On a type of non-classical boundary condition of Lagrangian field

Zaixing Huang
State Key Laboratory of Mechanics and Control of Mechanical Structures
Nanjing University of Aeronautics and Astronautics
Yudao Street 29, Nanjing, 210016, P R China
E-mail: huangzx@nuaa.edu.cn

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Abstract

In the framework of the Lagrangian field theory, we derive a type of new non-classical natural boundary condition to be correlated with the mean curvature of boundary surface. Under the condition of homogeneity and isotropy, this type of boundary condition can be simplified into the Tolman’s formula in which the size effect of surface tension is prescribed.

Key words: natural boundary condition, surface effect, Lagrangian field theory, Tolman’ formula, size effect

1 Introduction

Conventionally, boundary conditions of partial differential equation can be categorized into four types: Dirichlet, Neumann, Robin and periodic boundary condition. All of these boundary conditions are determined in terms of a self-adjoint extension of the differential operator of field, rather than concerning the surface effects of boundary. With entering micro/nano-scale, the surface effect has to be taken into account in the behaviors of material. This causes non-classical boundary conditions to appear in the boundary value problems of partial differential equations. Some typical examples can be found in capillary wave, surface elasticity and phase transition etc.

The first non-classical boundary condition is the Young-Laplace’s equation [1]. As a traction boundary condition, it was used to solve the oscillation of spherical droplet [2] and fission of nucleus [3]. Gurtin and Murdoch extended the Young-Laplace equation into the generalized Young-Laplace equation so as to characterize the surface of elastic solid [4]. Further, Steigmann and Ogden proposed reinforced boundary condition by taking into account the bending stiffness of the surface film [5]. Zhu, Ru and Chen discussed non-uniqueness of boundary value problems based on the generalized Young-Laplace equation [6]. Javili and Mosler et al revisited and carefully examined the surface/interface elasticity theory. They established a consistent linearized interface elasticity theory [7].

As a traction boundary condition, the generalized Young-Laplace equation has been applied to investigate physical behaviors of nano-structured materials. The relevant literatures can be found in the reviews by Wang et al. [8] and Sun [9]. Recently, Figotin and Reyes advanced a non-classical boundary condition, whose feature consists in that the boundary fields may differ from the boundary limit of the interior fields so as to characterize the interactions between the boundary and the interior fields [10]. Huang proposed a Shape-dependent natural boundary condition [11]. However, there is an error in [11] due to mistakenly using the divergence theorem on surface. So far, many studies have shown that the influences of surface effect on physical behaviors of field can be characterized by the boundary condition. However, how to introduce the surface effect in the boundary condition is still a problem awaiting to be further explored. So the aim of this paper is to propose a type of non-classical boundary condition that can simultaneously characterize the surface effect and its size effect in the framework of the Lagrangian field theory.

The paper is outlined as follows. In Section 2, we introduce a surface Lagrangian to describe the surface effect of field. The Lagrangian equation and curvature-dependent natural boundary condition are derived. In Section 3, by simplification to the curvature-dependent natural boundary condition, the Tolman’ formula is given. Finally, we summarize and comment on the results in this paper.

Notation: The index rules and summation convention are adopted. Latin indices run from 1 to 3. The Greece letter $\Omega$ stands for a bounded domain of $\mathbb{R}^3$, and $\partial \Omega$ is the boundary surface of $\Omega$. The covariant derivative with respect to coordinates is represented by the symbol $\partial_i$. The contravariant derivative operator corresponding to $\partial_i$ is denoted by $\partial^i = g^{ij} \partial_j$, where $g^{ij}$ is the metric tensor. The symbol $\partial_A$ ($A = 1, 2$) or $\nabla_s$ is the surface gradient.
operator defined on $\partial \Omega$. The derivative with respect to time is denoted by an upper dot, e.g., $\dot{a} = da/dt$. Other symbols will be introduced in the text where they appear for the first time.

