数理解析研究所講究録 1237 巻 2001 年 110-119

A variational problem with constraints for the modified Willmore functional with constraints

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1 Introduction

This is a joint work with Izumi Takagi, Tôhoku University.

The shape of human red blood cell is usually axially symmetric with the biconcave cross section. About 30 years ago several physicists proposed some models of cell ([1, 3, 4]). They considered that the shape minimizes the bending energy of the cell membrane.

One of models is the *spontaneous curvature* model. They regarded the cell as an oriented closed smooth surface embedded in $\mathbb{R}^3$, denoted by Σ. The mean curvature denotes h. The sign of mean curvature is positive if the surface is strictly convex. $A(\Sigma)$ and $V(\Sigma)$ mean the area and enclosed volume:

$$A(\Sigma)=\int_{\Sigma}dS, \quad V(\Sigma)=-\frac{1}{3}\int_{\Sigma}\boldsymbol{n}\cdot\boldsymbol{p}\,dS.$$

Here $\boldsymbol{p}$ and $\boldsymbol{n}$ are respectively the position vector and the inner unit normal vector at $\boldsymbol{p}$ on Σ. Usually the energy is defined the integral of squared curvature (the Willmore functional). Since the spheres are global minimizers for this functional, it is impossible to explain the concavity of cell. Then they modified the energy, and imposed some constraints on the minimizing problem. By the difference of the structure of cell membrane between the exterior and interior sides, it is considered that the cell bends spontaneously with constant curvature, say c_0. If so, the energy should minimize when $h\equiv c_0$. Taking this into account, they introduced the bending energy defined by

$$W(\Sigma)=\int_{\Sigma}(h-c_0)^2dS,$$

where c_0 is a given constant, not necessarily positive, called the spontaneous curvature.

Let A_0 and V_0 be given constant. Then they considered that a critical surface, in particular a minimizer, of the bending energy under the prescribed area A_0 and volume V_0 is the shape of the red blood cell. Of course A_0 and V_0 must satisfy the isoperimetric inequality. The spontaneous curvature c_0 determined by the structure of the cell membrane.

We formulate the problem mathematically. For a smooth function ϕ on a surface Σ and $t \in \mathbb{R}$, we shift Σ to the normal direction with length $t\phi$. If $|t|$ is sufficiently small, then we get a surface, denoted by Σ_t. This is called the normal variation. We denote the first and second variations by δ and δ^2 respectively, that is, for a functional F on Σ, $\delta F(\Sigma)$ and $\delta^2 F(\Sigma)$ are the first and second derivatives with respect to t at $t = 0$ of $F(\Sigma_t)$. Our problem is a variational one with two constraints. The theory of Lagrange multipliers gives the Euler-Lagrange equation

$$\delta W(\Sigma) + \lambda_1 \delta A(\Sigma) + \lambda_2 \delta V(\Sigma) = 0. \tag{1.1}$$

Here λ_1 and λ_2 are Lagrange multipliers.

There are other models about the red blood cells. One of them is called the *bilayer-coupled* model. This is the same variational problem but with different meaning of physical parameters λ_1 and λ_2 (see [3]).

2 Known results

By use of differential geometry, (1.1) is reduced to a second order elliptic equation

$$\Delta_g h + 2h(h^2 - k) + 2c_0 k - 2c_0^2 h - 2\lambda_1 h - \lambda_2 = 0 \tag{2.1}$$

for the mean curvature h. Here k is the Gauss curvature and Δ_g is the Laplace-Beltrami operator of Σ with the induced metric g from $\mathbb{R}^3$. The metric g is determined from the embedding of Σ, and therefore unknown. Hence this equation is quasi-linear, not semi-linear.

Several results are known about this problem. If $c_0 = \lambda_1 = \lambda_2 = 0$, then our functional is the Willmore functional, which has a long history in differential geometry, but we do not mention here.

Spheres are critical points for any c_0. That is, spheres satisfy the Euler-Lagrange equation for any c_0 and suitable λ_1 and λ_2, since h and k is constant. This is a direct calculation.

We have a lot of discussions of critical points other than spheres. Most of them are based on formal calculations or experiments, however, we would like to point out some of them.

Though the normal red blood cell has a biconcave shape when at rest in the plasma, this is not the only shape of the cell. Adding distilled water to the plasma, we can observe various shapes. At first cell loses the biconcavity, gradually shapes an oblate ellipsoid, and finally, spherical. It is considered that the shape is determined by the excess of osmotic pressure between interior and exterior of cell. The physical constant λ_2 corresponds to the excess of osmotic pressure. From the point of mathematical view, this shape transformation implies the existence of "a bifurcating family" of shapes of cell from the sphere with the bifurcation parameter of λ_2.

