interaction of the several waves.

In this and an accompanying paper[5] we turn our attention to materials possessing a spontaneous electric dipole moment. If the direction of the moment cannot be reoriented, they are called simply pyroelectrics; the subclass of pyroelectrics whose moment can be reoriented are called ferroelectrics. This work applies to either type. In addition to the spontaneous electric moment a spontaneous electric field may also be present. However, under typical laboratory conditions an extrinsic charge collects on the crystal surfaces so as to cancel the spontaneous electric field. Weak conductivity can also contribute to this cancelling process. Nevertheless, we will include the possible existence of the spontaneous field in our treatment.

Our interest is directed at determining whether the spontaneous electric moment or field will lead to indirect contributions to either linear elasticity or piezoelectricity. We further wish to find out whether rotations, in contrast to strains, will play a role in any such indirect effects. Toward this end we find it advantageous to set up the theory in a general way that includes all levels of nonlinearity. We will then specialize to linear elasticity and piezoelectricity in an accompanying paper.[5] In further papers we intend to apply the results of this paper to various nonlinear acoustic-wave–electromagnetic-wave interactions in pyroelectrics.

The treatment in this paper is based on our previous paper[1] on dielectrics and most of the justification of the approach will not be repeated here. Nevertheless, we will attempt to make the present treatment as self-contained as feasible.

Briefly, the organization of the paper is as follows: From the microscopic discrete position coordinates of the particles, continuum coordinates consisting of the center-of-mass position and a set of internal coordinates are defined (Sec. II). The total Lagrangian is then constructed in terms of these coordinates and the vector and scalar potentials which characterize the electromagnetic field (Sec. III). The total Lagrangian consists of the vacuum electromagnetic field Lagrangian, the matter-field interaction Lagrangian, the kinetic energy, and the stored energy of the matter. The latter is required to satisfy invariance under displacements, rotations, inversions, and crystal group operations. The Lagrange equations then yield the Maxwell-Lorentz electromagnetic equations (Sec. IV), the center-of-mass motion equation (Sec. V), and the internal coordinate motion equations (Sec. VI). Momentum, angular momentum, and energy conservation are presented briefly in Secs. VII–IX, respectively. The form that the sources of energy, momentum, and angular momentum take in the presence of external fields are presented in Sec. X. Boundary conditions on all the fields are given in Sec. XI.

II. CRYSTAL COORDINATES

The position of a particle (ion or electron) of type α, having a charge e^α, is $\vec{x}^{n\alpha}(t)$. The index n has three integral components that name the primitive cell n (the smallest unit of structural repetition). The particle type index α has values from 1 to N. For long-wavelength phenomena (wavelengths large compared to primitive-unit-cell dimensions) each discrete particle sublattice can be replaced by a continuum, giving a manifold of N continua to represent the crystal. In so doing the particle type index α is retained as a sublattice index but the cell index n is replaced by a continuous variable $\vec{X}$ which rides with the mass point, names it, and is called the material coordinate (vector). Thus

$$\vec{x}^{n\alpha}(t) \to \vec{x}^{\alpha}(\vec{X}, t) \ . \tag{2.1}$$

In the continuum limit cell sums become integrals over the body with respect to the material coordinate, i.e.,

$$\sum_n F(\vec{x}^{n\alpha}(t)) \to \frac{1}{\Omega} \int F(\vec{x}^{\alpha}(\vec{X}, t))\, d\vec{X} \ , \tag{2.2}$$

where Ω is the primitive-unit-cell volume. In terms of the continuum position coordinates $\vec{x}^\alpha$ the center-of-mass position is

$$\vec{x}(\vec{X}, t) \equiv \sum_{\alpha=1}^{N} \frac{\rho^\alpha \vec{x}^\alpha(\vec{X}, t)}{\rho^0} \ , \tag{2.3}$$

$$\rho^0 \equiv \sum_{\alpha=1}^{N} \rho^\alpha \equiv \sum_{\alpha=1}^{N} \frac{m^\alpha}{\Omega} \ . \tag{2.4}$$

Throughout this paper we will retain the distinction between the material coordinate $\vec{X}$ of the center of mass and the spatial coordinate $\vec{x}$ of the center of mass. To facilitate this distinction we will use upper case Latin letter subscripts to denote components in the material coordinate system, e.g., X_A, and lower case Latin letter subscripts to denote components in the spatial (laboratory) coordinate system, e.g., x_i. This notation serves to remind us that under a body rotation, the coordinates x_i change but the "names" X_A of the particles do not. Though we choose each of these coordinate systems to be Cartesian, we regard their transformations as independent. When this theory is applied to the calculation of a specific problem, it is then convenient to make these two coordinate systems identical and to make the material coordinate components X_A of the center of mass equal to the latter's spatial position components x_a when the body is in its natural state, that is, a homogeneous, time-independent state free from applied external influences. We also define the natural state as having no spontaneous strain or total stress. With this definition of $\vec{X}$ the ordinary displacement vector $\vec{u}$ used in the acoustic propagation equation, for instance, is defined by

$$\vec{u} \equiv \vec{x} - \vec{X} \ . \tag{2.5}$$

In place of the $\vec{x}^\alpha$ coordinates we find it more convenient to use a complete set of position coordinates which consist of the center-of-mass position $\vec{x}(\vec{X}, t)$ and internal coordinates $\vec{y}^{T\mu}(\vec{X}, t)$ ($\mu = 1, 2, \ldots, N-1$) which are displacement invariant. We define them by

$$\vec{y}^{T\mu}(\vec{X}, t) \equiv \sum_{\alpha=1}^{N} U^{\mu\alpha} \vec{x}^\alpha(\vec{X}, t) \tag{2.6}$$

$$\vec{x}^\alpha(\vec{X}, t) = \sum_{\mu=0}^{N-1} V^{\alpha\mu} \vec{y}^{T\mu}(\vec{X}, t) \ , \tag{2.7}$$

where

$$\sum_{\alpha=1}^{N} U^{\mu\alpha} V^{\alpha\nu} = \delta^{\mu\nu} \ , \tag{2.8}$$

$$\sum_{\mu=0}^{N-1} V^{\alpha\mu} U^{\mu\beta} = \delta^{\alpha\beta} \ , \tag{2.9}$$

$$\vec{y}^{T0}(\vec{X}, t) \equiv \vec{x}(\vec{X}, t) \ . \tag{2.10}$$

Displacement invariance of $\vec{y}^{T\mu}$ ($\mu \neq 0$) and its lack for $\mu = 0$ require

$$\sum_{\alpha=1}^{N} U^{\mu\alpha} = \delta^{\mu 0} \ . \tag{2.11}$$

Summing Eq. (2.9) over β with the use of Eq. (2.11) yields an alternate statement of displacement invariance,

$$V^{\alpha 0} = 1 \ . \tag{2.12}$$

Equations (2.3), (2.6), and (2.10) together imply

$$U^{0\alpha} = \rho^\alpha / \rho^0 \ . \tag{2.13}$$

Substitution of Eq. (2.13) into Eq. (2.8) yields

$$\sum_{\alpha=1}^{N} \frac{\rho^\alpha V^{\alpha\nu}}{\rho^0} = \delta^{0\nu} \ . \tag{2.14}$$

The superscript T on $\vec{y}^{T\mu}$, standing for total, is used to indicate that these internal coordinates possess a constant or spontaneous part $\vec{Y}^\mu$ in addition to a part $\vec{y}^\mu$ which may vary because of some external influence, i.e.,

$$y_i^{T\mu} = \delta_{iA} Y_A^\mu + y_i^\mu \ . \tag{2.15}$$

The special case $\mu = 0$ reduces to Eq. (2.5)

$$x_i = \delta_{iA} X_A + u_i \tag{2.16}$$

when we use Eq. (2.10) and identify

$$\vec{Y}^0 = \vec{X}, \quad \vec{y}^0 = \vec{u} \ . \tag{2.17}$$

The presence of the spontaneous parts $\vec{Y}^\mu$ is necessary to obtain a spontaneous electric dipole moment.

