Configurational forces in dynamics and electrodynamics

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Abstract. The notion of configurational force in mechanics and thermomechanics can be readily extended to electromagnetic elastic materials. By invariance arguments and through variational procedures, the Maxwell equations are transformed into a Lagrangian (or material) form and thus consistently coupled with the mechanical balance laws. In this context, the configurational forces and momenta depend also on the electromagnetic fields and specifically on the Lagrangian electromagnetic potentials. The question then arises as to whether the classical gauge conditions are still appropriate to the Lagrangian potentials. Eventually, gauge transformations for these potentials are examined for the full set of equations of interest.

Key words: configurational forces, continuum mechanics, electrodynamics, variational calculus.

1. INTRODUCTION

The singular behaviour of mechanical and electromagnetic fields can be assimilated to possibly time-dependent localized material inhomogeneities. In this view, the related thermodynamical potential, such as the free energy, may explicitly depend on time, the time evolution of the material response being governed by the laws of thermodynamics. However, in most cases these phenomena are better understood in the context of configurational mechanics, in terms of material forces and material momenta [1–6].

In the presence of electromagnetic fields, the problem of identifying forces and momenta may arise as a preliminary issue. This identification being established, configurational material forces and momenta can be introduced in terms of the electromagnetic quantities and specifically of the material electromagnetic potentials, which are defined in the reference configuration of the body. The Maxwell equations, written in terms of these potentials, are said to

be expressed in material or Lagrangian form. The request of invariance of the Maxwell equations for possible transformations of the aforementioned potentials addresses gauge transformations. These transformations for the Lagrangian potentials, though similar in form, radically differ from the classical gauge transformations, which are inherent in the electromagnetic fields and equations in the actual configuration. The electromagnetic potentials also address gauge conditions. These conditions can be reformulated for the Lagrangian potentials as a replica of those stated in the classical electromagnetic theory, but, unfortunately, the related results seem to be rather unsatisfactory.

These remarks suggest looking for new conditions or new equations in the Lagrangian framework. In this context, configurational forces and momenta may fail to be invariant with respect to the material gauge transformations [7,8]. A similar situation in which a physical quantity is not invariant with respect to gauge transformations of the classical electromagnetic potentials emerges in the case of a pointwise charged particle acted on by electromagnetic fields. A Lagrangian is associated with the particle from which the canonical momentum is derived. This momentum turns out to depend explicitly on the electromagnetic vector-potential and is thus gauge-dependent. However, the role of the electromagnetic potential in the canonical momentum deserves some further comments. In fact, on the basis of this momentum a Hamiltonian can also be associated with the particle through a classical Legendre transformation. As is known, the Hamiltonian provides the basis for a quantum mechanical description as it addresses the Schrödinger equation, the master equation of quantum mechanics [9–11]. This equation governs the so-called wave function, a complex-valued function of the position and time that is associated with the particle. It turns out that the presence of the electromagnetic potentials in the Hamiltonian and thus in the Schrödinger equation only affects the phase of the solution for the wave function. As this phase shift is essentially due to the vector potential, the gauge transformation of this potential also only affects the phase of the wave function of the particle. From the physical standpoint, the occurrence of such a phase shift is of minor relevance. In fact, the norm is physically relevant, as it is a candidate for representing the density of the particles in a phenomenological theory. As the norm of the wave function does not depend on its phase, it is clearly invariant under gauge transformations. Notwithstanding, the afore-mentioned phase shift due to gauge transformations turns out to be of interest in the presence of other particles or in the presence of a crystalline environment with which they may interact. In fact, the full set of the coupled equations possibly removes the indeterminacy of the potentials.

From the phenomenological standpoint, the particle may be conceived as an inhomogeneity of the elastic crystal. In this case, the equation that governs its motion is possibly coupled with the equations of configurational mechanics.