Jenkins [5] showed numerically the existence of families of solutions bifurcating from spheres when $c_0 = 0$. The solutions are surfaces of revolution. Subsequently Peterson [9] and Ou-Yang and Helfrich [8] investigated the stability and instability of surfaces of mode 2 by formal computation. We shall explain the meaning of "mode" in the next section. Unfortunately these results seemed to be based on formal calculations, and the rigorous proofs were expected.

The author jointly with Takagi succeeded in giving a rigorous proof of existence of solutions of mode n, $n \geq 2$. We can also analyze the stability and instability of solutions of general modes. The solutions are surfaces of revolution, however, it is to be emphasized that we include variations which are not axisymmetric in the stability question. Our results in this note have already announced in [6] without precise proofs. The full paper [7] is now in preparation.

3 Critical points bifurcating from spheres

We construct critical surfaces which are axisymmetric. Let Σ be a surface of revolution:

$$\Sigma = \{\boldsymbol{p} = (r(s)\cos\theta, r(s)\sin\theta, z(s)) \,|\, 0 \leq \theta < 2\pi,\ 0 \leq s \leq \bar{s}\}.$$

Here r and z are unknown functions, and s is the arch-length parameter of generating curve. The range of s is unknown, that is, the problem is the free boundary problem. This is one of the difficulties. To avoid this, we introduce a new coordinate. By scaling we may assume the area is 4π. A new coordinate ζ is defined by

$$s \mapsto \zeta = \int_0^s r(s)\,ds - 1 \in \{\zeta \,|\, -1 \leq \zeta \leq 1\}.$$

We may call this "the area-wise coordinate" in the following sense. The surface generates the curve parameterized by s. Let consider the segment of curve with the arch-length parameter between 0 and s, and the surface patch generating the segment. The area of the patch varies from 0 to 4π. Normalizing the range to the interval $[-1, 1]$, we get ζ. Changing an unknown function r to ρ, where ρ is the square of r. And put $\lambda = -2\lambda_1$ and $\mu = \lambda_2$. Then we reduce our problem (2.1) to

$$\begin{cases} (\rho h')' + 2(h - c_0)\{(h - z')^2 + c_0 h\} + \lambda h - \mu = 0, \\ \frac{1}{2}\rho'' - (h - z')^2 + h^2 = 0, \\ (\rho z')' - \rho' h = 0 \\ \qquad\qquad\qquad\qquad \text{for } -1 < \zeta < 1, \\ \sqrt{\rho} h' = \rho = \sqrt{\rho} z' = 0 \quad \text{at} \quad \zeta = \pm 1, \\ \rho' = \mp 2 \quad \text{at} \quad \zeta = \pm 1. \end{cases}$$

The first equation is the Euler-Lagrange equation. The second and third ones are the relations between ρ, z and h. The boundary conditions except the last one mean that the surface closes smoothly. The last condition comes from the normalization of area, or reduction of free boundary condition.

This system, however, is overdetermined as a system of second order ordinary differential equations. The normalization of area gives an extra condition. We would like to construct bifurcation solutions from the unit sphere S^2, but we cannot apply the standard bifurcation theory. Instead we consider the system of equations

$$\begin{cases} (\rho h')' + 2(h - c_0)\{(h - z')^2 + c_0 h\} + \lambda h - \mu + \nu_1 \rho' = 0, \\ \dfrac{1}{2}\rho'' - (h - z')^2 + h^2 + \dfrac{\nu_2}{4}\rho' = 0, \\ (\rho z')' - \rho' h + \dfrac{\nu_2}{2}\rho z' = 0 \\ \qquad\qquad\qquad\qquad \text{for } -1 < \zeta < 1 \end{cases}$$

with the same boundary conditions. The new system contains new parameters ν_1 and ν_2, and therefore it is not overdetermined. Furthermore we can show that if there exists a solution, then ν_1 and ν_2 are zero. Hence the solution satisfies the original system. Conversely solutions of the original system solve the new system putting ν_1 and ν_2 zero. Consequently two systems are equivalent. Using translation invariance of functional can show this fact. Of course we can show that by analytic argument, but we need length calculations.