Besides satisfying displacement invariance the internal coordinates can be chosen to retain the diagonality of the kinetic energy. Thus

$$\mathfrak{L}_K = \frac{1}{2} \sum_{\alpha=1}^{N} \rho^\alpha \left(\frac{d\vec{x}^\alpha}{dt}\right)^2 = \frac{1}{2} \sum_{\mu=0}^{N-1} m^\mu \left(\frac{d\vec{y}^{T\mu}}{dt}\right)^2 \tag{2.18}$$

provided

$$\sum_{\alpha=1}^{N} \rho^\alpha V^{\alpha\mu} V^{\alpha\nu} = m^\mu \delta^{\mu\nu}, \quad m^0 \equiv \rho^0 \ . \tag{2.19}$$

If we multiply Eq. (2.19) by $U^{\nu\beta}$, sum over ν, and use Eq. (2.9), we obtain the useful relation

$$\rho^\beta V^{\beta\mu} = m^\mu U^{\mu\beta} \ . \tag{2.20}$$

The newly introduced m^μ can be found from Eq. (2.19) by setting $\mu = \nu$.

III. TOTAL LAGRANGIAN

The total Lagrangian can be expressed in terms of a Lagrangian density in the spatial coordinate system or one in the material coordinate system:

$$L = \int \mathfrak{L}^S \, dv = \int \mathfrak{L}^M \, dV \ . \tag{3.1}$$

Here dv and dV are volume elements in the spatial and material frames. The total Lagrangian consists of the sum of three Lagrangians describing the field, the field-matter interaction, and the matter:

$$\mathfrak{L}^j = \mathfrak{L}_F^j + \mathfrak{L}_I^j + \mathfrak{L}_M^j \quad (j = S, M) \ . \tag{3.2}$$

The well-known field Lagrangian is expressed in terms of the vector potential $\vec{A}$ and the scalar potential Φ, regarded as generalized coordinates, by

$$\mathfrak{L}_F^S = \tfrac{1}{2}\epsilon_0 \{[\vec{E}(\vec{z}, t)]^2 - c^2 [\vec{B}(\vec{z}, t)]^2\} , \tag{3.3}$$

where c is the speed of light in vacuum and ϵ_0 is the permittivity of free space (mks units are used). The electric field $\vec{E}$, which may contain a constant spontaneous part $\vec{E}^S$, and the magnetic induction $\vec{B}$ are expressed as usual in terms of the potentials by

$$\vec{E} = -\vec{\nabla}\Phi - \frac{\partial \vec{A}}{\partial t} , \tag{3.4}$$

$$\vec{B} = \vec{\nabla} \times \vec{A} \ . \tag{3.5}$$

The interaction Lagrangian is given by

$$\mathfrak{L}_I^M = \sum_\alpha q^\alpha \left(\frac{d\vec{x}^\alpha}{dt}(\vec{X}, t) \cdot \vec{A}(\vec{x}^\alpha(\vec{X}, t), t) - \Phi(\vec{x}^\alpha(\vec{X}, t), t) \right) \tag{3.6}$$

or

$$\mathfrak{L}_I^S = \vec{j}(\vec{z}, t) \cdot \vec{A}(\vec{z}, t) - q(\vec{z}, t)\Phi(\vec{z}, t) , \tag{3.7}$$

where

$$q(\vec{z}, t) \equiv \sum_\alpha q^\alpha \int \delta(\vec{z} - \vec{x}^\alpha(\vec{X}, t)) \, dV , \tag{3.8}$$

$$\vec{j}(\vec{z}, t) \equiv \sum_\alpha q^\alpha \int \frac{d\vec{x}^\alpha}{dt}(\vec{X}, t) \delta(\vec{z} - \vec{x}^\alpha(\vec{X}, t)) \, dV , \tag{3.9}$$

$$q^\alpha \equiv e^\alpha / \Omega \ . \tag{3.10}$$

In either of the forms (3.6) and (3.7) the interaction Lagrangian contains multipoles of all orders. Since we wish to consider a dielectric material which contains no free charge, i.e., no monopole,

$$\sum_\alpha q^\alpha = 0 , \tag{3.11}$$

and since we do not wish to consider magnetic dipole or electric quadrupole effects[1] at present, we expand the functions of $\vec{x}^\alpha$ about $\vec{x}$ using Eq. (2.7). We obtain the interaction Lagrangian to electric dipole order by using Eq. (3.11) and by remembering that a total time (or space) derivative can be discarded from the Lagrangian since it cannot affect the equations of motion. In the material frame we find

$$\mathfrak{L}_I^M = \sum_\mu{}' q^\mu \vec{y}^{T\mu}(\vec{X}, t) \cdot \vec{\mathcal{E}}(\vec{x}(\vec{X}, t), t) , \tag{3.12}$$

while in the spatial frame we find

$$\mathfrak{L}_I^S = \vec{\mathcal{E}}(\vec{z}, t) \cdot \sum_\mu{}' q^\mu \left(\frac{\vec{y}^{T\mu}(\vec{X}, t)}{J(\vec{X}, t)} \right)_{\vec{z} = \vec{x}(\vec{X}, t)} , \tag{3.13}$$

where

$$\vec{\mathcal{E}} \equiv \vec{E} + \frac{d\vec{x}}{dt} \times \vec{B} \ . \tag{3.14}$$

In these equations the prime on the summation symbol indicates exclusion of the $\mu = 0$ term and q^μ is given by

$$q^\mu \equiv \sum_\alpha q^\alpha V^{\alpha\mu} \ . \tag{3.15}$$

Neutrality of the unit cell, Eq. (3.11), implies $q^0 = 0$. Note that we use a Greek letter early in the alphabet to denote a charge density associated with the position $\vec{x}^\alpha$ and one late in the alphabet to denote a charge density associated with the internal coordinate $\vec{y}^{T\mu}$. The Jacobian of the transformation from the $\vec{X}$ frame to the $\vec{x}$ frame is

$$J(\vec{X}, t) \equiv \det \frac{\partial x_i}{\partial X_A} = \det x_{i,A} , \tag{3.16}$$

where the comma denotes differentiation in the last expression.

The matter Lagrangian consists of the kinetic energy, as expressed in Eq. (2.18) minus the stored energy,

$$\mathcal{L}_M^M = \tfrac{1}{2}\rho^0\left(\frac{d\vec{x}}{dt}\right)^2 + \sum_\mu{}' \tfrac{1}{2}m^\mu\left(\frac{d\vec{y}^{T\mu}}{dt}\right)^2 - \rho^0\Sigma , \qquad (3.17)$$

where Σ is the stored energy per unit undeformed mass of the crystal. The form that Σ may take consistent with the conservation laws has been discussed in detail previously.[1,6] We will only summarize those arguments here.