2. DYNAMICS OF ELECTROMAGNETIC MATERIALS

The present treatment is based on a classical variational approach. Two configurations, the actual and the reference configuration, denoted by V and v, respectively, are introduced for the body of interest, both embedded in the physical Euclidean space E_3. Here V and v are two simply connected open sets such that $\mathbf{X} \in V$ and $\mathbf{x} \in v$; $\mathbf{x} = \boldsymbol{\chi}(\mathbf{X}, t)$, $t \in \mathbb{R}$, represents the motion, $\mathbf{F}$ the deformation gradient, and $\mathbf{v} = \mathbf{x}^{\cdot} \equiv \mathrm{d}/\mathrm{d}t[\boldsymbol{\chi}(\mathbf{X}, t)]$ the velocity. As usual, det $\mathbf{F} \equiv J > 0$ [12]. A Lagrangian density per unit volume of the reference configuration is introduced in [1–4,7,8,13]

$$L = \mathbb{L}(\mathbf{x}, \mathbf{F}, \mathbf{v}, \phi, (\nabla_R \phi), (\phi^{\cdot}), \boldsymbol{A}, (\nabla_R \boldsymbol{A}), (\boldsymbol{A}^{\cdot}), \mathbb{P}, (\nabla_R \mathbb{P}), \mathbb{P}^{\cdot}, \mathbb{M}, (\nabla_R \mathbb{M}), \mathbb{M}^{\cdot}, \mathbf{X}),$$
$$(2.1)$$

where ϕ and $\boldsymbol{A}$ represent the electromagnetic potentials in the Lagrangian form, ∇_R denotes the gradient operator in V, $\mathbb{P} = J\mathbf{F}^{-1}\mathbf{P}$ and $\mathbb{M} = \mathbf{F}^T \boldsymbol{M} \equiv \mathbf{F}^T(\boldsymbol{M} + \mathbf{v} \times \mathbf{P})$ represent the material polarization and magnetization, respectively. Details are found in [1–4,7,8,14]. The related Euler–Lagrange (E–L) equations provide the Maxwell equations in the Lagrangian form, the balance equation of momentum and additional constitutive-like equations for $\mathbb{P}$ and $\mathbb{M}$. A specific Lagrangian was introduced in aforementioned papers, in which the gradients of polarization and magnetization were neglected. With reference to these equations (although the result easily extends to the case in which the polarization and magnetization gradients are present), we can note that the E–L equations and all related physical quantities are invariant for the following gauge transformations:

$$\boldsymbol{A}^* = \boldsymbol{A} - (\nabla_R f), \tag{2.2}$$

$$\phi^* = \phi + f^{\cdot}, \tag{2.3}$$

where $f(\mathbf{x}(\mathbf{X}, t), t)$ represents an arbitrary scalar function, in fact, the material gauge function.

The momentum and the stress that are related to the aforementioned Lagrangian read, respectively,

$$(\partial \mathbb{L}/\partial \mathbf{v}) = \rho_0 \mathbf{v} + J\varepsilon_0 \mathbf{E} \times \mathbf{B}, \tag{2.4}$$

$$(\partial \mathbb{L}/\partial \mathbf{F}) = -J\mathbf{T}\mathbf{F}^{-T}. \tag{2.5}$$

In Eqs (2.4) and (2.5) ρ_0 denotes the mass density in V; $\mathbf{E}$ and $\mathbf{B}$ are the electric field and the magnetic induction in the current frame, respectively; ε_0 is the dielectric constant of a vacuum; $\mathbf{T}$ is a Cauchy-like stress that explicitly reads [1–4]

$$\mathbf{T} = \varepsilon_0 \mathbf{E} \otimes \mathbf{E} + (\mu_0)^{-1}\mathbf{B} \otimes \mathbf{B} + J^{-1}(\partial W / \partial \mathbf{F})_{\mathrm{ex}} \mathbf{F}^T - \{\tfrac{1}{2}[\varepsilon_0 E^2 + (\mu_0)^{-1}B^2] + \boldsymbol{M} \cdot \mathbf{B}\}\mathbf{I}$$
$$+ \boldsymbol{E} \otimes \mathbf{P} - \boldsymbol{M} \otimes \mathbf{B} + (\mathbf{E} \times \mathbf{B}) \otimes \mathbf{v}, \tag{2.6}$$

where μ_0 is the magnetic permeability of a vacuum, W is the stored energy, $\mathbf{I}$ is the identity tensor, and $\boldsymbol{E} = \mathbf{E} + \mathbf{v} \times \mathbf{B}$.

