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Integral Theorems Based on a New Gradient Operator Derived from Biomembranes (Part I): Fundamentals

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Abstract: A new gradient operator was derived in recent studies of topological structures and shape transitions in biomembranes. Because this operator has widespread potential uses in mechanics, physics, and biology, the operator's general mathematical characteristics should be investigated. This paper explores the integral characteristics of the operator. The second divergence and the differential properties of the operator are used to demonstrate new integral transformations for vector and scalar fields on curved surfaces, such as the second divergence theorem, the second gradient theorem, the second curl theorem, and the second circulation theorem. These new theorems provide a mathematical basis for the use of this operator in many disciplines.

Key words: gradient operator; integral theorem; curved surfaces; biomembranes

Introduction

The description of topological structures[1] and the prediction of shape transitions[2-5] in biomembranes are of special importance in cell biology[6-8]. Geometrically, a biomembrane, such as a cell membrane, may be regarded as a curved surface or a two-dimensional Riemann space. Special mathematical techniques have been developed to describe the equilibrium configuration of these curved surfaces in complicated micro bio-structures. Yin et al.[9] presented a new gradient operator $\bar{\nabla}$ which plays an important role in controlling the equilibrium configurations of the curvature bifurcations in closed biomembranes.

Besides its widespread uses in cell biology, $\bar{\nabla}$ also has potential applications in other disciplines, so $\bar{\nabla}$ may become a universal and fundamental differential operator. Therefore, the operator's general mathematical characteristics should be investigated systematically. This paper describes the new gradient operator and some possible physical meanings. Four fundamental integral theorems based on the operator are proven along with possible applications of these theorems in various disciplines.

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1 Second Gradient Operator

The equilibrium differential equation for heterogeneous closed biomembranes has been proven to be of the generalized form[9],

$$\nabla \cdot \left(\nabla \varphi + \bar{\nabla} \psi \right) + f = 0 \tag{1}$$

As shown in Eq. (1), the equilibrium configuration and topological structure of closed biomembranes are controlled by two differential operators: ∇ which is the classical 2-D gradient operator in differential geometry[10] and $\bar{\nabla}$ which is a new 2-D gradient operator[9] defined on the curved surface. The two gradient operators are given by:

$$\nabla = \boldsymbol{g}^i \frac{\partial}{\partial u^i}, \quad \bar{\nabla} = K\bar{L}^{ij} \boldsymbol{g}_i \frac{\partial}{\partial u^j} \quad \left(i, j = 1,2 \right) \tag{2}$$

In Eq. (1), $\varphi = \varphi\left(H, K\right)$, $\psi = \psi(H, K)$, and $f = f\left(H, K\right)$ are three known scalar functions derived from the free energy of the biomembrane. H is the mean curvature and K is the Gauss curvature. In Eq. (2), $\boldsymbol{g}_i$ and $\boldsymbol{g}^i$ are the covariant and contravariant base vectors. $\bar{L}^{ij}$ is the contravariant component of a tensor defined by $\bar{\boldsymbol{L}} = \boldsymbol{L}^{-1}$, with $\boldsymbol{L}$ being the second fundamental tensor. u^i are the Gauss parameter coordinates defined on the curved surface.

The second gradient operator, $\bar{\nabla}$, can be understood by comparison with ∇. They have obvious difference. ∇ is dominated by the first fundamental tensor and may be termed "the first gradient operator", while $\bar{\nabla}$ is dominated by the second fundamental tensor and may be named "the second gradient operator". The importance of ∇ and $\bar{\nabla}$ differs in different length scales. For example, on a spherical surface with radius R, $\nabla = R\bar{\nabla}$. Thus, in large geometries ∇ is much more important than $\bar{\nabla}$. However, for small geometries (e.g., nano scale), $\bar{\nabla}$ is much more important than ∇. For a differentiable scalar function φ on a curved surface, the first gradient $\nabla\varphi$ means that the change of φ is determined by changes of the location. With the second gradient, $\bar{\nabla}\varphi$, the variation of φ is affected not only by the variation of the location, but also by the curvature of the curved space. $\nabla\varphi$ defines the direction along which φ increases the fastest. $\bar{\nabla}\varphi$ also defines a special direction, but the exact meaning of this direction is still unknown.