The unit sphere S^2 corresponds to

$$h \equiv 1,\ \rho = 1 - \zeta^2,\ z = \zeta,\ \lambda = -2c_0 + 2c_0^2 + \mu.$$

We denote $C^2(-1,1)$, $L^2(-1,1)$, and $H^k(-1,1)$ simply by C^2, L^2, and H^k. Let P_n be the Legendre polynomial of order n, and

$\mathcal{D} =$ the graph closure in L^2 of

$$\left\{ u \in C^2 \cap L^2 \,\middle|\, \lim_{\zeta \to \pm 1} \sqrt{1-\zeta^2}\frac{du}{d\zeta} = 0,\ \frac{d}{d\zeta}\left\{(1-\zeta^2)\frac{du}{d\zeta}\right\} \in L^2 \right\},$$

$$\mathcal{D}_0^1 = \left\{ u \in \mathcal{D} \,\middle|\, \int_{-1}^{1} u\, d\zeta = 0,\ \frac{du}{d\zeta} \in \mathcal{D} \right\}.$$

H_0^2 is the completion of the space of smooth functions with compact support in H^2 topology. As an application of Crandall-Rabinowitz' theorem [2] to the new system, we have the existence theorem.

Theorem 3.1 *Let n be an integer greater than 1. Then we have families of solutions $\Sigma_n(\varepsilon) = (h(\varepsilon), \rho(\varepsilon), z(\varepsilon), \lambda(\varepsilon), \mu(\varepsilon)) \in \mathcal{D} \times (\{1-\zeta^2\} + H_0^2) \times \mathcal{D}_0^1 \times \mathbb{R} \times \mathbb{R}$:*

$$\begin{cases} h = 1 + \varepsilon P_n + \mathcal{O}(\varepsilon^2), \\ \rho = 1 - \zeta^2 - \dfrac{4\varepsilon(1-\zeta^2)^2 P_n''}{(n-1)n(n+1)(n+2)} + \mathcal{O}(\varepsilon^2), \\ z' = 1 + \dfrac{2\varepsilon(\zeta P_n' - P_n)}{(n-1)(n+2)} + \mathcal{O}(\varepsilon^2), \\ \lambda = n(n+1) - 4c_0 + 2c_0^2 + \mathcal{O}(\varepsilon)(= -2c_0 + 2c_0^2 + \mu + \mathcal{O}(\varepsilon)), \\ \mu = n(n+1) - 2c_0 + \mathcal{O}(\varepsilon), \\ (\nu_1 = \nu_2 = 0) \end{cases}$$

for sufficiently small $|\varepsilon|$, say $|\varepsilon| < \varepsilon_1$. The mapping from ε to the solution $\Sigma_n(\varepsilon)$ is analytic from $\mathbb{R}$ to the above class.

Note that the part of order 1 is the unit sphere. Therefore these are families of critical points bifurcating from S^2. We call the solution of Theorem 3.1 that of *mode n*.

The surfaces obtained in Theorem 3.1 are critical points of $W(\cdot)$ under the prescribed area $A_0 = 4\pi$ and volume V_0. Next we would like to discuss the result of stability of them. As usual we define the Nullity and the Index of critical points. That is, Nullity is the multiplicity of zero eigenfunction of the quadratic form associated with the second variation, and Index is the number of negative eigenvalues. Then we have the lower bound of Index and Nullity.

Theorem 3.2 *For the solution of mode n it holds that* $\mathrm{Index}(\Sigma_n(\varepsilon)) \geq (n-2)(n+2)$, *and* $\mathrm{Nullity}(\Sigma_n(\varepsilon)) \geq 5$ *provided* $|\varepsilon| > 0$ *is sufficiently small.*

The lower bound 5 of Nullity comes form the rigid motion. Since the surface is axially symmetric, the rotation around the axis of symmetry generates the tangential variation but not the normal variation. Therefore the space of normal variations coming from infinitesimal rigid motions of is a 5-dimensional space, not 6-dimensional. The lower bound of Index shows that the surfaces of mode n is unstable if n is greater than 2.

The theorem giving below is the more precise bounds in case of even n. Let γ be

$$\gamma = c_0(3n^4 + 6n^3 - 3n^2 - 6n + 8) + 3n^4 + 6n^3 - 7n^2 - 10n,$$

and let σ be the sign of $\varepsilon \times \gamma$. P_n^m is the associate Legendre functions of the first kind. $E_{n,+}$, $E_{n,-}$, and $E_{n,0}$ are the spaces defined by

$$E_{n,+} = \mathrm{span}\{P_n^m \cos m\theta,\ P_n^m \sin m\theta \,|\, 2 \leq m \leq n,\ S_n^m = 1\},$$
$$E_{n,-} = \mathrm{span}\{P_n^m \cos m\theta,\ P_n^m \sin m\theta \,|\, 2 \leq m \leq n,\ S_n^m = -1\},$$
$$E_{n,0} = \mathrm{span}\{P_n^m \cos m\theta,\ P_n^m \sin m\theta \,|\, 2 \leq m \leq n,\ S_n^m = 0\}.$$

Here

$$A_n^m = \int_{-1}^{1} P_n \,(P_n^m)^2 \, d\zeta,$$

and

$$S_n^m = \mathrm{sgn}\left\{ \frac{(n+m)!}{(n-m)!} A_n^0 - 2A_n^m \right\}.$$

Then dimensions of these spaces give the lower and upper bound of Nullity and Index.