In general, Σ could be a function of all the coordinates, $\vec{x}$ and $\vec{y}^{T\mu}$ ($\mu = 1, 2, \ldots, N-1$), their first and higher derivatives with respect to $\vec{X}$, and $\vec{X}$ itself. Momentum conservation requires invariance of Σ with respect to uniform displacements in the spatial coordinate system. Since all $\vec{y}^{T\mu}$ ($\mu = 1, 2, \ldots, N-1$) and all orders of derivatives of the $\vec{y}^{T\mu}$ and $\vec{X}$ possess such invariance, Σ may be a function of them. The center-of-mass position $\vec{x}$, however, does not possess such invariance and so Σ may not be a function of it. In the true long-wavelength limit we need only retain $\vec{x}_{,A}$ and $\vec{y}^{T\mu}$ ($\mu = 1, 2, \ldots, N-1$). Wave-vector dispersion effects, such as optical or acoustic activity, which are lowest-order corrections to the long-wavelength limit, require the retention of dependence of Σ upon $\vec{x}_{,AB}$ and $\vec{y}^{T\mu}_{,A}$ ($\mu = 1, 2, \ldots, N-1$). Though the latter can be incorporated into the present formalism,[1] their physical effects can be distinguished readily from those, caused by the presence of a permanent electric dipole moment, which we are considering here. We thus exclude the latter dependence.

Angular momentum conservation requires invariance of Σ with respect to uniform rotations in the spatial coordinate system. Such invariance is quaranteed if each of the independent variables of Σ is individually rotationally invariant. A complete set of such variables consists of E_{AB}, $\Lambda_A^{T\mu}$ ($\mu = 1, 2, \ldots, N-1$), X_A, and $\mathrm{sgn}(J)$. The Green finite strain tensor E_{AB} is defined by

$$E_{AB} \equiv \tfrac{1}{2}(C_{AB} - \delta_{AB}) , \qquad (3.18)$$

$$C_{AB} \equiv x_{i,A}x_{i,B} . \qquad (3.19)$$

Summation over repeated subscripts is implied. The rotationally invariant internal coordinates $\Lambda_A^{T\mu}$ are defined by

$$\Lambda_A^{T\mu} \equiv y_i^{T\mu}R_{iA} \quad (\mu = 1, 2, \ldots, N-1) , \qquad (3.20)$$

where R_{iA} is the finite rotation tensor[1] given by

$$R_{iA} \equiv x_{i,B}(C^{-1/2})_{BA} . \qquad (3.21)$$

The $\mathrm{sgn}(J)$ variable has values of $+1$ and -1 for proper and improper rotations, respectively.

Parity conservation is not a fundamental conservation law and its possible violation in crystal physics has been discussed.[1] Nevertheless, indications are that it is obeyed to a very high degree of accuracy. Thus, for the purposes of this paper we will assume its validity. Parity conservation requires the invariance of Σ with respect to inversion (improper rotation) of the spatial coordinate system. Thus $\mathrm{sgn}(J)$ must be removed from the set of variables for Σ.

We will for simplicity consider homogeneous crystals. In the continuum limit, this requires invariance of Σ with respect to arbitrary translations of the material coordinate system. Thus X_A must be deleted from the set of variables of Σ. In the language of conservation laws homogeneity is equivalent to crystal momentum conservation.

From the above arguments the functional dependence of Σ may be stated as

$$\Sigma = \Sigma(E_{AB}, \Lambda_C^{T\mu}) . \qquad (3.22)$$

It is worth emphasizing that by the nature of a potential energy Σ may not be a function of any characteristic of an external influence such as a frequency or wave vector.

Since the quantities E_{AB} and $\Lambda_C^{T\mu}$ are small quantities, it is convenient to expand $\rho^0\Sigma$ in a double power series in these variables. The first few terms are

$$\rho^0\Sigma = {}^{(0,1)}H_{AB}E_{AB} + {}^{(0,2)}H_{ABCD}E_{AB}E_{CD} + \sum_\mu{}' {}^{(1,0)}H_A^\mu\Lambda_A^{T\mu} + \sum_{\mu\nu}{}' {}^{(2,0)}H_{AB}^{\mu\nu}\Lambda_A^{T\mu}\Lambda_B^{T\nu} + \sum_\mu{}' {}^{(1,1)}H_{ABC}^\mu\Lambda_A^{T\mu}E_{BC} + \cdots . \qquad (3.23)$$

Now, the stored energy must also be invariant under crystal group operations. Since the terms of the series of different degree are independent, the requirement applies individually to the terms. Since both E_{AB} and $\Lambda_C^{T\mu}$ are altered by crystal group operations, conditions are imposed on the series coefficients, ${}^{(m,n)}H$. Such relations have been stated before[1] and need not be repeated here.

The choice of $\Lambda_A^{T\mu}$ as expansion parameters for $\rho^0\Sigma$ has one drawback. In the natural state of the crystal, i.e., when no external influences are applied to the crystal and all space and time derivatives vanish, $E_{AB} = 0$ but $\Lambda_A^{T\mu}$ has a spontaneous value of

$$\Lambda_A^{S\mu} \equiv Y_A^\mu \quad (\mu = 1, 2, \ldots, N-1) . \qquad (3.24)$$

This leads to the spontaneous value of $\rho^0\Sigma$ and $\partial\rho^0\Sigma/\partial\Lambda_A^{T\mu}$ having an infinite series of terms. This can be avoided if we introduce a new quantity

$$\Lambda_A^\mu \equiv \Lambda_A^{T\mu} - \Lambda_A^{S\mu} \quad (\mu = 1, 2, \ldots, N-1) , \qquad (3.25)$$

which is the difference of two rotational invariants. Using Eq. (2.15) we obtain

$$\Lambda_A^\mu = (R_{iA} - \delta_{iA})\delta_{iB}Y_B^\mu + R_{iA}y_i^\mu , \qquad (3.26)$$

a result whose invariance is less obvious.

Equation (3.23) can now be reexpressed as

$$\rho^0\Sigma(E_{AB},\Lambda_c^\mu)={}^{(0,1)}K_{AB}E_{AB}+{}^{(0,2)}K_{ABCD}E_{AB}E_{CD}+\sum_\mu{}'\,{}^{(1,0)}K_A^\mu\Lambda_A^\mu+\sum_{\mu\nu}{}'\,{}^{(2,0)}K_{AB}^{\mu\nu}\Lambda_A^\mu\Lambda_B^\nu+\sum_\mu{}'\,{}^{(1,1)}K_{ABC}^\mu\Lambda_A^\mu E_{BC}+\cdots\,. \tag{3.27}$$

Expressions for the new expansion coefficients ${}^{(m,n)}K$ in terms of the old expansion coefficients ${}^{(m,n)}H$ can easily be found from Eqs. (3.23), (3.25), and (3.27) but, since they will not be needed, they will not be presented here. The stored energy is now expanded in rotationally invariant variables which vanish in the natural state. The constant term in $\rho^0\Sigma$ which cannot contribute to the equations of motion has been dropped.