2 Boundary condition of Lagrangian field

Let $x = \{x^i\}$ be a 3-dimensional position vector in $\Omega$ and $t \in [t_0, t_1]$ be time. A vector field defined on $[t_0, t_1] \cup \Omega$ is denoted by $\phi_k = \phi_k(t, x)$. The Lagrangian of the field $\phi$ is written as $L = L(\phi, \dot{\phi}, \partial \phi_k)$. Let spatial domain $\Omega$ occupied by $\phi_k$ be bounded and the surface $\partial \Omega$ of $\Omega$ be a smooth surface. We believe that physical behaviors of $\phi_k$ in the interior of $\Omega$ are different from those on the boundary of $\Omega$. An additional Lagrangian $\Gamma$ is used to characterize the physical behaviors of $\phi_k$ on the boundary surface $\partial \Omega$. We refer to $\Gamma$ as the surface Lagrangian, which is supposed to have the form below

$$\Gamma = \Gamma_0(\phi, \dot{\phi}, \partial \phi_k) + \nabla_v \cdot S(\phi, \dot{\phi}, \partial \phi_k). \quad (1)$$

On $\partial \Omega$, the vector field $S(\phi, \dot{\phi}, \partial \phi_k)$ can be decomposed into $S(\phi, \dot{\phi}, \partial \phi_k) = S^A(\phi, \dot{\phi}, \partial \phi_k)g_A + \Gamma(\phi, \dot{\phi}, \partial \phi_k)n$, where $g_A$ is the unit base vector defined on the tangent plane of $\partial \Omega$ and $n$ the unit normal vector. As thus, Eq.(1) is rewritten as

$$\Gamma = \Gamma_0 + \partial_h S^A + 2H\dot{\Gamma}, \quad (2)$$

where $H$ is the mean curvature of $\partial \Omega$. In general, it is explicitly independent of time. In the process to derive Eq.(2), we use the identity $\nabla_v \cdot n = -2H$ [12, 13]. By Eq.(2), the action of field can be represented as

$$A[\phi_k] = \int_{t_0}^{t_1} \int_{\Omega} L(\phi, \dot{\phi}, \partial \phi_k) dv dt + \int_{t_0}^{t_1} \int_{\partial \Omega} \Gamma(\phi, \dot{\phi}, \partial \phi_k) d\sigma dt$$

$$= \int_{t_0}^{t_1} \int_{\Omega} L dv dt + \int_{t_0}^{t_1} \int_{\partial \Omega} (\Gamma_0 + \partial_h S^A + 2H\dot{\Gamma}) d\sigma dt$$

$$= \int_{t_0}^{t_1} \int_{\Omega} L dv dt + \int_{t_0}^{t_1} \int_{\partial \Omega} (\Gamma_0 - 2H\dot{\Gamma}) d\sigma dt, \quad (3)$$

where $dv$ and $d\sigma$ are a volume measure in $\Omega$ and an area measure on $\partial \Omega$, respectively. Let $\delta \phi_k(t_0) = \delta \phi_k(t_1) = 0$. Taking the variation of $A[\phi_k]$ leads to

$$\delta A = \int_{t_0}^{t_1} \int_{\Omega} \left\{ \frac{\partial L}{\partial \phi_k} \frac{d}{dt} \frac{\partial L}{\partial (\partial \phi_k)} - \frac{d}{dt} \frac{\partial L}{\partial (\partial \phi_k)} \right\} \delta \phi_k dv(x^k) dt$$

$$+ \int_{t_0}^{t_1} \int_{\Omega} \left\{ \frac{\partial L}{\partial (\partial \phi_k)} + \frac{\partial L}{\partial \dot{\phi}_k} \frac{d}{dt} \frac{\partial L}{\partial \dot{\phi}_k} - \frac{d}{dt} \frac{\partial L}{\partial \dot{\phi}_k} \right\} \delta \phi_k da(x^k) dt$$

$$- \int_{t_0}^{t_1} \int_{\partial \Omega} 2H \frac{\partial \Gamma}{\partial \phi_k} \frac{d}{dt} \frac{\partial \Gamma}{\partial \phi_k} - \frac{d}{dt} \frac{\partial \Gamma}{\partial \phi_k} - \frac{d}{dt} \frac{\partial \Gamma}{\partial \dot{\phi}_k} \frac{d}{dt} \frac{\partial \Gamma}{\partial \dot{\phi}_k} \right\} \delta \phi_k da(x^k) dt + \int_{t_0}^{t_1} \int_{\partial \Omega} 2 \frac{\partial \Gamma}{\partial \phi_k} \frac{\partial \Gamma}{\partial \dot{\phi}_k} \frac{d}{dt} \frac{\partial \Gamma}{\partial \dot{\phi}_k} \delta \phi_k da(x^k) dt, \quad (4)$$

where $n_k$ denotes the unit normal vector on $\partial \Omega$. The Hamilton’s principle asserts that $\delta A[\phi_k] = 0$. Therefore, according to the fundamental lemma of variation, we have

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{\phi}_k} - \frac{d}{dt} \frac{\partial L}{\partial \phi_k} = 0, \quad x^k \in \Omega. \quad (5)$$

Natural boundary condition:

$$\frac{\partial L}{\partial \phi_k} \frac{d}{dt} \frac{\partial L}{\partial \dot{\phi}_k} - \frac{d}{dt} \frac{\partial L}{\partial \phi_k} = 0, \quad x^k \in \partial \Omega. \quad (6)$$

Eq.(5) and (6) show that the surface Lagrangian has no influence on the Euler-Lagrange equation, but it contributes to the natural boundary condition and causes the natural boundary condition to be correlated with the mean curvature and its gradient of boundary surface. As a boundary condition, Eq.(6) is universal but complicated. Next, we turn to simplification to Eq.(6).

