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Validity of Post Constraint of Electromagnetism in Multiferroic Materials

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Abstract: We present a framework for modeling the boundary-value problem (frequency driven) for homogeneous multiferroic material under the validity of post constraint and apply it to fundamental differential equation of electromagnetism in valid new regimes (boundary conditions for material with simultaneous electric and magnetic order). Three facets of the model are addressed, which explicitly respect the validity of post constraint of modern electromagnetism. First, AFM (antiferromagnetic) ordering and magneto electric coupling are explained. Second, the energetic anaysis of multiferroic is expressed for ferroic-electric ordering. Third, the conflict of fundamental differential electromagnetism in multiferroic material under explicit application of boundary condition is resolved.

Key words: Multiferroic, antiferriomagnetic ordering, electromagnetic theory, post constraint, boundary conditions, Tellegen parameter.

Nomenclature

H:	Exchange interaction energy
C:	Elastic stiffness
B:	Magnetic induction
H:	Magnetic field
E:	Electric field
D:	Electric displacement
P:	Polarisation
M:	Magnetisation

Greek letters

κ:	Dielectric coefficient
ω:	Angular frequency
ν:	Impermeability coefficient
ζ_{m}:	Demagnetisation
ζ_{p}:	Depolarisation

1. Introduction

Multiferroic material has boomed enormously in recent years. Exponent growth in the development of accurate theoretical method accompanying the sophisticated synthesis techniques in both solid route methods like mechanical activation, sintering; and wet chemical methods like sol-gel method, pulsed laser deposit, liquid chemical epitaxy, hydrothermal synthesis etc; along with characterisation brings in the study of various types of multiferroic oxides [1-5]. The discussion of multiferroics is fascinating since this is rich in variety of physical mechanisms underplaying simultaneously evolving captivating scenario when ferroelectric and magnetic order simultaneously exhibit along with ferroelasticity [6-9].

This paper addresses the genesis of the post constraint of electromagnetic constitution relation of multiferroic material medium. The post constraint is the structural constraint with the linear medium exhibiting the magneto-electric coupling [10, 11]. With the origination from the microscopic nature of primitive electromagnetic fields and Lorentz covariance of the Maxwell equations, the post constraint has 35 independent complex-value parameters [12, 13]. We analyse the energetic analysis of multiferroic material for ferroelectric ordering and anti-ferromagnetic order with magneto electric coupling. We then have presented a framework for developing the validity of post constraint of multiferroics.

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We derive the magnetic ordering with magneto-electric coupling. It accommodates the energetic analysis of multiferroics. Thereafter, we introduce the framework. It is general in the sense and can be applied to the globally conserved distributed quantities born of the spatial homogeneous microscopic entities. The Maxwell postulates with its structural entities are included with envision to stipulate the framework for post-constraint analysis. Then, the boundary-value problems invoked to claim the validity of post constraint of multiferroics.

2. Anti-ferromagnetic Coupling

The term "multiferroic" was coined by Schimd in 1993 to describe the crystals exhibiting two or three types of ferroic order simultaneously. The functional crystal ABO_3 has a cation with lone pair of 6 electros and transition metal element B which transforms to inert gas upon removal of *s* and *d* shell electrons.

Let consider multiferroic crystal with simple cubic lattice having magnetic spins in (111) plane.

The nearest neighbors of the spin with respect to the considered spin in simple cubic lattice with lattice constant c are given by

$$ð^{i,j} = \pm \begin{pmatrix} c & 0 & 0 \\ 0 & c & 0 \\ 0 & 0 & c \end{pmatrix}$$

The relative coordinates of 12 second nearest coordinates are given by

$$\tilde{n}^{i,j} = \pm \begin{pmatrix} 0 & c & c & 0 & c & c \\ c & 0 & c & c & 0 & -c \\ c & c & 0 & -c & -c & 0 \end{pmatrix}$$

Generalised Hamilton for inter-spins exchange interaction is given by Ref. [14, 15]

$$H = -\sum_{ij} J^{ij} K_i K_j \tag{1}$$

where J^{ij} is the exchange integral of spins K. It is proportional to the distance of spins in consideration.