Theorem 3.3 *Let n be even. Then there exists* $\varepsilon_2 = \varepsilon_2(n, c_0) > 0$ *such that for* $0 < |\varepsilon| < \varepsilon_2$

$$(n-2)(n+2) + \dim E_{n,-\sigma} \leq \mathrm{Index}(\Sigma_n(\varepsilon))$$
$$\leq (n-2)(n+2) + \dim E_{n,-\sigma} + \dim E_{n,0}$$

$$5 \leq \mathrm{Nullity}(\Sigma_n(\varepsilon)) \leq 5 + \dim E_{n,0},$$

hold provided $\gamma \neq 0$.

Note that if $E_{n,0} = \emptyset$, then estimates are optimal (here we interpret $\dim \emptyset = 0$). When $n \leq 6$ and even, it can be shown that $E_{n,0} = \emptyset$ by direct calculation. When $8 \leq n \leq 30$ and even, we have $E_{n,0} = \emptyset$ with help of computer.

Furthermore when n is 2, 4, or 6, we can give $E_{n,\pm}$ explicitly. Consequently we can give the exact value of Index and Nullity. In particular, if $\varepsilon(5c_0 + 3) > 0$, then the solution of mode 2 is stable. All other solutions except $5c_0 + 3 = 0$ are unstable.

The result on the stability and instability in mode 2 coincides with formal results of Peterson [9] and Ou-Yang-Helfrich [8]. The result for higher modes is completely new. Note that we include variations which are not rotationally symmetric in the study of the stability and instability.

To show Theorems 3.2 and 3.3 we must check the sign of the second variation. In the following we sketch the proof of Theorem 3.3. Since the problem is the variational one with constraints, we must restrict the variations to those which satisfies the constraints. We call such variations *admissible*. Hence we need the second variation formula for admissible variations, and the necessary and sufficient condition of admissibility.

The first proposition gives the second variation formula of the bending energy under constraints.

Proposition 3.1 (The second variation formula) *Let* $\Sigma \to \Sigma(\psi(t)) = \{\boldsymbol{p} + \psi(t)\boldsymbol{n} \,|\, \boldsymbol{p} \in \Sigma\}$ *be a variation preserving the area and volume. Then we have*

$$\frac{d^2}{dt^2} W(\Sigma(\psi(t)))\bigg|_{t=0} = \delta^2 W(\Sigma)[\psi'(0)] + \lambda_1 \delta^2 A(\Sigma)[\psi'(0)] + \lambda_2 \delta^2 V(\Sigma)[\psi'(0)].$$

This formula is derived in the following way. If the variation is linear, then it does not satisfy the constraints. Therefore we must consider the nonlinear variations. If the variation is nonlinear, then the second derivative is

$$\frac{d^2}{dt^2} W(\Sigma(\psi(t)))\bigg|_{t=0} = \delta^2 W(\Sigma)[\psi'(0)] + \delta W(\Sigma)[\psi''(0)].$$

The second term in the right-hand side does not appear when the variation is linear. The Euler-Lagrange equation, and the constraints of the area and volume yield

$$\delta W(\Sigma)[\psi''(0)] = -\lambda_1 \delta A(\Sigma)[\psi''(0)] - \lambda_2 \delta V(\Sigma)[\psi''(0)],$$

$$-\delta A(\Sigma)[\psi''(0)] = \delta^2 A(\Sigma)[\psi'(0)], \quad -\delta V(\Sigma)[\psi''(0)] = \delta^2 V(\Sigma)[\psi'(0)]$$

respectively. Combining these, we get our formula.

Next proposition says the admissibility of variations.

Proposition 3.2 (Admissibility of test function) *The variation* $\Sigma \to \Sigma(\psi(t)) = \{\boldsymbol{p} + \psi(t)\boldsymbol{n} \,|\, \boldsymbol{p} \in \Sigma\}$ *preserves the area and volume, if and only if*

$$\int_{S^2} \psi'(0)\, dS = \int_{S^2} h\psi'(0)\, dS = 0.$$

This means that the first variation of area and volume vanish. Therefore the necessity is clear. The sufficiency is not trivial. We show this by use of the implicit function theorem. The class of admissible variations is not linear space, but manifold. The condition of Proposition 3.2 determines the tangent space of the manifold.