The Lagrange equations can be written in either the spatial or material frames depending on which Lagrangian density in Eq. (3.1) is used. In the spatial frame the Lagrange equation for a generalized coordinate q_i is

$$\frac{\partial}{\partial t}\frac{\partial\mathcal{L}^S}{\partial(\partial q_i/\partial t)}=\frac{\partial\mathcal{L}^S}{\partial q_i}-\frac{\partial}{\partial z_j}\frac{\partial\mathcal{L}^S}{\partial q_{i,j}}\,, \tag{3.28}$$

where $\vec{z}$ is the independent variable. In the material frame the Lagrange equation for the generalized coordinate q_i is

$$\frac{d}{dt}\frac{\partial\mathcal{L}^M}{\partial\dot{q}_i}=\frac{\partial\mathcal{L}^M}{\partial q_i}-\frac{\partial}{\partial X_A}\frac{\partial\mathcal{L}^M}{\partial q_{i,A}}\,, \tag{3.29}$$

where $\vec{X}$ is the independent variable. Note that a material time derivative is given by

$$\frac{dF}{dt}\equiv\dot{F}\equiv\frac{\partial F}{\partial t}+\dot{x}_i\frac{\partial F}{\partial x_i}\,. \tag{3.30}$$

IV. MAXWELL-LORENTZ EQUATIONS

The Lagrange equation (3.28) for the scalar potential Φ, regarded as a generalized coordinate, yields

$$\epsilon_0\vec{\nabla}\cdot\vec{E}=-\vec{\nabla}\cdot\vec{P}\equiv q^D\,, \tag{4.1}$$

with the aid of Eqs. (3.2)–(3.5) and (3.13). The right-hand side of Eq. (4.1) is the dielectric or bound charge in the electric dipole approximation and the polarization $\vec{P}$ is defined by

$$\vec{P}(\vec{z},t)\equiv\sum_\mu{}'\,q^\mu\left(\frac{\vec{y}^{T\mu}(\vec{X},t)}{J(\vec{X},t)}\right)_{\vec{z}=\vec{x}(\vec{X},t)}\,. \tag{4.2}$$

Note that the polarization $\vec{P}$ can contain a constant part, the spontaneous polarization $\vec{P}^S$, given by

$$P_i^S\equiv\delta_{iA}\sum_\mu{}'\,q^\mu Y_A^\mu\,. \tag{4.3}$$

The Lagrange equation (3.28) for the vector potential $\vec{A}$, regarded as a generalized coordinate, yields

$$\frac{\vec{\nabla}\times\vec{B}}{\mu_0}-\frac{1}{\epsilon_0}\frac{\partial\vec{E}}{\partial t}=\frac{\partial\vec{P}}{\partial t}+\vec{\nabla}\times\left(\vec{P}\times\frac{d\vec{x}}{dt}\right)\equiv\vec{j}^D\,, \tag{4.4}$$

with the aid of Eqs. (3.2)–(3.5) and (3.13). The right-hand side of Eq. (4.4) is the dielectric or bound charge current in the electric dipole approximation.

We see from Eqs. (4.1) and (4.4) that to obtain the Maxwell equations in the conventional form we must define the electric displacement vector $\vec{D}$ and the magnetic field $\vec{H}$ by

$$\vec{D}\equiv\epsilon_0\vec{E}+\vec{P} \tag{4.5}$$

$$\vec{H}\equiv\frac{\vec{B}}{\mu_0}-\vec{P}\times\frac{d\vec{x}}{dt}\,, \tag{4.6}$$

which are functions, of course, of $\vec{z}$ and t.

The two remaining Maxwell equations,

$$\vec{\nabla}\times\vec{E}+\frac{\partial\vec{B}}{\partial t}=0 \tag{4.7}$$

$$\vec{\nabla}\cdot\vec{B}=0\,, \tag{4.8}$$

are direct consequences of the definitions, Eqs. (3.4) and (3.5), of the $\vec{E}$ and $\vec{B}$ fields in terms of $\vec{A}$ and Φ, the basic Lagrangian coordinates.

V. CENTER-OF-MASS EQUATION

The material frame Lagrange equation (3.29) for the center-of-mass position $\vec{x}$ yields

$$\rho^0\ddot{x}_i=\left(\vec{p}\times\frac{d\vec{B}}{dt}\right)_i+\left(\frac{d\vec{p}}{dt}\times\vec{B}\right)_i+\vec{p}\cdot\vec{E}_{,i}+\vec{p}\cdot\left(\frac{d\vec{x}}{dt}\times\vec{B}_{,i}\right)+T_{iA,A}\,, \tag{5.1}$$

with the aid of Eqs. (3.2), (3.12), (3.17), and (3.27). Here

$$\vec{p}\equiv\sum_\mu{}'\,q^\mu\vec{y}^{T\mu}\,, \tag{5.2}$$

and the Piola-Kirchoff mixed-frame stress tensor T_{iA} is defined by

$$T_{iA}\equiv\frac{\rho^0\partial\Sigma}{\partial x_{i,A}}\,. \tag{5.3}$$

With the use of vector identities and Eq. (4.7) the center-of-mass equation (5.1) can be reexpressed as

$$\rho^0\ddot{x}_i=T_{iA,A}+(\vec{p}\cdot\vec{\nabla})E_i+\left(\frac{d\vec{p}}{dt}\times\vec{B}\right)_i+\left(\frac{d\vec{x}}{dt}\times(\vec{p}\cdot\vec{\nabla})\vec{B}\right)_i\,. \tag{5.4}$$

This equation can be transformed to a spatial frame equation by multiplying by J^{-1}, defined in Eq. (3.16), and rearranging terms. With the use of the Euler-Piola-Jacobi identity,

$$(J^{-1}x_{j,A})_{,j}=0\ ,\tag{5.5}$$

it is easy to show that

$$J^{-1}T_{iA,A}=t^{y}_{ij,j}\ ,\tag{5.6}$$

where the local stress tensor t^{y}_{ij} is defined by

$$t^{y}_{ij}\equiv \rho x_{j,B}\frac{\partial \Sigma}{\partial x_{i,B}}\ ,\tag{5.7}$$

the y indicating that the $\vec{y}^{\nu}$ variables are held fixed while taking the derivative. The symbol

$$\rho \equiv J^{-1}\rho^{0}\tag{5.8}$$

is used as an abbreviation for the mass density associated with the single continuum defined by the center-of-mass motion $\vec{x}(\vec{X},t)$. We also use the identity[7]

$$J^{-1}\frac{d\vec{p}}{dt}=\frac{\partial \vec{P}}{\partial t}+\vec{\nabla}\times\left(\vec{P}\times\frac{d\vec{x}}{dt}\right)+\left(P_i\frac{d\vec{x}}{dt}\right)_{,i}\ .\tag{5.9}$$

Equation (5.4) can then be put in the spatial frame form

$$\rho\ddot{x}_i=(t^{y}_{ij}+\mathcal{E}_iP_j)_{,j}+q^{D}E_i+(\vec{j}^{D}\times\vec{B})_i\ .\tag{5.10}$$

Note, however, that we have left the inertial term expressed as a material time derivative. By substituting the dielectric charge and current from Eqs. (4.1) and (4.4) we have put the body force terms into the Lorentz force form.

VI. INTERNAL-MOTION EQUATIONS

The material frame Lagrange equation (3.29) for the internal coordinate $\vec{y}^{T\mu}$ ($\mu\neq 0$) yields

$$m^{\mu}\ddot{y}^{T\mu}_i=q^{\mu}\mathcal{E}_i-R_{iA}\frac{\partial \rho^{0}\Sigma}{\partial \Lambda^{\mu}_{A}}\ ,\tag{6.1}$$

with the use of Eqs. (3.2), (3.12), (3.14), (3.17), (3.20), (3.25), and (3.27). In the natural state (NS) of the pyroelectric crystal $\vec{E}=\vec{E}^{S}$ and $R_{iA}=\delta_{iA}$. Equation (6.1) then yields

$$q^{\mu}E^{S}_i=\left(\frac{\partial \rho^{0}\Sigma}{\partial \Lambda^{\mu}_{A}}\right)^{\rm NS}\delta_{iA}={}^{(1,0)}K^{\mu}_{A}\delta_{iA}\ .\tag{6.2}$$

We may subtract Eq. (6.2) from Eq. (6.1) in order to remove the constant terms from Eq. (6.1). Thus

$$m^{\mu}\ddot{y}^{\mu}_i=q^{\mu}\mathcal{E}^{V}_i-R_{iA}\frac{\partial \rho^{0}\Sigma}{\partial \Lambda^{\mu}_{A}}+\delta_{iA}\left(\frac{\partial \rho^{0}\Sigma}{\partial \Lambda^{\mu}_{A}}\right)^{\rm NS}\ ,\tag{6.3}$$

where

$$\vec{\mathcal{E}}^{V}\equiv \vec{E}^{V}+\frac{d\vec{x}}{dt}\times\vec{B}\ ,\tag{6.4}$$

$$\vec{E}^{V}\equiv\vec{E}-\vec{E}^{S}\ .\tag{6.5}$$

VII. MOMENTUM CONSERVATION

The momentum-conservation equation states that the sum of the partial time derivative of the total momentum density and the divergence of the flow of total momentum density is zero. The total momentum consists of both matter momentum and electromagnetic field momentum.