From the aforementioned E–L equations the configurational material stress and the configurational material momentum density can be derived [8]. These read, respectively,

$$\boldsymbol{b} = \{W - \mathbb{P} \cdot \boldsymbol{E} - \boldsymbol{B} \cdot (\mathbf{V} \times \boldsymbol{D_0}) - \tfrac{1}{2}\rho_0 \mathbf{V} \cdot \mathbf{C}\mathbf{V}\}\mathbf{I} - \mathbf{F}^T(\partial W / \partial \mathbf{F}) + \boldsymbol{E} \otimes \mathbb{P} - \mathbb{M} \otimes \boldsymbol{B}$$
$$+ (\mathbf{V} \times \boldsymbol{D_0}) \otimes \boldsymbol{B} - (\boldsymbol{B} \times \mathbf{V}) \otimes \boldsymbol{D_0} + (\boldsymbol{D_0} \times \boldsymbol{B}) \otimes \mathbf{V}, \tag{2.7}$$

$$\boldsymbol{p} = \rho_0 \mathbf{C}\mathbf{v} + \mathbb{P} \times \boldsymbol{B}, \tag{2.8}$$

where $\mathbf{C} \equiv \mathbf{F}^T\mathbf{F}$, $\mathbf{V} \equiv -\mathbf{F}^{-1}\mathbf{v}$; $\boldsymbol{E}$, $\boldsymbol{B}$, and $\boldsymbol{D}$ are the electric field, the magnetic and the electric induction, respectively, in the Lagrangian form; $\boldsymbol{D_0} \equiv \boldsymbol{D} - \mathbb{P} \equiv J\varepsilon_0 \mathbf{C}^{-1}(\boldsymbol{E} + \mathbf{V} \times \boldsymbol{B})$.

All these quantities are evidently unaffected by the transformations (2.2) and (2.3). This is not the case if the configurational forces and the related equations are introduced as primary equations, independently of the classical balance equations.

2.1. Configurational dynamics and inverse motion

Introduce the inverse motion $\mathbf{X} = \boldsymbol{\chi}^{-1}(\mathbf{x},t)$ and the following Lagrangian density per unit volume of the current configuration:

$$L = L(\phi, (\phi,_t), \nabla\phi, \boldsymbol{A}, (\boldsymbol{A},_t), \nabla\boldsymbol{A}, \mathbb{P}, (\mathbb{P},_t), \nabla\mathbb{P}, \mathbb{M}, (\mathbb{M},_t), \nabla\mathbb{M}, \mathbf{X}, (\mathbf{X},_t), \mathbf{F}^{-1}, \mathbf{x}),$$
$$\tag{2.9}$$

where ∇ denotes the gradient operator in V; $(h,_t) \equiv \partial h(\mathbf{X}(\mathbf{x},t),t)/\partial t$ at fixed $\mathbf{x}$, for any function h. Through a nonstandard variational procedure, it is possible to recover the equations of the configurational electrodynamics and the Maxwell equations, having assumed that $JL = L$. With reference to the specific Lagrangian, introduced in papers [1–4,7,8], these equations are now established in the current frame of reference and eventually transformed in the referential frame. The E–L equations that are related to the Lagrangian (2.9) are invariant with respect to the gauge transformations (2.2) and (2.3), whereas, by contrast, the configurational material stress and momentum are not. In fact, from this nonclassical variational approach these quantities are derived as follows:

$$(\partial L / \partial \mathbf{V}) = \boldsymbol{p} + (\nabla_R A)\boldsymbol{D}, \tag{2.10}$$

$$-J(\partial L / \partial \mathbf{F}^{-1})\mathbf{F}^{-T} = \boldsymbol{b} + (\nabla_R A)(\partial L / \partial \nabla_R A) + \boldsymbol{A}^{\boldsymbol{\cdot}} \otimes \boldsymbol{D}, \tag{2.11}$$

where b and p are defined by the relationships (2.7) and (2.8), respectively [8]. Note that

$$(\nabla_R A) \equiv \mathbf{F}^T (\nabla A) \text{ and } A^{\cdot} \equiv (A_{,t}) + (\nabla A)\mathbf{v}. \qquad (2.12)$$

The second term on the right-hand side of the expression (2.10) and the second and third terms of the expression (2.11) fail to be invariant with respect to the gauge transformations (2.2) and (2.3), as does the invariance of the material momentum and stress. A failure of gauge invariance may also appear in different contexts, which are introduced in the next sections.

