Supplementary notes for
"Electric displacement as the fundamental variable in electronic-structure calculations"

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1 Introduction

In these supplementary notes, we spell out some details of the definitions of the various electric energy functionals introduced in the main text, and of the Legendre transformations that connect them.

2 Basic relations between energy functionals

2.1 Units

We use Gaussian units so that $\mathbf{D} = \boldsymbol{\mathcal{E}} + 4\pi\mathbf{P}$, etc. In the present Sec. 2 energies like E are energy densities, i.e., energy per unit volume, until specified otherwise. (We change this convention in Sec. 3.)

2.2 Legendre transformations

If the concave-up function $f(x)$ and the concave-down function $g(y)$ are related by

$$g(y) = \min_x \Big[f(x) - yx \Big] \qquad \Leftrightarrow \qquad f(x) = \max_y \Big[g(y) + yx \Big] \tag{1}$$

they are said to form a Legendre-transform pair. We have $dg = -x\,dy$, $df = y\,dx$, so that

$$y = \frac{df}{dx}\,, \qquad x = -\frac{dg}{dy}\,. \tag{2}$$

2.3 Legendre transform between $E(\mathbf{P})$ and $\mathcal{F}(\boldsymbol{\mathcal{E}})$

We start with $E(\mathbf{P})$, the energy as a functional of polarization, which is

$$E(\mathbf{P}) = \min_{v \to \mathbf{P}} E(v) \tag{3}$$

where v refers to all internal degrees of freedom (atomic displacements and wave-function coefficients) and the minimization is carried out over the restricted set of

v having their polarization equal to $\mathbf{P}$. It is not entirely straightforward to compute $E(\mathbf{P})$ in the context of Kohn-Sham (KS) density-functional theory (DFT), but methods for doing so have been introduced by Diéguez and Vanderbilt [1]. To clarify exactly what is, and is not, included in $E(\mathbf{P})$, we note that the local electric field can be decomposed into its macroscopic average, which we denote by $\boldsymbol{\mathcal{E}}$, and the remainder

$$\boldsymbol{\mathcal{E}}_{\text{mic}}(\mathbf{r}) = \sum_{\mathbf{G} \neq 0} \boldsymbol{\mathcal{E}}(\mathbf{G}) \, e^{i\mathbf{G}\cdot\mathbf{r}} \, , \tag{4}$$

which is the part that would come from solving Poisson's equation $\nabla^2\phi = 4\pi\rho$ with *periodic boundary conditions* on ϕ. In particular, $\boldsymbol{\mathcal{E}}_{\text{mic}}(\mathbf{r})$ is defined by Gauss's equation

$$\nabla \cdot \boldsymbol{\mathcal{E}}_{\text{mic}}(\mathbf{r}) = 4\pi\rho(\mathbf{r}) \, , \tag{5}$$

which in reciprocal space reads

$$\boldsymbol{\mathcal{E}}(\mathbf{G} \neq 0) = -i4\pi\rho(\mathbf{G})\frac{\mathbf{G}}{G^2} \, , \qquad \boldsymbol{\mathcal{E}}(\mathbf{G} = 0) = \boldsymbol{\mathcal{E}} \, . \tag{6}$$

$E(\mathbf{P})$ contains the usual ingredients of the KS energy including kinetic and exchange-correlation terms, and its electrostatic part is computed as

$$E_{\text{elec}}(\mathbf{P}) = \frac{1}{8\pi} \sum_{\mathbf{G} \neq 0} \boldsymbol{\mathcal{E}}(\mathbf{G})^2 = 2\pi \sum_{\mathbf{G} \neq 0} \frac{\rho(\mathbf{G})^2}{G^2} \, . \tag{7}$$

Note that the $\mathbf{G} = 0$ term is absent from this sum. Then, only the part of the field energy coming from the integral of $\boldsymbol{\mathcal{E}}_{\text{mic}}(\mathbf{r})^2/8\pi$ is included in $E_{\text{elec}}(\mathbf{P})$. This is just the definition of the energy that is implicit in all ordinary KS DFT calculations.