The change of momentum of the center of mass is given by Eq. (5.10). The left-hand side of this equation can be rearranged using a well-known identity[7] to be

$$\rho\ddot{x}_i=\frac{\partial(\rho\dot{x}_i)}{\partial t}+\frac{\partial(\rho\mathring{x}_i\dot{x}_j)}{\partial z_j}\ .\tag{7.1}$$

The body force terms of Eq. (5.10) can be regarded as momentum transfer terms between the matter and field. Corresponding terms of opposite sign should thus appear in the momentum equation of the electromagnetic field.

The latter can be found by forming the vector product of Eq. (4.7) with $\epsilon_0\vec{E}$ and the vector product of Eq. (4.4) with $\vec{B}$ and adding the results. After use of Eqs. (4.1) and (4.8) to reexpress the terms this yields

$$\frac{\partial(\epsilon_0\vec{E}\times\vec{B})_i}{\partial t}-m_{ij,j}=-q^{D}E_i-(\vec{j}^{D}\times\vec{B})_i\ ,\tag{7.2}$$

with the Maxwell stress tensor defined by

$$m_{ij}\equiv\epsilon_0E_iE_j+B_iB_j/\mu_0-\tfrac{1}{2}(\epsilon_0E_kE_k+B_kB_k/\mu_0)\delta_{ij}\ .\tag{7.3}$$

Since the internal coordinates $\vec{y}^{T\mu}$ are displacement invariant, they do not carry any momentum. It is thus sufficient to add Eqs. (5.9) and (7.2) with the use of Eq. (7.1). This yields the spatial frame statement of momentum conservation

$$\frac{\partial}{\partial t}\left[\rho\dot{x}_i+\epsilon_0(\vec{E}\times\vec{B})_i\right]+\frac{\partial}{\partial z_j}(\rho\mathring{x}_i\dot{x}_j-t^{y}_{ij}-\mathcal{E}_iP_j-m_{ij})=0\ .\tag{7.4}$$

We show in an accompanying paper[8] that the quantity included within the divergence in this equation may be properly identified as the total stress tensor t^{L}_{ij} in the laboratory or spatial frame,

$$t^{L}_{ij}\equiv t^{y}_{ij}+\mathcal{E}_iP_j+m_{ij}-\rho\dot{x}_i\dot{x}_j\ .\tag{7.5}$$

The sign change of this quantity from that within the divergence is chosen to give the stress tensor the conventional sign. We show in the accompanying paper[8] that t^{L}_{ij} is asymmetric. The meaning of the antisymmetric part will be interpreted in Sec. VIII.

It is usually assumed that the natural state (NS) of a perfect crystal is a stress-free state. If we adopt this viewpoint, we find

$$(t^{L}_{ij})^{\rm NS}=t^{S}_{ij}+E^{S}_{(i}P^{S}_{j)}+\epsilon_0E^{S}_iE^{S}_j-\tfrac{1}{2}\epsilon_0E^{S}_kE^{S}_K\delta_{ij}=0\ ,\tag{7.6}$$

where the spontaneous elastic stress t^{S}_{ij} is

$$t^{S}_{ij}\equiv{}^{(0,1)}K_{AB}\delta_{iA}\delta_{iB}\ .\tag{7.7}$$

We are not concerned with temperature-dependent effects in this paper. It should be noted, however, that the stress-free condition leads, in general, to a different natural state at each temperature. The effect of Eq. (7.6) is to fix the spontaneous elastic stress in terms of spontaneous electric field stresses. If $E_i^S=0$, so also will $t_{ij}^S=0$.

Equation (7.6) is in the spirit of a boundless medium, as considered up to this point. For a finite body possessing a spontaneous electric field a spontaneous Maxwell stress will exist outside the body. Continuity of the scalar product of the unit normal and the total stress tensor at the boundary can lead to a different condition for the natural state than Eq. (7.6). This will be discussed in Sec. XI.

VIII. ANGULAR MOMENTUM CONSERVATION

The angular momentum conservation law may be found by combining contributions from the center-of-mass motion, each of the internal motions, and the electromagnetic field. The center-of-mass contribution is found by forming the vector product of the equation of motion [Eq. (5.10)] with $\vec{x}$ and by using Eq. (7.1) with the result

$$\epsilon_{ijk}x_j\left(\frac{\partial}{\partial t}(\rho\dot{x}_k)+\frac{\partial}{\partial z_l}(\rho\dot{x}_k\dot{x}_l)\right)=\epsilon_{ijk}x_j(t_{kl}^y+\mathcal{E}_kP_l)_{,l}+q^D(\vec{x}\times\vec{E})_i+[\vec{x}\times(\vec{j}^D\times\vec{B})]_i\ . \tag{8.1}$$

This may be rearranged into

$$\frac{\partial}{\partial t}\left[\rho\left(\vec{x}\times\frac{d\vec{x}}{dt}\right)_i\right]+\frac{\partial}{\partial z_l}\left[\rho\left(\vec{x}\times\frac{d\vec{x}}{dt}\right)_i\dot{x}_l\right]=[\epsilon_{ijk}x_j(t_{kl}^y+\mathcal{E}_kP_l)]_{,l}-\epsilon_{ilk}(t_{kl}^y+\mathcal{E}_kP_l)+q^D(\vec{x}\times\vec{E})_i+[\vec{x}\times(\vec{j}^D\times\vec{B})]_i\ , \tag{8.2}$$

because a spatial frame time derivative of $\vec{x}$ is zero since $\vec{z}=\vec{x}$ is held fixed.

The contribution from the internal motions is found by forming the vector product of the equation of motion (6.1) of the internal coordinates with $\vec{y}^{T\mu}$ and multiplying by J^{-1} to obtain

$$\frac{1}{J}\frac{d}{dt}\left(J\rho^\mu\vec{y}^{T\mu}\times\frac{d\vec{y}^{T\mu}}{dt}\right)_i=\frac{1}{J}q^\mu(\vec{y}^{T\mu}\times\vec{\mathcal{E}})_i-\frac{1}{J}\epsilon_{ijk}y_j^{T\mu}\frac{\partial\rho^0\Sigma}{\partial y_k^{T\mu}}\ , \tag{8.3}$$

where

$$\rho^\mu\equiv m^\mu/J\ . \tag{8.4}$$

We now define the internal angular momentum $\vec{l}$ by

$$\vec{l}\equiv\sum_\mu{}'\rho^\mu\vec{y}^{T\mu}\times\frac{d\vec{y}^{T\mu}}{dt}\ , \tag{8.5}$$

sum Eq. (8.3) over μ from 1 to $N-1$, rearrange the left-hand side by a well-known identity,[7] and use the definition of the polarization, Eq. (4.2). The result is

$$\frac{\partial l_i}{\partial t}+\frac{\partial}{\partial z_l}(l_i\dot{x}_l)=(\vec{P}\times\vec{\mathcal{E}})_i-\frac{1}{J}\epsilon_{ijk}\sum_\mu{}'y_j^{T\mu}\frac{\partial\rho^0\Sigma}{\partial y_k^{T\mu}}\ . \tag{8.6}$$

