# A parametrized variational principle of nonlinear piezoelectricity

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The variational theory is the theoretical basis of the finite element method, meshfree particle methods and other modern numerical techniques. The present paper establishes a family of variational principles for nonlinear piezoelectricity. A new constitutive relation is suggested, which is deduced as a stationary condition of a generalized variational principle.

**Keywords:** variational theory, piezoelectricity, constitutive equations.

## 1. INTRODUCTION

The phenomenon of piezoelectricity was first discovered by the Curie brothers, Pierre and Jaques in 1880 when Pierre Curie was only 21 years old. The brothers [6] discovered that a crystal of sufficiently low symmetry develops an electric polarization under the influence of an external mechanical force, and about one year later the inverse effect was predicted, i.e. deformation of a crystal experiences an electric field. Piezoelectricity is one of the basic properties of crystals, ceramics, polymers, liquid crystals and some biological tissues (e.g. bone and tendon). Recent interest in piezoelectric materials stems from their potential applications in intelligent structural systems, and piezoelectricity is currently enjoying a greatest resurgence in both fundamental research and technical applications. Much achievement has been made in recently years [1–3, 5, 19, 20, 13, 17].

The rapid development of computer science and the finite element applications reveals the importance of searching for a classical variational principle for the piezoelectricity, which is the theoretical basis of the finite element methods. Recent research also reveals that variational theory is also a powerful tool for meshless particle method or element-free method [9]. The present author has successfully established variational theory for linear piezoelectricity [17] and linear thermopiezoelectricity [13], and in this paper we will establish a variational functional for nonlinear piezoelectricity by the semi-inverse method [7–18].

## 2. MATHEMATICAL FORMULATION

The basic equations for nonlinear piezoelectric media can be written in the forms [5, 13, 17]

*a) Equilibrium equations*

$$\sigma_{ij,j} + f_i = 0, \qquad (1)$$

in which $\sigma_{ij}$ is the symmetric stress tensor, $\sigma_{ij,j} = \partial \sigma_{ij}/\partial x_j$, $f_i$ represents the mechanical body force.

## b) Constitutive equations

$$\sigma_{ij} = a_{ijkl}r_{kl} - e_{mij}E_m + \frac{1}{2}C_{ijklpq}r_{kl}r_{pq} - g_{mijkl}E_m r_{kl} - \frac{1}{2}Q_{ijmn}E_m E_n, \tag{2}$$

$$D_m = \varepsilon_{mj}E_j + e_{mij}r_{ij} + \frac{1}{2}g_{mijkl}r_{ij}r_{kl} + \frac{1}{2}\varepsilon_{mnl}E_n E_l + Q_{mnij}E_n r_{ij}, \tag{3}$$

in which $r_{ij}$ is the symmetric strain tensor $D_i$ is the vector of the electric displacement, $E_i$ is the vector of the electric field. $a_{ijkl}$ and $C_{ijklpq}$ – second and third-order moduli of elasticity are respectively fourth and sixth-rank tensors being measured on condition that electric field is constant(zero); $\varepsilon_{mn}$ and $\varepsilon_{mnl}$ – second and third-order dielectric penetrabilities which are second and third-rank tensors being measured on condition that deformation is constant(zero); $e_{mij}$ are the piezoelectric moduli which are third-rank tensor components; $g_{mijkl}$ are elastoelectric coefficients which are fifth-rank tensor components; $Q_{ijmn}$ are electrostriction coefficients which are fourth-rank tensor components.

For linear piezoelectric media it follows

$$C_{ijklpq} = 0, \quad g_{mijkl} = 0, \quad Q_{ijmn} = 0, \quad \text{and} \quad \varepsilon_{mnl} = 0.$$

## c) Strain-displacement relations

$$r_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}), \tag{4}$$

where $u_i$ is the vector of the elastic displacement.

## d) Maxwell's equations for piezoelectric materials

$$D_{i,i} = 0 \quad \text{or} \quad \nabla \cdot \mathbf{D} = 0, \tag{5}$$

$$E_i = \Phi_{,i} \quad \text{or} \quad \mathbf{E} = \nabla\Phi, \tag{6}$$

where $\Phi$ is the electric potential.