The Legendre transformation (LT) leading to the electric enthalpy functional $\mathcal{F}(\boldsymbol{\mathcal{E}})$ is then

$$\mathcal{F}(\boldsymbol{\mathcal{E}}) = \min_{\mathbf{P}} \left[E(\mathbf{P}) - \boldsymbol{\mathcal{E}} \cdot \mathbf{P} \right] \qquad \Leftrightarrow \qquad E(\mathbf{P}) = \max_{\boldsymbol{\mathcal{E}}} \left[\mathcal{F}(\boldsymbol{\mathcal{E}}) + \boldsymbol{\mathcal{E}} \cdot \mathbf{P} \right] \tag{8}$$

with

$$\mathbf{P} = -\frac{d\mathcal{F}}{d\boldsymbol{\mathcal{E}}} \, , \tag{9}$$

$$\boldsymbol{\mathcal{E}} = \frac{dE}{d\mathbf{P}} \, . \tag{10}$$

The field energy $\mathcal{E}^2/8\pi$ is still not included in $\mathcal{F}(\boldsymbol{\mathcal{E}})$. In the KS context ($E = E_{\text{KS}}$), calculations at finite electric field are performed by carrying out the minimization

$$\mathcal{F}(\boldsymbol{\mathcal{E}}) = \min_{v} \mathcal{F}(\boldsymbol{\mathcal{E}}, v) = \min_{v} \left[E_{\text{KS}}(v) - \boldsymbol{\mathcal{E}} \cdot \mathbf{P}(v) \right] \tag{11}$$

where the dependence on the internal degrees of freedom v (atomic coordinates and electronic wavefunctions) has been made explicit. Such an approach has been introduced in Refs. [2] and [3] based on the Berry-phase formulation of the polarization $\mathbf{P}(v)$ [4]. Ordinary KS DFT calculations, which implicitly assume a vanishing electric field, just corresponding to minimizing $E_{\text{KS}}(v)$.

2.4 Legendre transform between $\widetilde{\mathcal{F}}(\boldsymbol{\mathcal{E}})$ and $U(\mathbf{D})$

Next, starting with $\mathcal{F}(\boldsymbol{\mathcal{E}})$, we want to do a LT such that the conjugate variable will turn out to be not $\mathbf{P}$, but $\mathbf{D}$. To this end, we define

$$\widetilde{\mathcal{F}}(\boldsymbol{\mathcal{E}}) = \mathcal{F}(\boldsymbol{\mathcal{E}}) - \frac{1}{8\pi}\,\mathcal{E}^2 \tag{12}$$

and also introduce a factor of 4π in the definition of the conjugate variable, leading to the LT pair

$$U(\mathbf{D}) = \max_{\boldsymbol{\mathcal{E}}}\left[\widetilde{\mathcal{F}}(\boldsymbol{\mathcal{E}}) + \frac{1}{4\pi}\mathbf{D}\cdot\boldsymbol{\mathcal{E}}\right] \qquad \Leftrightarrow \qquad \widetilde{\mathcal{F}}(\boldsymbol{\mathcal{E}}) = \min_{\mathbf{D}}\left[U(\mathbf{D}) - \frac{1}{4\pi}\mathbf{D}\cdot\boldsymbol{\mathcal{E}}\right] \tag{13}$$

with

$$\boldsymbol{\mathcal{E}} = 4\pi\frac{dU}{d\mathbf{D}}\,, \tag{14}$$

$$\mathbf{D} = -4\pi\frac{d\widetilde{\mathcal{F}}}{d\boldsymbol{\mathcal{E}}}\,. \tag{15}$$

Using $\widetilde{\mathcal{F}}(\boldsymbol{\mathcal{E}}) = E - \boldsymbol{\mathcal{E}}\cdot\mathbf{P} - \mathcal{E}^2/8\pi$, this last equation gives $\mathbf{D} = \boldsymbol{\mathcal{E}} + 4\pi\mathbf{P}$ as it should.