Hence, we deduced the exchange interaction of the nearest 6 spins neighbors of simple cubic multiferroic crystal with respect to 2 antiferromagnetic coupled lattice spins K_a and K_b is derived as

$$H_{m1} = -12\sum_{i=1}^{n/2} K_a \,.K_b - Jc^2\sum_{i=1}^{n/2}[K_a.\Delta K_b + K_b.\Delta K_a] \tag{2}$$

Similarly, the exchange interaction by the second nearest neighbors with respect to same lattice spins K_a and K_b is derived as

$$H_{m2} = 4J'c^2\sum_{i=1}^{n/2}[K_a.\Delta K_b + K_b.\Delta K_a] \tag{3}$$

Whereas J and J' are the exchange integrals for the nearest neighbors and second nearest neighbors respectively, Δ is the Laplace operator and n is the number of neighboring lattice points considered.

Henceforth the total exchange interaction is given by

$$H = H_{m1} + H_{m2} \tag{4}$$

According to the continuum approximation, in the material with size larger than the lattice constant, the distribution of spins is assumed as continuous and the summation of exchange energy can be treated as integral.

Hence, the exchange integral is assayed as

$$H = \frac{-6J}{c^3}\int K_a \,.K_b \,dV - \frac{J}{2c}\int [K_a.\Delta K_b + K_b.\Delta K_a]dV + \frac{2J'}{c}\int [K_a.\Delta K_a + K_b.\Delta K_b]dV \tag{5}$$

With divergence theorem and periodic boundary condition, the exchange integral is simplified as

$$\begin{aligned} H &= \frac{-6J}{c^3}\int K_a \,.K_b \,dV - \frac{J}{2c}\int [\nabla K_a.\nabla K_b + \nabla K_b.\nabla K_a]dV + \frac{2J'}{c}\int [\nabla K_a.\nabla K_a + \nabla K_b.\nabla K_b]dV \\ &= \frac{-6J}{c^3}\int K_a \,.K_b \,dV - \frac{J}{c}\int [\nabla K_a.\nabla K_b]dV + \frac{2J'}{c}\int [(\nabla K_a)^2 + (\nabla K_b)^2]dV \end{aligned}$$

Substitute F = $\frac{6J}{c^3}$, A = $\frac{-J}{2c}$ and J'=$\frac{J}{4}$

$$H = \int [A|\nabla K_a - \nabla K_b|^2 - FK_a.K_b]dV \qquad (6)$$

The exchange constitutive parameters F and A depend on c and J; former retards magnetic polarization and latter accelerates antiferromagnetic coupling between spins.

3. Energetic of Multiferroic Crystal

3.1 Potential Energy

Potential energy of multiferroic crystal with simple cubic lattice in region under external stress σ and electric field E and magnetic field H is influenced by

- interfacial energy at domain wall H_i,
- anisotropy ferroelectric energy due to both ferroic ordering H_{an0} and magneto electric coupling H_{an1},
- energy due to antiferromagnetic ordering H_{afm},
- and due to elasticity H_e.

The total potential energy is demoted under external loadings, demagnetization energy ζ_m and depolarization energy ζ_p.

Interfacial energy at domain wall is deduced from Eq. (1) as

$$H_i = \int [A|\nabla K_a - \nabla K_b|^2]dV + F_e\,|\nabla\emptyset|^2 \qquad (7)$$

Whereas F_e is exchange constant due to ferroelectric coupling; $\emptyset$ is the charactersistic function for phase field variable to stimulate the domain patterns [16-18]

$$\text{P.E} = H_i + H_{an0} + H_{an1} + H_{afm} + H_e - \sigma.\varepsilon - \mathbf{E}.\text{p} - \text{M}\mathbf{H}(m_a + m_b) + \zeta_p + \zeta_m \qquad (8)$$

3.2 Kinetic Energy

Similarly, kinetic energy is influenced by the driving force and effective magnetization field developed respectively under influence of

- interfacial energy at domain wall F_i and H_i,
- anisotropy ferroelectric energy due to both ferroic ordering F_{an0} and $H_{an0;}$ and magneto electric coupling F_{an1} and H_{an1},
- energy due to antiferromagnetic ordering $\mathbf{F}_{afm}$ and $\mathbf{H}_{afm}$,
- and due to elasticity F_e and H_e

$$\text{K.E} = -\int \text{F}.\delta\emptyset dV - \int M\text{H}.\delta m_{a,b}\, dV \qquad (9)$$

4. Multiferroics under Effective Fields

The effect of demagnetisation ζ_m and depolarisation ζ_p under the influence of elastic, electric and magnetic field, the multiferroic energetic state is calculated using governing equations and boundary conditions.