## f) Boundary conditions

On $A_1$ surface displacement is prescribed

$$u_i = \overline{u}_i \qquad (\text{on } A_1) \tag{7}$$

and on the complementary part $A_2$ the traction is given

$$\sigma_{ij}n_j = \overline{p}_i \qquad (\text{on } A_2) \tag{8}$$

where $A_1 + A_2 = A$ covers the total boundary surface.

Suppose that on $A_3$, the electric potential and on $A_4$, the surface charges are given as

$$\Phi = \overline{\Phi} \qquad (\text{on } A_3) \tag{9}$$

$$D_i n_i = \overline{D}_n \qquad (\text{on } A_4) \tag{10}$$

where $A_3 + A_4 = A$ covers the total boundary surface.

Our aim of this paper is to establish a generalized variational principle for the above discussed problem, whose stationary conditions should satisfy all the field equations and boundary conditions. The present paper deals in facts with the very difficult inverse problem of the calculus of variations, and the semi-inverse method of establishing generalized variational principle will be applied hereby.

## 3. GENERALIZED VARIATIONAL PRINCIPLE

The traditional approach to establishing generalized variational principles is the well-known Lagrange multiplier method. By such method the constraints of a known functional can be eliminated. In sometime, however, the variational crisis (some multipliers become zero) might occur during the derivation of generalized variational principles [4, 11, 12]. On the other hand, the Lagrange multiplier method is not valid to deduce a variational representation directly from the field equations and boundary conditions for the present problem.

We will use the semi-inverse method [7–18] to search a variational functional for the present study. The basic idea of the semi-inverse method is to construct an energy-like integrate with some an unknown function as a trial-functional. There are various methods to construct trial-functionals for practical problems. Details can be found in Ref. [7].

If we want to establish a functional with 6 kinds of independent variations $(\sigma_{ij}, r_{ij}, u_i, D_i, E_i$ and $\Phi)$, we can construct an energy-like trial-functional as follows

$$J(\sigma_{ij}, r_{ij}, u_i, D_i, E_i, \Phi) = \iiint L\,dV + IB, \tag{11a}$$

where

$$L = \sigma_{ij} r_{ij} + F, \tag{11b}$$

$$IB = \sum_{k=1}^{4} \iint_{A_k} G_k\,dA, \tag{11c}$$

in which $F$ and $G_i$ $(i = 1 \sim 4)$ are unknowns, $L$ is a trial-Lagrangian.

Now we will identify the unknowns step by step.

**Step 1**

Calculating variation of functional (11) with respect to $\sigma_{ij}$ results in the following trial-Euler equation:

$$r_{ij} + \frac{\delta F}{\delta \sigma_{ij}} = 0, \tag{12}$$

where $\delta F / \delta \Psi$ is call variational derivative, which is defined in $xyz$ coordinates as

$$\frac{\delta F}{\delta \Psi} = \frac{\partial F}{\partial \Psi} - \frac{\partial}{\partial x}\left(\frac{\partial F}{\partial \Psi_x}\right) - \frac{\partial}{\partial y}\left(\frac{\partial F}{\partial \Psi_y}\right) - \frac{\partial}{\partial z}\left(\frac{\partial F}{\partial \Psi_z}\right).$$

We search for such an $F$ that the above trial-Euler Eq. (12) satisfies one of its field equations, saying, the Eq. (4).
If

$$\frac{\delta F}{\delta \sigma_{ij}} = -\frac{1}{2}(u_{i,j} + u_{j,i}), \tag{13}$$

then the Eq. (12) turns out to be (4). From (13) the unknown $F$ can be identified as

$$F = -\frac{1}{2}\eta \sigma_{ij}(u_{i,j} + u_{j,i}) + \mu \sigma_{ij,j} u_i + F_1, \tag{14}$$

where $\eta$ and $\mu$ are constants and should satisfy the identity $\eta + \mu = 1$, $F_1$ is a newly introduced unknown function, which should be free from $\sigma_{ij}$.