The functional $U(\mathbf{D})$ is known as the internal energy. When expressed in terms of $\boldsymbol{\mathcal{E}}$ it takes the form $U = \widetilde{\mathcal{F}} + \mathbf{D}\cdot\boldsymbol{\mathcal{E}}/4\pi = E + \mathcal{E}^2/8\pi$. The last term $\mathcal{E}^2/8\pi$ is precisely the field energy coming from the uniform part of the field, which was absent in E, $\mathcal{F}$, and $\widetilde{\mathcal{F}}$. Thus, the the electrostatic part of $U(\mathbf{D})$ is simply

$$U_{\text{elec}}(\mathbf{D}) = \frac{1}{8\pi}\sum_{\mathbf{G}}\mathcal{E}(\mathbf{G})^2 \tag{16}$$

where the sum now runs over all reciprocal lattice vectors including $\mathbf{G} = 0$. In the KS context context, one carries out the minimization

$$U(\mathbf{D}) = \min_{v} U(\mathbf{D}, v) = \min_{v}\left[E_{\text{KS}}(v) + \frac{1}{8\pi}\left(\mathbf{D} - 4\pi\mathbf{P}(v)\right)^2\right]\,. \tag{17}$$

where the dependence on the internal degrees of freedom v has again been made explicit.

2.5 Additional comments

In a similar way, defining $\widetilde{E}(\mathbf{P}) = E(\mathbf{P}) + 2\pi P^2$ and $\widetilde{U}(\mathbf{D}) = U(\mathbf{D}) - D^2/8\pi$, it is possible to set up a LT that directly connects $\widetilde{E}(\mathbf{P}) \Leftrightarrow \widetilde{U}(\mathbf{D})$. We shall not pursue this further here.

For the special case of a linear dielectric medium of polarizability $\chi > 0$ and $\epsilon = 1 + 4\pi\chi$, it follows that

$$E(\mathbf{P}) = E_0 + \frac{1}{2\chi}P^2\,, \tag{18}$$

$$\mathcal{F}(\boldsymbol{\mathcal{E}}) = E_0 - \frac{\chi}{2}\mathcal{E}^2\,, \tag{19}$$

$$\widetilde{\mathcal{F}}(\boldsymbol{\mathcal{E}}) = E_0 - \frac{\epsilon}{2}\,\boldsymbol{\mathcal{E}}^2 \;, \tag{20}$$

$$U(\mathbf{D}) = E_0 + \frac{1}{8\pi\epsilon}\,D^2 \;. \tag{21}$$

From this it is clear that $E(\mathbf{P})$ and $U(\mathbf{D})$ are concave-up functions, while $\mathcal{F}(\boldsymbol{\mathcal{E}})$ and $\widetilde{\mathcal{F}}(\boldsymbol{\mathcal{E}})$ are concave-down.

3 Hellmann-Feynman forces

Here we need to separate v into atomic coordinates R and electronic coordinates w, and minimize only with respect to w. Thus, $\mathcal{F}(\boldsymbol{\mathcal{E}}, R) = \min_w \mathcal{F}(\boldsymbol{\mathcal{E}}, R, w)$, $U(\mathbf{D}, R) = \min_w U(\mathbf{D}, R, w)$, etc. The Hellmann-Feynman argument for $\mathcal{F}$ proceeds by writing

$$\frac{d\mathcal{F}}{dR_j} = \frac{\partial\mathcal{F}}{\partial R_j} + \sum_i \frac{\partial\mathcal{F}}{\partial w_i}\frac{\partial w_i}{\partial R_j} \tag{22}$$

and noting that since $\partial\mathcal{F}/\partial w_i$ is already zero at the electronic minimum, we can drop the second term, getting

$$\frac{d\mathcal{F}}{dR_j} = \frac{\partial E}{\partial R_j} - \boldsymbol{\mathcal{E}} \cdot \frac{\partial\mathbf{P}}{\partial R_j} \;. \tag{23}$$

This formula was derived in Refs. [2, 3]. The first term on the RHS is just the force as calculated in ordinary KS theory. In the case of a plane-wave basis and norm-conserving pseudopotentials, the second term is given just by multiplying the electric field by the *bare* ionic charge of the atom in question, while in ultrasoft-pseudopotential (USPP) and projector-augmented-wave (PAW) approaches, augmentation terms are also needed. A similar argument works for $U(\mathbf{D})$, yielding in the end the same Eq. (23). The same formula can also be derived from the $E(\mathbf{P})$ context, but this time the second term on the RHS of Eq. (23) arises as a constraint force with the electric field $\boldsymbol{\mathcal{E}}$ playing the role of a Lagrange multiplier [2].