3. CLASSICAL GAUGE CONDITIONS AND GAUGE TRANSFORMATIONS

The transformations (2.2) and (2.3) formally reproduce the classical gauge transformations that are inherent in the electromagnetic potentials in the current frame. If φ and $\mathbf{a}$ denote these potentials, the classical gauge transformations read

$$\mathbf{a}^* = \mathbf{a} - \nabla g, \qquad (3.1)$$

$$\varphi^* = \varphi - (g_{,t}), \qquad (3.2)$$

where $g(\mathbf{x},t)$ represents the classical gauge function [15–18]. Note that the space and time differential operators act on in the current configuration here, contrary to the case of section 2, in which the corresponding operators act on in the reference configuration. As is known, the Maxwell equations are invariant with respect to these transformations.

It is worth recalling the relationships between $(\varphi, \mathbf{a})$ and $(\phi, \mathbf{A})$, which are [1]

$$A = \mathbf{F}^T \mathbf{a}, \qquad (3.3)$$

$$\phi = \varphi - \mathbf{v} \cdot \mathbf{a}. \qquad (3.4)$$

In order to determine uniquely the electromagnetic potentials, additional equations are needed. In the classical electromagnetic theory, these are typically given as two alternate conditions, known as the gauge conditions. Specifically, they are either the Coulomb (or transverse condition) or the Lorenz-Lorentz condition [16,17]. If these are combined with the Maxwell equations in homogeneous materials or in a vacuum, the resulting equations are two decoupled hyperbolic wave equations for φ and $\mathbf{a}$. This outcome is remarkable as it addresses the notion of retarded potentials and causality. The equivalence between the Coulomb and the Lorenz-Lorentz condition is discussed by Brill and Goodman [18].

A condition that in the Lagrangian context is similar to the classical Lorenz-Lorentz-like condition is

$$\mathrm{Div}\,A - (c^{-2})\dot{\phi} = 0, \qquad (3.5)$$

where c denotes the light velocity. Unfortunately, this condition leads neither to wave equations nor to any interesting results from the physical standpoint.

To understand better the role of the gauge conditions, the effect of gauge transformations (3.1) and (3.2) on a pointwise charged particle will be examined closely hereafter.

3.1. Pointwise particle in external fields

A pointwise charged particle is acted on by the Lorentz force $q(\mathbf{v}\times\mathbf{B})$. The mechanics of this particle is governed by the Lagrangian [9,11,19]

$$\lambda = \tfrac{1}{2}mv^2 - q(\varphi - \mathbf{v}\cdot\mathbf{a}), \qquad (3.6)$$

where m, q, and $\mathbf{v}$ are the mass, the electric charge, and the velocity of the particle, respectively. With reference to this Lagrangian, the canonical momentum associated with this particle is

$$(\partial\lambda/\partial\mathbf{v}) = \mathbf{p} = m\mathbf{v} + q\mathbf{a}. \qquad (3.7)$$

Note that this momentum is clearly gauge-dependent under the transformations (3.1) and (3.2).

The following Hamiltonian can be associated with the particle, through a classical Legendre transformation:

$$H = [1/(2m)]\mathbf{p}_{\mathbf{a}}^2 + q\varphi, \qquad (3.8)$$

where

$$\mathbf{p}_{\mathbf{a}} = \mathbf{p} - q\mathbf{a} = m\mathbf{v}. \qquad (3.9)$$

The quantum mechanical description of the particle in the presence of electromagnetic fields is based on the Hamiltonian (3.8).