The trial-Lagrangian, therefore, can be renewed as follows

$$L = \sigma_{ij}r_{ij} - \frac{1}{2}\eta\sigma_{ij}(u_{i,j} + u_{j,i}) + \mu\sigma_{ij,j}u_i + F_1. \tag{15}$$

**Step 2**

Making the renewed trial-functional (11) stationary with respect to $u_i$ yields the following trial-Euler equation

$$(\eta + \mu)\sigma_{ij,j} + \frac{\delta F_1}{\delta u_i} = 0. \tag{16}$$

Supposing that the above equation is the field Eq. (1), we can identify the unknown $F_1$ as follows

$$F_1 = f_i u_i + F_2, \tag{17}$$

where $F_2$ is free from $u_i$.

The substitution of the Eq. (17) into the trial-Lagrangian (15) yields a new one, which reads

$$L = \sigma_{ij}r_{ij} - \frac{1}{2}\eta\sigma_{ij}(u_{i,j} + u_{j,i}) + \mu\sigma_{ij,j}u_i + f_i u_i + F_2. \tag{18}$$

**Step 3**

The stationary condition with respect to $r_{ij}$ reads

$$\sigma_{ij} + \frac{\delta F_2}{\delta r_{ij}} = 0. \tag{19}$$

We set

$$\frac{\delta F_2}{\delta r_{ij}} = -(a_{ijkl}r_{kl} - e_{mij}E_m + \frac{1}{2}C_{ijklpq}r_{kl}r_{pq} - g_{mijkl}E_m r_{kl} - \frac{1}{2}Q_{ijmn}E_m E_n) \tag{20}$$

in Eq. (19), so that the Euler equation (19) becomes (2). From (20), one can readily obtain

$$F_2 = -\frac{1}{2}r_{ij}a_{ijkl}r_{kl} + r_{ij}e_{mij}E_m - \frac{1}{6}r_{ij}C_{ijklpq}r_{kl}r_{pq}$$
$$+ \frac{1}{2}r_{ij}g_{mijkl}E_m r_{kl} + \frac{1}{2}r_{ij}Q_{ijmn}E_m E_n + F_3, \tag{21}$$

The trial-Lagrangrian (18), therefore, can be further renewed as

$$L = \sigma_{ij}r_{ij} - \frac{1}{2}\eta\sigma_{ij}(u_{i,j} + u_{j,i}) + \mu\sigma_{ij,j}u_i + f_i u_i - \frac{1}{2}r_{ij}a_{ijkl}r_{kl} + r_{ij}e_{mij}E_m$$
$$- \frac{1}{6}r_{ij}C_{ijklpq}r_{kl}r_{pq} + \frac{1}{2}r_{ij}g_{mijkl}E_m r_{kl} + \frac{1}{2}r_{ij}Q_{ijmn}E_m E_n + F_3 \tag{22}$$

where $F_3$ is free from $r_{ij}$.

**Step 4**

Processing as the previous steps, the trial-Euler equation for $\delta E_m$ reads

$$r_{ij}e_{mij} + \frac{1}{2}r_{ij}g_{mijkl}r_{kl} + r_{ij}Q_{ijmn}E_m + \frac{\delta F_3}{\delta E_m} = 0. \tag{23}$$

We set

$$\frac{\delta F_3}{\delta E_m} = -D_m + \varepsilon_{mj}E_j + \frac{1}{2}\varepsilon_{mnl}E_n E_l \tag{24}$$

so that Eq. (23) satisfies the field Eqs. (3). From (24) we have

$$F_3 = -E_m D_m + \frac{1}{2} E_m \varepsilon_{mj} E_j + \frac{1}{6} E_m \varepsilon_{mnl} E_n E_l + F_4. \tag{25}$$