Although the physical meaning of the second gradient operator needs to be explored further, the operator's general mathematical characteristics such as the integral properties can be investigated without difficulty. In classical geometry, various classical integral theorems, which may be called "the first category of integral theorems", can be derived on the basis of the first gradient operator, ∇. In this paper, various new integral theorems, which may be termed "the second category of integral theorems", can be derived based on the second gradient operator, $\bar{\nabla}$. Four new integral theorems will be developed in the next section.

2 Second Category of Integral Theorems

Various theorems connecting line integrals round a closed curve drawn on the surface, with surface integrals taken over the enclosed region, will be proven. Let $\boldsymbol{n}$ be the outward unit normal of the surface and C be any closed curve drawn on the surface. At any point of this curve, let $\boldsymbol{m}$ be the unit vector tangent to the surface and normal to the curve, drawn outward from the region enclosed by C. Let $\boldsymbol{t}$ be the unit tangent to the curve, in that sense for which $\boldsymbol{m}$, $\boldsymbol{t}$, and $\boldsymbol{n}$ form a right-handed system of unit vectors (Fig. 1), so that $\boldsymbol{m} = \boldsymbol{t} \times \boldsymbol{n}$, $\boldsymbol{t} = \boldsymbol{n} \times \boldsymbol{m}$, and $\boldsymbol{n} = \boldsymbol{m} \times \boldsymbol{t}$. The sense of $\boldsymbol{t}$ is the positive sense for a description of the curve. With the aid of the unit vectors, three element vectors may be formulated as $\mathrm{d}\boldsymbol{s} = \boldsymbol{m}\mathrm{d}s$, $\mathrm{d}\boldsymbol{r} = \boldsymbol{t}\mathrm{d}s$, and $\mathrm{d}\boldsymbol{A} = \boldsymbol{n}\mathrm{d}A$. Here, $\mathrm{d}s$ is the length of an element on the curve, $\mathrm{d}\boldsymbol{r}$ is the displacement along the curve in the positive sense, and A is the area enclosed by C.

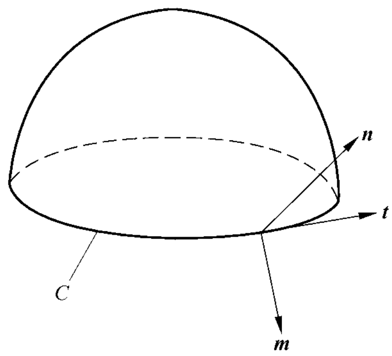

Fig. 1 Schematic of the unit vectors $\boldsymbol{m}$, $\boldsymbol{t}$, and $\boldsymbol{n}$

2.1 Second divergence theorem for a vector field

Consider the surface integral of the second divergence of a differentiable vector given by

$$\boldsymbol{v} = v_i \boldsymbol{g}^i + v_3 \boldsymbol{n} \tag{3}$$

The second divergence of the vector can be proven to be

$$\bar{\nabla}\bullet\boldsymbol{v} = \frac{1}{\sqrt{g}} \frac{\partial\left(\sqrt{g} K \bar{L}^{ij} v_i\right)}{\partial u^j} - 2Kv_3 \tag{4}$$

Here, $g = \left|g_{ij}\right|$ is the determinant of the metric tensor. The surface integral taken over the region enclosed by C is

$$\iint_A \bar{\nabla}\bullet\boldsymbol{v}\mathrm{d}A = \iint_A \frac{\partial\left(\sqrt{g} K \bar{L}^{ij} v_i\right)}{\partial u^j} \mathrm{d}u^1 \mathrm{d}u^2 - \iint_A 2Kv_3 \mathrm{d}A \tag{5}$$

The two terms on the right side may also be respectively written as:

$$\iint_A \frac{\partial\left(\sqrt{g} K \bar{L}^{ij} v_i\right)}{\partial u^j} \mathrm{d}u^1 \mathrm{d}u^2 = \oint_C \mathrm{d}\boldsymbol{s} \bullet \hat{\boldsymbol{L}} \bullet \boldsymbol{v},$$