The electromagnetic field contribution is easily found by forming the vector product of the electromagnetic momentum equation (7.2) with $\vec{x}$ and rearranging the left-hand side in the manner done to Eq. (8.2) with the result

$$\frac{\partial}{\partial t}[\epsilon_0\vec{x}\times(\vec{E}\times\vec{B})]_i-\frac{\partial}{\partial z_l}(\epsilon_{ijk}x_jm_{kl})=-q^D(\vec{x}\times\vec{E})_i-[\vec{x}\times(\vec{j}^D\times\vec{B})]_i\ . \tag{8.7}$$

We now add the angular momentum contributions represented by Eqs. (8.2), (8.6), and (8.7) to obtain

$$\frac{\partial}{\partial t}\left\{\left[\vec{x}\times\left(\rho\frac{d\vec{x}}{dt}+\epsilon_0\vec{E}\times\vec{B}\right)\right]_i+l_i\right\}+\frac{\partial}{\partial z_l}(l_i\dot{x}_l-\epsilon_{ijk}x_jt_{kl}^L)=-\frac{1}{J}\epsilon_{ijk}\left(\sum_\mu{}'y_j^{T\mu}\frac{\partial\rho^0\Sigma}{\partial y_k^{T\mu}}+t_{kj}^y\right)\ . \tag{8.8}$$

This equation has the conservation law form if we can show the right-hand side vanishes. We do this by using the rotational invariance of Σ discussed in Sec. III.

Consider an infinitesimal rotation of the spatial coordinates,

$$z_i'=z_i+\delta z_{[i,j]}z_j\ , \tag{8.9}$$

where the brackets denote antisymmetric interchange symmetry. This induces changes in the spatial vectors $y_i^{T\mu}$ and $x_{i,A}$ of the form

$$(y_i^{T\mu})'=y_i^{T\mu}+\delta z_{[i,j]}y_j^{T\mu}\ , \tag{8.10}$$

$$x_{i,A}'=x_{i,A}+\delta z_{[i,j]}x_{j,A}\ . \tag{8.11}$$

Rotational invariance requires the stored energy to obey

$$\Sigma((y_i^{T\mu})',x_{i,A}')=\Sigma(y_i^{T\mu},x_{i,A})\ . \tag{8.12}$$

A first-order Taylor series expansion in all the arguments on the left-hand side leads to

$$\sum_\mu{}'\frac{\partial\Sigma}{\partial y_k^{T\mu}}\delta z_{[k,j]}y_j^{T\mu}+\frac{\partial\Sigma}{\partial x_{k,B}}\delta z_{[k,j]}x_{j,B}=0\ . \tag{8.13}$$

Since $\delta z_{[k,j]}$ is an arbitrary infinitesimal antisymmetric tensor, we must have

$$\sum_\mu{}'\frac{\partial\Sigma}{\partial y_{[k}^{T\mu}}y_{j]}^{T\mu}+\frac{\partial\Sigma}{\partial x_{[k,B}}x_{j],B}=0\ . \tag{8.14}$$

Forming a scalar product of this equation with the permutation symbol ϵ_{ijk} and multiplying by $-\rho^0/J$ now yields

$$-\frac{1}{J}\epsilon_{ijk}\sum_\mu{}'y_j^{T\mu}\frac{\partial\rho^0\Sigma}{\partial y_k^{T\mu}}-\epsilon_{ijk}t_{kj}^y=0\ , \tag{8.15}$$

with the use of the definition Eq. (5.7) for t_{ij}^y. This proves that the right-hand side of Eq. (8.8) vanishes and so gives us

$$\frac{\partial}{\partial t}\left\{\left[\vec{x}\times\left(\rho\frac{d\vec{x}}{dt}+\epsilon_0\vec{E}\times\vec{B}\right)\right]_i+l_i\right\}+\frac{\partial}{\partial z_l}(l_i\dot{x}_l-\epsilon_{ijk}x_jt^L_{kl})=0\,, \tag{8.16}$$

the spatial frame angular momentum conservation law. From the reasoning of the accompanying paper[8] we are justified in interpreting the quantity in the time derivative as the spatial frame density of angular momentum and the quantity in the divergence as the flow of angular momentum across a surface fixed in the spatial frame.

It is important to realize that this closed system consisting of a crystal in interaction with the electromagnetic field possesses conservation of *total* angular momentum even though the *total* stress tensor is not symmetric. This results from the crystal being represented not simply by the center-of-mass continuum but by a manifold of N vector matter continua, $N-1$ of them representing internal motions. We see in Eq. (8.16) that there is an internal angular momentum density and a corresponding flow of internal angular momentum density produced by these internal motions. The balancing role played by the internal angular momentum with respect to the antisymmetric part of the total stress tensor can be seen by combining Eqs. (8.15) and (8.6) and returning the left-hand side of Eq. (8.15) to the form present in Eq. (8.3). We then get

$$\frac{1}{J}\frac{d}{dt}(Jl_i)=(\vec{P}\times\vec{\mathcal{E}})_i+\epsilon_{ijk}t^y_{kj}=\epsilon_{ijk}t^L_{kj}\,. \tag{8.17}$$

This can be interpreted as an equation of motion for the internal angular momentum with the antisymmetric part of the total stress tensor acting as the driving torque.

IX. ENERGY CONSERVATION

To obtain the energy conservation statement we must add the contributions from the center-of-mass motion, the internal motions, and the electromagnetic field. The center-of-mass contribution is found by forming the scalar product of Eq. (5.10) with $d\vec{x}/dt$ and manipulating the inertial term in a manner[7] similar to Eq. (7.1). The result is

$$\frac{\partial}{\partial t}\left[\frac{1}{2}\rho\left(\frac{d\vec{x}}{dt}\right)^2\right]+\frac{\partial}{\partial z_j}\left\{\left[\frac{1}{2}\rho\left(\frac{d\vec{x}}{dt}\right)^2\delta_{ij}-t^y_{ij}-\mathcal{E}_iP_j\right]\dot{x}_i\right\}$$
$$=-(t^y_{ij}+\mathcal{E}_iP_j)\dot{x}_{i,j}+[q^DE_i+(\vec{j}^D\times\vec{B})_i]\dot{x}_i\,. \tag{9.1}$$

Similar handling of the internal coordinate equation (6.1) yields

$$\frac{\partial}{\partial t}\left[\frac{1}{2}\rho^\mu\left(\frac{d\vec{y}^\mu}{dt}\right)^2\right]+\frac{\partial}{\partial z_i}\left[\frac{1}{2}\rho^\mu\left(\frac{d\vec{y}^\mu}{dt}\right)^2\mathring{x}_i\right]$$
$$=\rho q^\mu\mathring{y}^{T\mu}_i\mathcal{E}_i-\rho\mathring{y}^{T\mu}_i\frac{\partial\Sigma}{\partial y^{T\mu}_i}\,. \tag{9.2}$$

The electromagnetic field contribution is found by forming the scalar product of Eq. (4.4) with $-\vec{E}$ and the scalar product of Eq. (4.7) with $\vec{B}/\mu_0$ and adding the results. This yields

$$\frac{\partial}{\partial t}\left(\tfrac{1}{2}\epsilon_0\vec{E}^2+\frac{\vec{B}^2}{2\mu_0}\right)+\frac{\partial}{\partial z_i}\left(\frac{(\vec{E}\times\vec{B})_i}{\mu_0}\right)=-\vec{E}\cdot\vec{j}^D\,. \tag{9.3}$$