We, therefore, obtain the following renewed trial-Lagrange function

$$
\begin{aligned}
L = {} & \sigma_{ij} r_{ij} - \frac{1}{2} \eta \sigma_{ij} (u_{i,j} + u_{j,i}) + \mu \sigma_{ij,j} u_i + f_i u_i - \frac{1}{2} r_{ij} a_{ijkl} r_{kl} + r_{ij} e_{mij} E_m \\
& - \frac{1}{6} r_{ij} C_{ijklpq} r_{kl} r_{pq} + \frac{1}{2} r_{ij} g_{mijkl} E_m r_{kl} + \frac{1}{2} r_{ij} Q_{ijmn} E_m E_n \\
& - E_m D_m + \frac{1}{2} E_m \varepsilon_{mj} E_j + \frac{1}{6} E_m \varepsilon_{mnl} E_n E_l + F_4,
\end{aligned}
\tag{26}
$$

where $F_4$ is free from $E_i$.

## Step 5

The stationary condition for $\delta D_i$ and $\delta \Phi$ read

$$-E_i + \frac{\delta F_4}{\delta D_i} = 0, \tag{27}$$

$$\frac{\delta F_4}{\delta \Phi} = 0. \tag{28}$$

The above two equations should satisfy the Eqs. (6) and (5) respectively. So we can determine the unknown $F_4$ as

$$F_4 = \xi D_i \Phi_{,i} - \varsigma D_{i,i} \Phi \tag{29}$$

with $\xi + \varsigma = 1$, where $\xi$ and $\varsigma$ are constants. The Lagrangrian, therefore, has the following final form

$$
\begin{aligned}
L = {} & \sigma_{ij} r_{ij} - \frac{1}{2} \eta \sigma_{ij} (u_{i,j} + u_{j,i}) + \mu \sigma_{ij,j} u_i + f_i u_i - \frac{1}{2} r_{ij} a_{ijkl} r_{kl} + r_{ij} e_{mij} E_m \\
& - \frac{1}{6} r_{ij} C_{ijklpq} r_{kl} r_{pq} + \frac{1}{2} r_{ij} g_{mijkl} E_m r_{kl} + \frac{1}{2} r_{ij} Q_{ijmn} E_m E_n - E_m D_m \\
& + \frac{1}{2} E_m \varepsilon_{mj} E_j + \frac{1}{6} E_m \varepsilon_{mnl} E_n E_l + \xi D_i \Phi_{,i} - \varsigma D_{i,i} \Phi.
\end{aligned}
\tag{30}
$$

Applying the Green's theory, on the boundaries, we obtain the following trial-Euler equations:

$$\delta u_i: \quad -\eta \sigma_{ij} n_j + \frac{\partial G_k}{\partial u_i} = 0 \quad (k = 1 \sim 2), \tag{31}$$

$$\delta \sigma_{ij}: \quad \mu u_i n_j + \frac{\partial G_k}{\partial \sigma_{ij}} = 0 \quad (k = 1 \sim 2), \tag{32}$$

$$\delta \Phi: \quad \xi D_i n_i + \frac{\partial G_k}{\partial \Phi} = 0 \quad (k = 3 \sim 4), \tag{33}$$

$$\delta D_i: \quad -\varsigma \Phi n_i + \frac{\partial G_k}{\partial D_i} = 0 \quad (k = 3 \sim 4). \tag{34}$$

On $A_1$, the above trial-Euler equations should satisfy the boundary condition (7) or an identity, so the unknown $G_1$ can be identified as follows

$$G_1 = \eta \sigma_{ij} n_j (u_i - \bar{u}_i) - \mu \sigma_{ij} n_j \bar{u}_i. \tag{35}$$

It is easy to prove that the stationary conditions for $\delta u_i$ and $\delta \sigma_{ij}$ on the $A_1$ are an identity and the Eq. (7) respectively.