3 Simplification of boundary condition: Tolman’s formula

In the classical theory of partial differential equation, the boundary conditions usually exhibit two features: (1) they are rate-independent; and (2) they have lower order derivatives than differential equations themselves. If such two features are inherited in Eq.(6), $\Gamma_0(\phi, \phi, \partial \phi_k)$ and $\Gamma(\phi, \dot{\phi}, \partial \phi_k)$ necessarily take the form below

$$\Gamma_0(\phi, \dot{\phi}, \partial \phi_k) = \mathcal{P}(\phi) + \chi^A \partial_1 \gamma_0 \phi_k + \chi^A \partial_1 \phi_k. \quad (7)$$
Let us set a local coordinate system with the base vectors \( \mathbf{e}_A \) and \( \mathbf{e}_B \). We shall discuss them more fully later on.

where \( \gamma(\phi_k) \) and \( \dot{\gamma}(\phi_k) \) are two surface potential energy density functions, while \( \chi^{AB} \) and \( \kappa^{AB} \) are two surface stresses conjugated to \( \partial_A \phi_k \). The surface stress \( \partial_A \phi_k \) and \( \kappa^{AB} \) are determined by physical property of boundary surface. We shall discuss them more fully later on.

Let us set a local coordinate system with the base vectors \( (\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3) = (\mathbf{g}_4, \mathbf{n}) \), where \( \mathbf{g}_4 (A = 1, 2) \) is the the covariant base vectors corresponding to the curvilinear coordinate on the surface \( \partial \Omega \) and \( \mathbf{n} \) the unit normal vector.

In such a coordinate system, Eq.(9) can be expanded into

\[
\frac{\partial L}{\partial (\partial_j \phi_k)} n_j = \chi^{AC} \frac{\partial \phi_C}{\partial \phi_k} + 2H \frac{\partial \gamma}{\partial \phi_k} - \chi^{AC} \kappa^{AB} \frac{\partial \phi_C}{\partial \phi_k} - 2\kappa^{AC} \partial_A H, \quad x^k \in \partial \Omega, \tag{9}
\]

where \( \gamma(\phi_k) \) and \( \dot{\gamma}(\phi_k) \) are two surface potential energy density functions, while \( \chi^{AB} \) and \( \kappa^{AB} \) are two surface stresses conjugated to \( \partial_A \phi_k \).

Furthermore, if the field is also isotropic, we have \( \chi^{AB} = \sigma g^{AB} \), \( \chi^{AC} = 0 \), \( \kappa^{AB} = \tau g^{AB} \) and \( \kappa^{AC} = 0 \). Therefore, Eq.(13) and (14) lead to

\[
\frac{\partial L}{\partial (\partial_j \phi_k)} n_j = \sigma g^{BC} \frac{\partial \phi_C}{\partial \phi_k} + 2H \frac{\partial \gamma}{\partial \phi_k} - \tau \sigma g^{BC} - 2\tau \kappa^{AC} \partial_A H, \quad x^k \in \partial \Omega, \tag{15}
\]

Here, \( \sigma \) and \( \tau \) are two surface tensions, and \( g^{AB} \) is the metric tensor of surface. It is easy to see that Eq.(16) can be equivalently represented as

\[
\frac{\partial L}{\partial (\partial_j \phi_k)} n_j n_k = 2\sigma H - \frac{\partial \gamma}{\partial \phi_k} + 4H \frac{\partial \gamma}{\partial \phi_k} - 2\tau \kappa^{AC} \partial_A H, \quad x^k \in \partial \Omega. \tag{17}
\]

Consider a liquid droplet. Let \( \phi_k \) be a displacement field. Because the surface potential energies are invariant under the transformation of rigid motion, it is necessary that \( \dot{\gamma}(\phi_k) \) and \( \dot{\gamma}(\phi_k) \) are independent of \( \phi_k \). As a result, Eq.(18) and (17) reduce to

\[
\frac{\partial L}{\partial (\partial_j \phi_k)} n_j n_k = 2\sigma H - 2\tau H \frac{\partial \gamma}{\partial \phi_k} - 2\tau \kappa^{AC} \partial_A H, \quad x^k \in \partial \Omega. \tag{18}
\]