The rules and the assumptions for the quantum mechanical representation of the pointwise particle are summarized and listed hereafter without entering the details. The interested reader is referred to the related literature [9–11,19,20].

3.2. Quantum mechanical description

A complex-valued function $\psi(\mathbf{x},t)$, known as the wave function, is associated with the particle of interest in the quantum mechanical treatment. The norm of the wave function is a candidate for representing the density of a large number of pointwise particles in the Euclidean space. A differential operator $(-i\hbar)\nabla$ is

associated with the momentum $\mathbf{p}$. Here i denotes the imaginary unit and $\hbar$ the reduced Planck's constant. The operator introduced above is assumed to act on the wave function ψ. With reference to Eqs (3.8) and (3.9), a differential operator H that also acts on ψ is associated with H, so that

$$H\psi \equiv \{-(\hbar^2/2m)[\nabla - (\mathsf{i}q/\hbar)\mathbf{a}]^2 + q\varphi\}\psi. \tag{3.10}$$

The final assumption is that the function ψ is governed by the Schrödinger equation, which reads

$$H\psi = \mathsf{i}\hbar(\partial\psi/\partial t). \tag{3.11}$$

In many cases of interest, this equation reduces to the so-called stationary Schrödinger equation [9–11], which is

$$\{-(\hbar^2/2m)[\nabla - (\mathsf{i}q/\hbar)\mathbf{a}]^2 + q\varphi\}\psi = \mathcal{E}\psi. \tag{3.12}$$

Here $\mathcal{E}$ represents the possible eigenvalue of the partial differential equation (3.12) and ψ the related eigenfunction. In the absence of $\mathbf{A}$, Eq. (3.12) modifies accordingly, and if ψ denotes the eigenfunction that is related to the unchanged eigenvalue $\mathcal{E}$, it is straightforward to show that

$$\psi = \psi \exp[(\mathsf{i}q/\hbar)(\mathbf{a}\cdot\mathbf{x})]. \tag{3.13}$$

According to this result, the presence of $\mathbf{A}$ turns out to affect only the phase of the wave function by shifting it for the amount $(q/\hbar)(\mathbf{a}\cdot\mathbf{x})$, whereas the norm of the wave function remains unaltered as $\psi\psi^+ = \psi\psi^+$, with ψ^+ and ψ^+ denoting the complex conjugate of ψ and ψ, respectively.

3.3. Gauge transformations in the momentum and in the Hamiltonian

Under the gauge transformations (3.1) and (3.2) the differential operator associated with $\mathbf{p_a}$ transforms as

$$\mathbf{p_a}^* = -\mathsf{i}\hbar[\nabla - (\mathsf{i}q/\hbar)\mathbf{a} + (\mathsf{i}q/\hbar)\nabla g]. \tag{3.14}$$

The operator H transforms into H^* and Eq. (3.10) transforms accordingly as follows:

$$\{-(\hbar^2/2m)[\nabla - (\mathsf{i}q/\hbar)\mathbf{a} + (\mathsf{i}q/\hbar)\nabla g]^2 + q\varphi\}\psi^* = \mathcal{E}\psi^*, \tag{3.15}$$

with ψ^* being the new eigenfunction that is related with the unchanged eigenvalue $\mathcal{E}$.

It is worth noting that $\psi^* = \psi\exp[(\mathsf{i}q/\hbar)g]$ is a solution of Eq. (3.14). The proof relies on the following two equalities:

$$\mathbf{p_a}^*\psi^* = \exp[(\mathsf{i}q/\hbar)g]\mathbf{p_a}\psi, \tag{3.16}$$

$$(\mathbf{p_a}^*)^2 \psi^* = \exp[(\mathrm{i}q/\hbar)g](\mathbf{p_a})^2 \psi, \tag{3.17}$$

and on the remark that $(\mathbf{p_a})^2$ and $(\mathbf{p_a}^*)^2$ represent the differential operators on the left-hand sides of Eqs (3.12) and (3.15), respectively.

This result shows that the gauge transformations (3.1) and (3.2) produce in the wave function an additional phase shift that is equal to $[(\mathrm{i}q/\hbar)g]$. Therefore, the norm of the wave function is not affected by these gauge transformations [20,21].