4 Strains and strain derivatives

4.1 Introducing reduced field variables

For treating variable strain, it is strongly advantageous to change to internal variables. For *energies*, this means that the energy functionals like E, $\mathcal{F}$, and U will be *energies per unit cell* with units of energy (not energy/volume). Thus, an equation like Eq. (8) becomes $\mathcal{F}(\boldsymbol{\mathcal{E}}) = \min_{\mathbf{P}}[E(\mathbf{P}) - \Omega\,\boldsymbol{\mathcal{E}} \cdot \mathbf{P}]$, where Ω is the cell volume, and similarly elsewhere.

To define internal variables for the fields, we let $\mathbf{a}_j$ be the lattice vectors, and $g_{ij} = \mathbf{a}_i \cdot \mathbf{a}_j$ be the metric. We also let $\mathbf{b}_i$ be dual vectors defined as in the main manuscript, in which the conventional factor of 2π is *not included*, so that $\mathbf{a}_i \cdot \mathbf{b}_j = \delta_{ij}$ and $\mathbf{b}_i \cdot \mathbf{b}_j = (g^{-1})_{ij}$. There are now two choices of reduced variables. Referencing to the reciprocal vectors, we get reduced variables

$$p_i = \Omega\,\mathbf{b}_i \cdot \mathbf{P} \qquad \Longleftrightarrow \qquad \mathbf{P} = \frac{1}{\Omega}\sum_i p_i\,\mathbf{a}_i \;, \tag{24}$$

$$\varepsilon_i = \frac{\Omega}{4\pi}\, \mathbf{b}_i \cdot \boldsymbol{\mathcal{E}} \qquad \Longleftrightarrow \qquad \boldsymbol{\mathcal{E}} = \frac{4\pi}{\Omega} \sum_i \varepsilon_i\, \mathbf{a}_i \ , \tag{25}$$

$$d_i = \frac{\Omega}{4\pi}\, \mathbf{b}_i \cdot \mathbf{D} \qquad \Longleftrightarrow \qquad \mathbf{D} = \frac{4\pi}{\Omega} \sum_i d_i\, \mathbf{a}_i \ . \tag{26}$$

where the inverse relations are given to the right. The relation $\mathbf{D} = \boldsymbol{\mathcal{E}} + 4\pi\mathbf{P}$ becomes $d_i = \varepsilon_i + p_i$. The reduced variables d_i, ε_i, and p_i have units of charge, and are related to the free charge, total charge, and bound charge, respectively, found on a surface of orientation $\hat{\mathbf{b}}_i$ if the fields vanish in the vacuum. Note that, aside from a factor of $e/2\pi$, the p_i are nothing other than the Berry phases ϕ_i as given, e.g., in Eq. (23) of Ref. [5].

The other choice is to refer to the real-space lattice vectors, i.e.,

$$\bar{p}_i = 4\pi\, \mathbf{a}_i \cdot \mathbf{P} \qquad \Longleftrightarrow \qquad \mathbf{P} = \frac{1}{4\pi} \sum_i \bar{p}_i\, \mathbf{b}_i \ , \tag{27}$$

$$\bar{\varepsilon}_i = \mathbf{a}_i \cdot \boldsymbol{\mathcal{E}} \qquad \Longleftrightarrow \qquad \boldsymbol{\mathcal{E}} = \sum_i \bar{\varepsilon}_i\, \mathbf{b}_i \ , \tag{28}$$

$$\bar{d}_i = \mathbf{a}_i \cdot \mathbf{D} \qquad \Longleftrightarrow \qquad \mathbf{D} = \sum_i \bar{d}_i\, \mathbf{b}_i \ . \tag{29}$$

The relation $\mathbf{D} = \boldsymbol{\mathcal{E}} + 4\pi\mathbf{P}$ becomes $\bar{d}_i = \bar{\varepsilon}_i + \bar{p}_i$. The reduced variables $\bar{p}_i$, $\bar{\varepsilon}_i$, and $\bar{d}_i$ have units of electric potential (energy/charge), and are related to the potential drop across the unit cell in direction $\hat{\mathbf{a}}_i$ arising from the displacement field, the total field, and the depolarization field, respectively. They are related to the unbarred quantities by

$$\bar{p}_i = \frac{4\pi}{\Omega}\, g_{ij}\, p_j \ , \qquad \bar{\varepsilon}_i = \frac{4\pi}{\Omega}\, g_{ij}\, \varepsilon_j \ , \qquad \bar{d}_i = \frac{4\pi}{\Omega}\, g_{ij}\, d_j \ , \tag{30}$$

where an implied sum notation is used.