In physics, the right-side term of Eq.(19) represents the pressure, denoted by \( \Delta p \). Let \( \delta = 2\tau / \sigma \). Clearly, it has the dimension of length. As thus, Eq.(19) is rewritten as

\[
\Delta p = 2\sigma H (1 - \delta H), \quad x^k \in \partial \Omega. \tag{20}
\]
Eq. (20) is just the Tolman’s formula [14]. It has been extensively applied to analyze the surface size effects of micro/nano-scale liquid droplet and solid particle [15, 16]. Interestingly, if we assume \( \hat{\Gamma} = \delta \Gamma_0 / 2 \), Eq. (6) will lead to

\[
\frac{\partial L}{\partial (\partial_j \phi_k)} n_j = (1 - \delta H)(\frac{d}{dt} \frac{\partial \Gamma_0}{\partial \phi_k} + \frac{\partial}{\partial (\partial_k \phi)} \frac{\partial \Gamma_0}{\partial \phi_k} - \frac{\partial \Gamma_0}{\partial (\partial_k \phi)} \partial A(\delta H), \quad x^k \in \partial \Omega. \tag{21}
\]

Eq. (21) can be regarded as a extension of the Tolman formula.

4 Conclusion

In the framework of the Lagrangian field theory, we propose the so-called surface Lagrangian to characterize the surface effects of field. The surface Lagrangian has no influence on the Euler-Lagrange equation, but it contributes to the natural boundary condition and causes a type of new non-classical natural boundary condition to be correlated with the mean curvature of boundary surface. The well-known Tolman’s formula is derived from simplification to this new natural boundary condition.

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References

[1] P.R. Pujado, C. Huh, L.E. Scriven, On the contribution of an equation of capillary to Young and Laplace, Journal of Colloid and Interface Science 38 (1972) 662-663.
[2] L. Rayleigh, On the capillary phenomena of jets, Proceedings of the Royal Society of London 29 (1879) 71-97.
[3] N. Bohr, J.A. Wheeler, The mechanism of nuclear fission, Physical Review 56 (1939) 426-450.
[4] M.E. Gurtin, A.I. Murdoch, A continuum theory of elastic material surfaces, Archive for Rational Mechanics and Analysis 57 (1975) 291-323.
[5] D.J. Steigmann, R.W. Ogden, Elastic surface-substrate interactions, Proceedings of the Royal Society of London A 455 (1999) 437-474.
[6] J. Zhu, C.Q. Ru, W.Q. Chen, On the non-uniqueness of solution in surface elasticity theory, Mathematics and Mechanics of solid 17 (2012) 329-337.
[7] A. Javili, N.S. Ottosen, M. Ristinmaa, J. Aspects of interface elasticity theory, Mathematics and Mechanics of Solids DOI: 10.1177/1081286517699041 (2017) 1-21.
[8] J. Wang, Z. Huang, H. Duan, S. Yu, X. Feng, G. Wang, et al, Surface stress effect in mechanics of nanostructured materials, Acta Mechanica Solida Sinica 24 (2011) 52-82.
[9] C.Q. Sun, Size dependence of nanostructures: Impact of bond order deficiency, Prog. Solid State Chem. 35 (2007) 1-159.
[10] A. Figotin, G. Reyes, Lagrangian variational framework for boundary value problems, Journal of Mathematical Physics 56 (2015) 093506.
[11] Zaixing Huang, Shape-dependent natural boundary condition of Lagrangian field, Applied Mathematics Letters 61 (2016) 56-61.
[12] J.G. Simmonds, A Brief on Tensor Analysis, Springer, New York, 1994.
[13] Y. Yin, J. Wu, J. Yin, Symmetrical fundamental tensor, differential operators and integral theorems in differential geometry, Tsinghua Science & Technology 13 (2008) 121-126.
[14] R.C. Tolman, The effect of droplet size on surface tension, Journal of Chemical Physics 17 (1949) 333-337.
[15] A. Malijevsky, G. Jackson, A perspective on the interfacial properties of nanoscopic drops, Journal of Physics: Condensed Matter 24 (2012) 464121.

[16] Z. Huang, P. Thomson, S.L. Di, Lattice contractions of nanoparticle due to the surface tension: A model of elasticity, J. Phys. Chem. Solids 68 (2007) 30-535.