According to Maxwell's equations

$$\nabla.E(x,t) = \kappa^{-1}\rho(x,t) \qquad (10)$$

$$\nabla.B(x,t) = 0 \qquad (11)$$

$$\nabla \times B(x,t) - \kappa\mu\frac{\partial}{\partial t}E(x,t) = \mu J(x,t) \qquad (12)$$

$$\nabla \times E(x,t) + \frac{\partial}{\partial t}B(x,t) = 0 \qquad (13)$$

At mechanical equilibrium, the total stress is evaluated as [19, 20]

$$\nabla.\sigma(x,t) = 0 \;\; \sigma = C(x,t)\Delta\varepsilon \qquad (14)$$

κ is the dielectric constant used in relation to constrained theory of ferroelectric**.** $C(x,t)$ is the elastic stiffness and ε is strain.

The demagnetisation ζ_m and depolarisation ζ_p fields existe in entire region. They can be analysed by quantifying the source densities $\text{J}(x,t)$ and $\rho(x,t)$ into bounded components (frequency driven) polarization and magnetisation. P and M is the average polarisation and magnetisation distributed in the domain. Hence the electric induction D (x,t) and magnetic induction B (x,t) is evolved

$$\text{D}\;(x,t) = -\kappa E(x,t) + \text{P}\;(x,t) \qquad (15)$$

$$\text{B}(x,t) = -\mu\text{H}(x,t) + \text{M}(x,t) \qquad (16)$$

5. Linear Constitutive Relations

The linear constitutive relation for the demagnetisation ζ_m and depolarisation ζ_p field is expressed as

$$\text{D}(x,t) = \iint -\kappa(x,t).\text{E}(x-x',t-t')dx'dt' + \iint q(x,t).\text{B}(x-x',t-t')dx'dt' \qquad (17)$$

$$\mathrm{H(x,t)} = \iint \mathrm{r(x,t).E(x-x',t-t')dx'dt'} + \iint \nu\mathrm{(x,t).B(x-x',t-t')dx'dt'} \quad (18)$$

where κ is the di-electric tensor, ν is the impermeability tensor; q and r are magneto-electric tensor.

$$\mathrm{Trace}\ (\mathrm{q(x,t)} - \mathrm{r(x,t)} = 0 \quad (19)$$

Eqs. (17) and (18) will emanate mathematical complexities while solving Maxwell postulates. With execution of the convolution theorem, and using the temporal Fourier transformation, the frequency-domain constitutive relations evolved in dyadic notation as

$\mathbf{U}$(x,ω)= $\mathbf{V}$(x,ω).$\mathbf{W}$(x,ω)

With 6 vectors

$$\mathrm{U(x,\omega)}=\begin{bmatrix}\mathrm{D(x,\omega)}\\ \mathrm{H(x,\omega)}\end{bmatrix}$$

$$\mathrm{W(x,\omega)}=\begin{bmatrix}\mathrm{E(x,\omega)}\\ \mathrm{B(x,\omega)}\end{bmatrix}$$

With 6 × 6 constitutive dyadic

$$\mathrm{V(x,\omega)} = \begin{bmatrix}-\kappa & q\\ r & \nu\end{bmatrix}_{EB} \quad (20a)$$

In the modern analysis of electromagnetism of homogeneous material deals with EH-electromagnetism with electric field E(x,t) and magnetic field H(x,t) as proponent. Henceforth, the analysis of boundary condition of electric and magnetic fields is accounted.

$$\mathrm{U(x,\omega)}=\begin{bmatrix}\mathrm{D(x,\omega)}\\ \mathrm{H(x,\omega)}\end{bmatrix}$$

$$\mathrm{W(x,\omega)}=\begin{bmatrix}\mathrm{E(x,\omega)}\\ \mathrm{H(x,\omega)}\end{bmatrix}$$

$$\text{where } \mathbf{V}\mathrm{(x,\omega)} = \begin{bmatrix}-\kappa & q & s\\ r & \nu & s\end{bmatrix}_{EH} \quad (20\ b)$$

s is the Tellegen parameter.