4. GAUGE TRANSFORMATIONS INDUCED BY THE QUANTUM MECHANICAL DESCRIPTION

The quantum mechanical treatment expounded above addresses the following additional transformations for the space- and time-differential operators, respectively:

$$\nabla^{\mathrm{G}} = \nabla - (\mathrm{i}q/\hbar)\mathbf{a}, \tag{4.1}$$

$$(\partial/\partial t)^{\mathrm{G}} = (\partial/\partial t) + (\mathrm{i}q/\hbar)\varphi. \tag{4.2}$$

These transformations, known as gauge transformations of the first kind, leave invariant the Maxwell equations and the norm of the wave function of the particle of interest as well. By contrast, they affect the wave phase, as shown in section 3.2.

With reference to the Lagrangian form (2.9) and with reference to the specific Lagrangian such as introduced in previous papers [1–4,7,8,14], it is feasible to extend the transformations (4.1) and (4.2) to the space- and time-differential operators in the reference configuration of a deformable solid and write

$$\nabla_R^{\mathrm{G}} = \nabla_R - (\mathrm{i}q/\hbar)A, \tag{4.3}$$

$$(\mathrm{d}/\mathrm{d}t)^{\mathrm{G}} = (\mathrm{d}/\mathrm{d}t) + (\mathrm{i}q/\hbar)\phi. \tag{4.4}$$

With reference to the relationships (2.11), (3.3), and (3.9), the momentum operator that is associated with $\mathbf{p_a}$ can be written in terms of the Lagrangian potentials ϕ and A as follows:

$$(\mathbf{p_a})_R = -\mathrm{i}\hbar\mathbf{F}^{-T}[\nabla_R - (\mathrm{i}q/\hbar)A]. \tag{4.5}$$

Accordingly, the Hamiltonian operator H is written as

$$H = \{-(\hbar^2/2m)[\nabla_R - (\mathrm{i}q/\hbar)A] \cdot \mathbf{C}^{-1}[\nabla_R - (\mathrm{i}q/\hbar)A] + q\phi. \tag{4.6}$$

It is worth noting that the operator (4.3) is associated with the quantity $(\mathbf{F}^T\mathbf{p_a})$. This quantity, upon which the differential operator (4.6) is based, is a configurational quantity like the material momentum. Hence, according to this

remark, a particle moving in a deformable solid in the presence of electro-magnetic fields would interact with the environment through the material momentum rather than through the physical momentum.

It is also worth comparing the operator (4.6) with that on the left-hand side of Eq. (3.10) and note the role of a metric tensor played in the expression (4.6) by $\mathbf{C}^{-1}$, the inverse right-Cauchy–Green deformation tensor.

5. FINAL REMARKS

In certain circumstances the indeterminacy of physical quantities due to a gauge dependence may address possible coupling with other fields and other equations rather than classical gauge conditions. According to the results of section 4, in the presence of deformations this coupling has to be through material Lagrangian fields and configurational quantities such as the material momentum.

The operators (4.3) and (4.4) play a crucial role in the phenomenological description of superconductors [22]. This issue, however, deserves a more extensive discussion that is beyond the scope of this paper and will possibly be considered in a future work.

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Konfiguratsioonilised jõud dünaamikas ja elektrodünaamikas

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Konfiguratsioonilise jõu mõistet mehaanikas ja termomehaanikas võib lihtsalt laiendada elektromagnetilisele elastsele ainele. Invariantsete muutujate ja variatsioonmeetodi abil teisendatakse Maxwelli võrrandid Lagrange'i (ehk materiaalsele) kujule ja seega seostatakse need mehaanilise tasakaalu seadustega. Selles kontekstis sõltuvad konfiguratsioonilised jõud ja momendid ka elektromagnetväljast ja nimelt Lagrange'i elektromagnetilisest potentsiaalist. Tõstatub küsimus, kas klassikalised standardtingimused on ikka Lagrange'i potentsiaalide korral sobivad. Lõpptulemusena on neid potentsiaale uuritud huvipakkuvate võrrandite täieliku kogumi jaoks.