Equations (9.1), (9.2) for each μ, and (9.3) are added to obtain the total energy equation. All terms on the right of those equations cancel one another with the exception of

$$t^y_{ij}\dot{x}_{i,j}+\rho{\sum_\mu}'\mathring{y}^{T\mu}_i\frac{\partial\Sigma}{\partial y^{T\mu}_i}=\frac{\partial\rho\Sigma}{\partial t}+\frac{\partial}{\partial z_i}(\rho\Sigma\dot{x}_i)\,. \tag{9.4}$$

Hence we obtain

$$\frac{\partial W}{\partial t}+\frac{\partial S_j}{\partial z_j}=0\,, \tag{9.5}$$

where

$$W\equiv\tfrac{1}{2}\rho\left(\frac{d\vec{x}}{dt}\right)^2+{\sum_\mu}'\tfrac{1}{2}\rho^\mu\left(\frac{d\vec{y}^{T\mu}}{dt}\right)^2+\tfrac{1}{2}\epsilon_0\vec{E}^2+\vec{B}^2/2\mu_0+\rho\Sigma\,, \tag{9.6}$$

$$S_j\equiv\left[\tfrac{1}{2}\rho\left(\frac{d\vec{x}}{dt}\right)^2\delta_{ij}+{\sum_\mu}'\tfrac{1}{2}\rho^\mu\left(\frac{d\vec{y}^{T\mu}}{dt}\right)^2\delta_{ij}+\rho\Sigma\delta_{ij}-t^y_{ij}-\mathcal{E}_iP_j\right]\dot{x}_i+(\vec{E}\times\vec{B}/\mu_0)_j\,, \tag{9.7}$$

which states energy conservation in the spatial frame. By the arguments of the accompanying paper[8] we may interpret W as the energy density and S_j as the energy-flow vector.

At first glance it appears that Eq. (9.5) is sensitive to an arbitrary constant which could have been inserted in the definition Eq. (3.27) of $\rho^0\Sigma$, the stored energy. However, the two terms in $\rho\Sigma$ in Eq. (9.5) can be reexpressed as

$$\frac{\partial\rho\Sigma}{\partial t}+\frac{\partial\rho\Sigma\dot{x}_j}{\partial z_j}=\rho^0\Sigma\left(\frac{\partial\rho}{\partial t}+\frac{\partial\rho\dot{x}_j}{\partial z_j}\right)\Big/\rho^0+\frac{\rho}{\rho_0}\left(\frac{\partial\rho^0\Sigma}{\partial t}+\frac{\dot{x}_j\partial\rho^0\Sigma}{\partial z_j}\right)\,. \tag{9.8}$$

Any constant in $\rho^0\Sigma$ clearly disappears from the second pair of terms because of the derivatives acting on it. The first pair of terms, whose coefficient contains the constant in question, disappear because of mass conservation,

$$\frac{\partial\rho}{\partial t}+\frac{\partial\rho\dot{x}_j}{\partial z_j}=0\,, \tag{9.9}$$

a condition implicit throughout this work.[7] These remarks apply here because this theory is nonrelativistic. Were it relativistic, mass conservation would not be a conservation law separate from energy conservation, and the theory would be sensitive to the constant term in $\rho^0\Sigma$ since it would be the rest energy of all the mass of the system.

X. CONTINUITY EQUATIONS IN PRESENCE OF EXTERNAL FIELDS

In some problems it is of interest to consider certain electromagnetic fields $\vec{E}^e$ and $\vec{B}^e$ acting on the body under study as external fields. By this we mean that the external fields are specified fields, that we are interested in the action on the body, but not interested in the action of the body on the external fields. Thus we wish to ignore the sources q^e and $\vec{j}^e$ of the external fields and ignore the matter equations relating to q^e and $\vec{j}^e$. The energy, momentum, and angular momentum equations for the body and its fields will not contain source terms for these quantities arising from the action of the external fields on the body.

With this view the energy continuity equation in the spatial frame can be found by adding Eqs. (9.1) and (9.2) (for each μ), regarded as depending on the fields $\vec{E}+\vec{E}^e$ and $\vec{B}+\vec{B}^e$, to Eq. (9.3). The result is

$$\frac{\partial}{\partial t}\left[\tfrac{1}{2}\rho\left(\frac{d\vec{x}}{dt}\right)^2+\sum_\mu{}'\tfrac{1}{2}\rho^\mu\left(\frac{d\vec{y}^{T\mu}}{dt}\right)^2+\tfrac{1}{2}\epsilon_0\vec{E}^2+\frac{\vec{B}^2}{2\mu_0}+\rho\Sigma\right]$$
$$+\frac{\partial}{\partial z_j}\left\{\left[\tfrac{1}{2}\rho\left(\frac{d\vec{x}}{dt}\right)^2\delta_{ij}+\sum_\mu{}'\tfrac{1}{2}\rho^\mu\left(\frac{d\vec{y}^{T\mu}}{dt}\right)^2\delta_{ij}\right.\right.$$
$$\left.\left.+\rho\Sigma\delta_{ij}-t^{v}_{ij}-\mathcal{E}_iP_j\right]\mathring{x}_i+\frac{(\vec{E}\times\vec{B})_j}{\mu_0}\right\}=\vec{j}^D\cdot\vec{E}^e\,. \qquad (10.1)$$

A similar procedure applied to the momentum equations yields

$$\frac{\partial}{\partial t}[\rho\dot{x}_i+\epsilon_0(\vec{E}\times\vec{B})_i]-\frac{\partial t^L_{ij}}{\partial z_j}=q^DE^e_i+(\vec{j}^D\times\vec{B}^e)_i \qquad (10.2)$$

for momentum continuity in the spatial frame in the presence of external fields. Applying the procedure to the angular momentum equations yields

$$\frac{\partial}{\partial t}\left[\vec{x}\times\left(\rho\frac{d\vec{x}}{dt}+\epsilon_0(\vec{E}\times\vec{B})\right)+\vec{l}\right]_i+\frac{\partial}{\partial z_m}(l_i\dot{x}_m-\epsilon_{ijk}x_jt^L_{km})$$
$$=\{\vec{x}\times[q^D\vec{E}^e+(\vec{j}^D\times\vec{B}^e)]\}_i \qquad (10.3)$$

for angular momentum continuity in the spatial frame in the presence of external fields.

XI. BOUNDARY CONDITIONS

The boundary conditions on the four electromagnetic fields needed for this work are those which hold at the material surface of a moving, deforming body. Previous discussions have derived the boundary conditions at the surface of a rigidly moving body. Even in this simpler situation significant disagreement exists. Sommerfeld in his book on electrodynamics[9] presents a derivation which shows that the tangential components of the magnetic intensity $\vec{H}$ are continuous at the body surface of a body having no surface currents and moving at a uniform velocity with respect to a spatial coordinate frame to which $\vec{H}$ is referred. Moller,[10] on the other hand, asserts that the tangential components of $\vec{H}-(d\vec{x}/dt)\times\vec{D}$ are continuous under these conditions.

In order to resolve this question and to generalize the result to moving, deforming bodies we have in an accompanying paper[11] transformed the Maxwell equations to the material coordinate system of a moving, deforming body. The boundary conditions, found very simply in this system, are then transformed[11] back to the usual spatial coordinate system. Our result resolves the disagreement in favor of the Moller result and shows that Sommerfeld's error was in assuming that the material velocity $d\vec{x}/dt$ was discontinuous at the body surface.