The EH-electromagnetism so developed may introduce an anomaly which has to be eliminated. This develops the Post Constraint or the structural constraint

6. Boundary Condition Problems

Let us consider the multiferroic material filled in region R. It is uniaxial magnetic–dielectric anisotropic, homogeneous, temporally invariant and spatially local. It is characterized by constitutive relation with dyadic notation as follows

$$\mathrm{U(x,\omega)}=\begin{bmatrix}\mathrm{D(x,\omega)}\\ \mathrm{H(x,\omega)}\end{bmatrix}$$

$$\mathbf{W}\mathrm{(x,\omega)}=\begin{bmatrix}E\mathrm{(x,\omega)}\\ H\mathrm{(x,\omega)}\\ H\mathrm{(x,\omega)}\end{bmatrix}$$

$$\text{where } \mathbf{V}\mathrm{(x,\omega)} = \begin{bmatrix}-\kappa_{ani} & q & s\\ r & \nu_{ani} & s\end{bmatrix}_{EH} \quad (21)$$

The uniaxial anisotropic medium is determined by single axis with unit vector i .

$\kappa_{ani}(\omega)$ and ν_{ani} are dyadic di-electric tensor and impermeability with 3 × 3 diagonal matrix expressed as

$$\kappa_{ani}(\omega) = \kappa(\omega)(I - \mathrm{i\,i}) + \kappa_{ani}(\omega)\mathrm{i\,i} \quad (22)$$

$$\nu_{ani}(\omega) = \nu(\omega)(I - \mathrm{i\,i}) + \nu_{ani}(\omega)\mathrm{i\,i} \quad (23)$$

where I is identity dyad.

The boundary conditions imposed on this region R are

$B^n(x^+, \omega) = B^n(x^-, \omega)$

$E^t(x^+, \omega) = E^t(x^-, \omega)$

$D^n(x^+, \omega) = D^n(x^-, \omega)$

$H^t(x^+, \omega) = H^t(x^-, \omega)$

where x ϵ R; n and t represent normal and tangent components, respectively.

Among the Maxwell postulates, Eqs. (10) and (12) deal with matter-free space

$$\nabla.\boldsymbol{E}(x,\omega) = \kappa^{-1}\boldsymbol{\rho}(x,\omega) \quad (24)$$

$$\nabla \times \boldsymbol{B}(x,\omega) - \kappa\mu\frac{\partial}{\partial t}\boldsymbol{E}(x,\omega) = \mu\boldsymbol{J}(x,\omega) \quad (25)$$

Hence, we express Eqs. (11) and (13) succinctly in terms of frequency domain are expressed

$$\nabla.\boldsymbol{B}(x,\omega) = 0 \quad (26)$$

$$\nabla \times E(x,\omega) - i\omega\boldsymbol{B}(x,\omega) = 0 \quad (27)$$

And in terms of induction fields (DH) in region R.

$$\nabla. \mathrm{D}(x,\omega)=0 \quad (28)$$

$$\nabla\times \ \mathrm{H}(x,\omega)+i\omega \mathrm{D}(x,\omega)=0 \quad (29)$$

Substituting the equation 21 in the eq 28 and 29, we deduced

$$\nabla.[-\kappa_{ani}(\omega).E(x,\omega)+q(\omega).B(x,\omega)]=0 \quad (30)$$

And

$$\nabla\times[\nabla\times[r(\omega).\boldsymbol{E}(x,\omega)]-i\omega\kappa_{ani}(\omega).\boldsymbol{E}(x,\omega)+ \nabla\times[\nu_{ani}(\omega).\boldsymbol{B}(x,\omega)]+i\omega q(\omega).\boldsymbol{B}(x,\omega)-s\omega[\nabla\times E(x,\omega)-i\omega\boldsymbol{B}(x,\omega)]=0$$

$$\nabla.[-\kappa_{ani}(\omega).\boldsymbol{E}(x,\omega)+q(\omega).\boldsymbol{B}(x,\omega)]=0 \quad (31)$$

$$\nabla\times[r(\omega).E(x,\omega)]-i\omega\kappa_{ani}(\omega).E(x,\omega)+ \nabla\times[\nu_{ani}(\omega).B(x,\omega)]+i\omega q(\omega).B(x,\omega)=0 \quad (32)$$

7. Conclusion: The Conflict and Its Resolution

We have analysed the effective fields on multiferroic material. It involves the uniaxial anisotropic magnetic energy along with the potential for demagnetization and depolarization. Further scrutinising the effect boundary condition in frequency domain electromagnetism analysis, we found the presence of excess parameter (Tellegen) in Eq. (21). This excess-parameter is filtered out in Eq. (29). Hitherto, it does not affect the boundary condition of the multiferroic matter.

This theory augments the study for switching of antiferomagnetic domains by electric and magnetic loading and proponent for study of magnetoelectric materials with coupled ferroelastic, ferroelectric and antiferromagnetic domains.

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