By the same manipulation, we have

$$G_2 = \eta \bar{p}_i u_i - \mu u_i (\sigma_{ij} n_j - \bar{p}_i), \tag{36}$$

$$G_3 = -\xi (\Phi - \overline{\Phi}) D_i n_i + \varsigma \overline{\Phi} D_i n_i, \tag{37}$$

$$G_4 = -\xi \Phi \overline{D}_n + \varsigma \Phi (D_i n_i - \overline{D}_n). \tag{38}$$

**Note**: If the electrical and heat effects are not taken into consideration, then we have

$$J(\sigma_{ij}, r_{ij}, u_i) = \int L' dV\, dt + IB' \tag{39a}$$

where

$$L' = \sigma_{ij} \gamma_{ij} - \frac{1}{2} \eta \sigma_{ij} (u_{i,j} + u_{j,i}) + \mu \sigma_{ij,j} u_i - \frac{1}{2} \gamma_{ij} a_{ijkl} \gamma_{kl} + f_i u_i + \frac{1}{2} \rho u_{i,t} u_{i,t} \tag{39b}$$

and

$$IB' = \iint_{A_1} \{\eta \sigma_{ij} n_j (u_i - \bar{u}_i) - \mu \sigma_{ij} n_j \bar{u}_i\} dA + \iint_{A_2} \{\eta \bar{p}_i u_i - \mu u_i (\sigma_{ij} n_j - \bar{p}_i)\} dA. \tag{39c}$$

Setting $\eta = 1$, $\mu = 0$ in Eq. (39) results in the well-known Hu-Washizu principle of elasticity [21]. So we obtain Hu-Washizu-like principle for nonlinear piezoelectricity by setting $\eta = 1$, $\mu = 0$, $\xi = 1$, $\varsigma = 0$. The Lagrangian of Hu-Washizu-like principle can be expressed as

$$L_1 = \sigma_{ij} \left[ r_{ij} - \frac{1}{2} (u_{i,j} + u_{j,i}) \right] + f_i u_i - \frac{1}{2} r_{ij} a_{ijkl} r_{kl} + r_{ij} e_{mij} E_m$$

$$- \frac{1}{6} r_{ij} C_{ijklpq} r_{kl} r_{pq} + \frac{1}{2} r_{ij} g_{mijkl} E_m r_{kl} + \frac{1}{2} r_{ij} Q_{ijmn} E_m E_n - D_m (E_m - \Phi_{,m})$$

$$+ \frac{1}{2} E_m \varepsilon_{mj} E_j + \frac{1}{6} E_m \varepsilon_{mnl} E_n E_l. \tag{40}$$

For simplicity, we introduce a generalized strain-piezoelectric energy density defined as

$$A = \frac{1}{2} r_{ij} a_{ijkl} r_{kl} - r_{ij} e_{mij} E_m + \frac{1}{6} r_{ij} C_{ijklpq} r_{kl} r_{pq} - \frac{1}{2} r_{ij} g_{mijkl} E_m r_{kl}$$

$$- \frac{1}{2} r_{ij} Q_{ijmn} E_m E_n - \frac{1}{2} E_m \varepsilon_{mj} E_j - \frac{1}{6} E_m \varepsilon_{mnl} E_n E_l. \tag{41}$$

From (41), we have the following relations

$$\frac{\partial A}{\partial r_{ij}} = a_{ijkl} r_{kl} - e_{mij} E_m + \frac{1}{2} C_{ijklpq} r_{kl} r_{pq} - g_{mijkl} E_m r_{kl} - \frac{1}{2} Q_{ijmn} E_m E_n = \sigma_{ij}, \tag{42}$$

$$\frac{\partial A}{\partial E_m} = -r_{ij} e_{mij} - \frac{1}{2} r_{ij} g_{mijkl} r_{kl} - r_{ij} Q_{ijmn} E_n - \varepsilon_{mj} E_j - \frac{1}{2} \varepsilon_{mnl} E_n E_l = -D_m. \tag{43}$$

Constraining the functional by selectively field equations (1), (6) and boundary conditions (7) and (9), we can obtain

$$J(u_i, \Phi) = \iiint (A - f_i u_i) dV - \iint_{A_2} \bar{p}_i u_i dA + \iint_{A_2} \Phi \overline{D}_n dA, \tag{44}$$

which is the minimum principle for nonlinear piezoelectricity.

## 4. CONCLUSION

In the paper, we have succeeded in obtaining a generalized variational principle with some arbitrary constants, from which various variational principles (including the minimum principle) can be obtained by constraining the functional by selectively field equations or boundary/initial conditions.

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