The spatial frame electromagnetic boundary conditions that we find[11] hold at the surface of a dielectric body moving and deforming with respect to that frame are

$$\vec{n}\times\left(\vec{H}-\frac{d\vec{x}}{dt}\times\vec{D}\right)=0\,, \qquad (11.1)$$

$$\vec{n}\times\left(\vec{E}+\frac{d\vec{x}}{dt}\times\vec{B}\right)=0\,, \qquad (11.2)$$

$$\vec{n}\cdot[\vec{D}]=\sigma\,, \qquad (11.3)$$

$$\vec{n}\cdot[\vec{B}]=0\,, \qquad (11.4)$$

where the brackets here denote the jump in the quantity contained within,

$$[V]\equiv V^{\text{out}}-V^{\text{in}}\,, \qquad (11.5)$$

$\vec{n}$ is the outward unit normal and σ is the surface charge density. A surface charge has been included since an immobile, extrinsic charge usually collects on the surface of a pyroelectric in order to cancel the spontaneous electric field. One would expect that this surface charge multiplied by the component of the material velocity $d\vec{x}/dt$ tangential to the surface would produce a convective surface current in the $\vec{H}$ field boundary condition (11.1). However, we show in the accompanying paper[11] that an exactly cancelling term arises in the boundary condition from the $\partial\vec{D}/\partial t$ term of the differential equation with the result that no surface current of any kind appears in the boundary condition (11.1) for a dielectric.

To find the effects of deformation on $\vec{n}$ and σ we use Nanson's formula[12]

$$da_i=JX_{M,i}\,dA_M\,, \qquad (11.6)$$

which relates vector area elements in the spatial and material frames. Since

$$da_i=n_i\,da\,,\quad dA_M=N_m\,dA\,, \qquad (11.7)$$

where $\vec{N}$ and dA are the material frame (undeformed) unit normal and area element and $\vec{n}$ and da are the corresponding spatial frame (deformed) quantities, we obtain the area ratio

$$da=J[N_L(C^{-1})_{LM}N_M]^{1/2}\,dA\,, \qquad (11.8)$$

where

$$(C^{-1})_{MN}=X_{M,j}X_{N,j} \qquad (11.9)$$

follows from Eq. (3.19). We also obtain the relation between the unit normals,

$$n_i = N_A X_{A,i}[N_L(C^{-1})_{LM}N_M]^{-1/2} , \qquad (11.10)$$

by dividing Eq. (11.6) by Eq. (11.8). This expression relates the deformed normal $\vec{n}$, needed in Eqs. (11.1)–(11.4), to the undeformed normal $\vec{N}$. The deformed state surface charge density σ is related[11] to the undeformed state (or spontaneous) surface charge density Σ^S by

$$\sigma = \Sigma^S \frac{dA}{da} = J^{-1}[N_L(C^{-1})_{LM}N_M]^{-1/2}\Sigma^S . \qquad (11.11)$$

This expression is to be used in Eq. (11.3).

The remaining boundary condition needed is that for the stress tensor. In the accompanying paper on the stress tensor[8] the boundary condition on the stress,

$$[t^y_{ij} + \mathcal{E}_i P_j + m_{ij} + \epsilon_0(\vec{E}\times\vec{B})_i \dot{x}_j]n_j = 0 , \qquad (11.12)$$

is found for a deforming body surface moving at velocity $d\vec{x}/dt$. The brackets here denote the jump in the quantity as defined in Eq. (11.5). If a surface traction T_i could somehow be applied from the outside to the surface between the two media, it would appear on the left-hand side of Eq. (11.12). If such a surface traction is used to represent the effect of the outside medium on the inside medium, the stress tensor term for the outside medium in Eq. (11.12) must be dropped. If the stress tensors for each of the two media are retained, it is difficult to conceive of what an extra surface traction means. The only one applicable to pyroelectrics that comes to mind is the electric force on an immobile, extrinsic surface charge. However, an examination of the derivation of the stress boundary condition in the accompanying paper[8] reveals that this effect is not an extra surface traction but is included within the stress tensor effects through the discontinuity in the normal component of the polarization at such a surface.

Note that the stress boundary condition (11.12) includes the Maxwell stress tensor which can exist outside the material body. In particular there is a nonzero total stress outside the material body in the natural state if $\vec{E}^S \neq 0$. This fact leads us to reconsider the condition placed on the total stress by the definition of the natural state. In Sec. VII we considered the infinite body; here we wish to consider a finite body. Just as throughout this paper we consider here a homogeneous body. The question thus is whether a homogeneous solution of Eq. (11.12) exists for the natural state of a finite body. Equation (11.12) can be reexpressed in the natural state as

$$N_A\delta_{Ak}(t^S_{mk} + E^S_{(m}P^S_{k)} + \epsilon_0 E^S_m E^S_k - \tfrac{1}{2}\epsilon_0 E^S_n E^S_n \delta_{mk})^i$$
$$= N_A\delta_{Ak}(\epsilon_0 E^S_m E^S_k - \tfrac{1}{2}\epsilon_0 E^S_n E^S_n \delta_{mk})^o , \qquad (11.13)$$

where the superscripts i and o refer to inside and outside, respectively. Here $\vec{N}$ is regarded as a function of its position on the surface. Since it is well known that there is no electric field which is separately homogeneous inside and outside a finite, homogeneously polarized body, it would appear that there is no desired solution to Eq. (11.13). However, our objective would be met if a solution which is homogeneous *only* inside the body is found.

We thus are led to divide the outside electric field into normal and tangential parts (with respect to the surface) and use Eqs. (11.2) and (11.3) to eliminate the outside field in terms of the inside field. Since only the latter now appears, we can drop the superscript i. We also denote $N_k = \delta_{kA}N_A$. Equation (11.13) then yields

$$2N_k t^S_{mk} = \epsilon_0^{-1}(N_k P^S_k)^2 N_m + N_k P^S_k E^S_m - N_k E^S_k P^S_m . \qquad (11.14)$$

The most general shape isotropic body which possesses both a homogeneous electric field and polarization interior to the body is an ellipsoid.[13] Because of the cubic dependence on $\vec{N}$ of the first term on the right-hand side compared to the linear dependence of the other terms, Eq. (11.14) cannot be satisfied for such a shape for a homogeneous t^S_{mk}. The addition of anisotropy to the problem does not help. Thus we conclude that no pyroelectric body having a spontaneous electric field and having *all* dimensions finite can have a homogeneous natural state. A consistent treatment of such bodies will require inclusion of explicit dependence of the stored energy on $\vec{X}$.

Consider an infinite cylinder of arbitrary cross section with the spontaneous polarization parallel to the sides of the cylinder. A consideration of the depolarization field[13] yields the trivial solution of $\vec{E}^S = 0$ and so $t^S_{ij} = 0$. Hence a homogeneous natural state exists for this shape.

Consider next an infinite plate, that is, a body of one finite (and constant) dimension. A consideration of the depolarization field[13] yields the relation inside the plate

$$\vec{E}^S = -\epsilon_0^{-1}\vec{N}(\vec{N}\cdot\vec{P}^S) , \qquad (11.15)$$

where $\vec{N}$ is normal to the natural state surface and $\vec{P}^S$ is allowed to have any orientation. Outside the plate $\vec{E}^S$ vanishes. If we require t^S_{ij} to satisfy Eq. (11.14), to be a symmetric tensor, see Eq. (7.7), and to vanish when $\vec{N}\cdot\vec{P}^S = 0$ which corresponds to the solution of the previous paragraph, then

$$t^S_{ij} = P^S_k N_k(N_{(i}P^S_{j)} - \tfrac{1}{2}P^S_m N_m N_i N_j)/\epsilon_0 . \qquad (11.16)$$

Last, we remark that for a finite-sized body in all dimensions which, because of collected extrinsic surface charge or its own small conductivity, has its spontaneous electric field cancelled there exists a homogeneous natural state with $t^S_{ij} = 0$.

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