The reduced field variables introduced here are closely related to those discussed in Ref. [2] (see, e.g., Eq. (5) therein) and in Sec. II.C.3 and the Appendix of of Ref. [6]. Eqs. (A4) and (A5) of Ref. [6] introduce field variables that are reminiscent of p_i and $\bar{\varepsilon}_i$ here, but there they were defined in such a way as to coincide with the ordinary $\mathbf{P}$ and $\boldsymbol{\mathcal{E}}$ in the absence of strains or rotations. More closely related are the $\mathbf{P}'$ and ε_μ variables defined in (A13) and (A14) of Ref. [6], which are identical to our p_i and $\bar{\varepsilon}_i$ except for a factor of the charge quantum e.

4.2 Energy functionals and Legendre transformations

The equation analogous to Eq. (8) is

$$\mathcal{F}(\bar{\varepsilon}) = \min_p \left[E(p) - \frac{4\pi}{\Omega}\, g_{ij}\, \varepsilon_i\, p_j \right] = \min_p \left[E(p) - \bar{\varepsilon}_i\, p_i \right] \ . \tag{31}$$

Note that the natural variable of function $\mathcal{F}$ is $\bar{\varepsilon}$, not ε. That is, the variable conjugate to p_i is $(4\pi/\Omega)g_{ij}\varepsilon_j = \bar{\varepsilon}_i$, and this should be the natural variable of the Legendre-transformed function. We also have

$$\bar{\varepsilon}_i = \frac{dE}{dp_i} \ , \qquad p_i = -\frac{d\mathcal{F}}{d\bar{\varepsilon}} \ . \tag{32}$$

Then Eq. (12) becomes

$$\widetilde{\mathcal{F}}(\bar{\varepsilon}) = \mathcal{F}(\bar{\varepsilon}) - \frac{1}{8\pi}\,(g^{-1})_{ij}\,\bar{\varepsilon}_i\,\bar{\varepsilon}_j \tag{33}$$

and Eq. (13) becomes

$$U(d) = \max_{\bar{\varepsilon}}\left[\,\widetilde{\mathcal{F}}(\bar{\varepsilon}) + \bar{\varepsilon}_i\,d_i\,\right] \tag{34}$$

with

$$d_i = -\frac{d\widetilde{\mathcal{F}}}{d\bar{\varepsilon}_i}\,, \qquad \bar{\varepsilon}_i = \frac{dU}{dd_i}\,. \tag{35}$$

$$U = E + \frac{2\pi}{\Omega}\,g_{ij}\,\varepsilon_i\,\varepsilon_i = E + \frac{1}{2}\,\bar{\varepsilon}_i\,\varepsilon_i\,. \tag{36}$$

Thus, the sequence of LT's transforms the natural variables from p_i to $\bar{\varepsilon}_i$ to d_i. This is consistent with physical interpretations, in the following sense.

For the electric enthalpy function, we can imagine a large number N of crystalline cell layers sandwiched between capacitor electrodes with a voltage V applied across the electrodes. If the cell is strained as a result of the applied voltage or for any other reason, the voltage drop per cell will remain V/N, corresponding to a fixed $\bar{\varepsilon}$. It thus makes sense that this is the natural variable for this kind of problem. On the other hand, the variable ε would change with strain, and so is not an appropriate choice of variable in this context.

On the other hand, instead of a capacitor with fixed voltage across the plates, we can imagine a slab with fixed free charge on the surfaces. More specifically, it would be fixed free charge per surface cell, not per unit area, under general strain deformations. This corresponds to fixed d, and so it is natural that $U(d)$ has natural variable d, not $\bar{d}$.

4.3 Strain, strain derivatives, and the stress tensor

Let $\eta_{\mu\nu}$ be the strain tensor, and define the stresses $\sigma_{\mu\nu}^E = \Omega^{-1}dE/d\eta_{\mu\nu}$, $\sigma_{\mu\nu}^{\mathcal{F}} = \Omega^{-1}d\mathcal{F}/d\eta_{\mu\nu}$, $\sigma_{\mu\nu}^{\widetilde{\mathcal{F}}} = \Omega^{-1}d\widetilde{\mathcal{F}}/d\eta_{\mu\nu}$, and $\sigma_{\mu\nu}^U = \Omega^{-1}dU/d\eta_{\mu\nu}$. Then

$$\frac{d\Omega}{d\eta_{\mu\nu}} = \Omega\delta_{\mu\nu} \tag{37}$$

and

$$\frac{dg_{ij}}{d\eta_{\mu\nu}} = a_{i\mu}\,a_{j\nu} + a_{j\mu}\,a_{i\nu}\,. \tag{38}$$

The Hellmann-Feynman theorem applied to the electric enthalphy is

$$\left(\frac{d\mathcal{F}(\bar{\varepsilon},\eta;v)}{d\eta_{\mu\nu}}\right)_{\bar{\varepsilon}} = \frac{\partial\mathcal{F}(\bar{\varepsilon},\eta;v)}{\partial\eta_{\mu\nu}} + \frac{\partial\mathcal{F}(\bar{\varepsilon},\eta;v)}{\partial v}\,\frac{dv}{d\eta_{\mu\nu}} \tag{39}$$

but since $\partial \mathcal{F}/\partial v = 0$ at the equilibrium state of the internal variables $\{v\}$, the second term vanishes. Using $\mathcal{F}(\bar{\varepsilon}) = E(p) - \bar{\varepsilon}_i \, p_i$ we find

$$\frac{d\mathcal{F}(\bar{\varepsilon}, \eta)}{d\eta_{\mu\nu}} = \frac{\partial E(p, \eta)}{\partial \eta_{\mu\nu}} - \bar{\varepsilon}_i \, \frac{\partial p_i}{\partial \eta_{\mu\nu}} \ . \tag{40}$$

But if we assume that the internal variables are atomic coordinates in lattice-vector units and coefficients of plane-wave basis functions in a norm-conserving context, it follows that $\partial p_i/\partial \eta_{\mu\nu} = 0$. Thus

$$\sigma^{\mathcal{F}}_{\mu\nu} = \frac{1}{\Omega} \frac{d\mathcal{F}}{d\eta_{\mu\nu}} = \frac{1}{\Omega} \frac{\partial E}{\partial \eta_{\mu\nu}} = \sigma^E_{\mu\nu} \tag{41}$$

which is just the stress tensor appearing in the usual KS theory. In the case of USPP or PAW approaches, $\partial p_i/\partial \eta_{\mu\nu}$ does not vanish, and augmentation terms need to be included.

For the internal energy, we again use the Hellmann-Feynman argument to write $dU/d\eta_{\mu\nu} = \partial U/\partial d\eta_{\mu\nu}$. Now the natural variable being held fixed is d, and again p is unchanged under a homogeneous strain if the internal variables are chosen properly, and since $d_i = \varepsilon_i + p_i$, this means ε is also fixed (while $\bar{\varepsilon}$ is not). We choose to write Eq. (36) as

$$U(\eta, d) = E + \frac{2\pi}{\Omega} \, g_{ij} \, \varepsilon_i \, \varepsilon_j \tag{42}$$

so that, using Eqs. (37) and (38),

$$\sigma^U_{\mu\nu} = \frac{1}{\Omega} \frac{dU}{d\eta_{\mu\nu}} = \frac{1}{\Omega} \frac{\partial E}{\partial \eta_{\mu\nu}} + \frac{2\pi}{\Omega^2} \Big[2 \, a_{i\mu} \, a_{j\nu} \, \varepsilon_i \, \varepsilon_j - \delta_{\mu\nu} \, g_{ij} \, \varepsilon_i \, \varepsilon_i \Big] \tag{43}$$

or

$$\sigma^U_{\mu\nu} = \sigma^{\mathrm{KS}}_{\mu\nu} + \frac{1}{8\pi} \Big[2 \, \mathcal{E}_\mu \, \mathcal{E}_\nu - \delta_{\mu\nu} \, \mathcal{E}^2 \Big] \tag{44}$$

where the second term is just the Maxwell stress tensor arising from the macroscopic electric field. It is straightforward to show that $\sigma^{\widetilde{\mathcal{F}}} = \sigma^U$. Thus, there are basically two stress tensors, one ($\sigma^{\mathcal{F}}_{\mu\nu} = \sigma^E_{\mu\nu}$) that does not include the Maxwell stress, and another ($\sigma^{\widetilde{\mathcal{F}}} = \sigma^U$) that does.

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