Put $\psi'(0) = \phi$. Now we define the quadratic from II associated with the second variation by

$$\begin{aligned}
\mathrm{II}[\phi,\phi] &= \delta^2 W(\Sigma)[\phi] + \lambda_1 \delta^2 A(\Sigma)[\phi] + \lambda_2 \delta^2 V(\Sigma)[\phi] \\
&= 2\int_{S^2} \Bigg(\left[\frac{1}{2}\Delta_g (h^2 - k) + (4h^2 - k)(h^2 - k) + \frac{1}{\sqrt{g}} \left\{ \sqrt{g} h^{ij} (h)_i \right\}_j \right] \phi^2 \\
&\quad - hh^{ij}\phi_i\phi_j - \frac{1}{2}(h^2 - 2k)|\nabla_g \phi|^2 + \frac{1}{4}(\Delta_g \phi)^2 - 2c_0 \left(-\frac{1}{2} h^{ij}\phi_i\phi_j + h|\nabla_g\phi|^2 \right) \\
&\quad + \left(c_0^2 - \frac{\lambda}{2} \right) \left(k\phi^2 + \frac{1}{2}|\nabla_g \phi|^2 \right) + \mu h \phi^2 \Bigg)\, dS.
\end{aligned}$$

Here Δ_g and ∇_g are the Laplacian and the gradient on the surface with the induced metric. g_{ij} and h_{ij} are the first and second fundamental forms.

Inserting the expansion of solution $h = 1 + \varepsilon h_1 + \mathcal{O}(\varepsilon^2)$ etc. in the formula above, we get

$$\mathrm{II}[\phi,\phi] = \mathrm{II}_0[\phi,\phi] + \varepsilon \mathrm{II}_1[\phi,\phi] + \cdots,$$

where

$$\mathrm{II}_0[\phi,\psi] = \int_{S^2} \left\{ \frac{1}{2}(\Delta_0\phi)(\Delta_0\psi) - \frac{n^2+n+2}{2}\nabla_0\phi \cdot \nabla_0\psi + n(n+1)\phi\psi \right\} dS,$$

$$\mathrm{II}_1[\phi,\psi]=\int_{S^2}\Bigg(\left[\{4c_0-2n(n+1)\}h_1+\mu_1\right]\varphi\psi$$

$$-\left[\frac{n^2+n+2}{2}\rho_1+\rho_0\left\{4h_1+(c_0-1)\frac{dz_1}{d\zeta}+\frac{\mu_1}{2}\right\}\right]\frac{\partial\varphi}{\partial\zeta}\frac{\partial\psi}{\partial\zeta}$$

$$+\left[\frac{n^2+n+2}{2}\frac{\rho_1}{\rho_0^2}+\frac{1}{\rho_0}\left\{-4c_0h_1+2(c_0-1)\frac{dz_1}{d\zeta}-\frac{\mu_1}{2}\right\}\right]\frac{\partial\varphi}{\partial\theta}\frac{\partial\psi}{\partial\theta}$$

$$+\frac{1}{2}(\Delta_0\varphi)\left\{\frac{\partial}{\partial\zeta}\left(\rho_1\frac{\partial\psi}{\partial\zeta}\right)-\frac{\rho_1}{\rho_0^2}\frac{\partial^2\psi}{\partial\theta^2}\right\}+\frac{1}{2}(\Delta_0\psi)\left\{\frac{\partial}{\partial\zeta}\left(\rho_1\frac{\partial\varphi}{\partial\zeta}\right)-\frac{\rho_1}{\rho_0^2}\frac{\partial^2\varphi}{\partial\theta^2}\right\}\Bigg)\,dS.$$

Using the expansion of solution in Theorem 3.1, we compute the sign on II_0 and II_1 for admissible function ϕ.

Proposition 3.3 *Let $\mathcal{A}$ and $\mathcal{R}$ be spaces of admissible variations and rigid motions respectively. $E_{n,+}$, $E_{n,-}$, and $E_{n,0}$ are as before. There exist linear spaces $E_{n,1}$ and $E_{n,2}$ such that*

$$E_{n,1}\simeq\mathrm{span}\{P_\ell,P_\ell^m\cos m\theta,\ P_\ell^m\sin m\theta\,|\,2\le\ell\le n,\ 1\le m\le\ell\},$$

$$E_{n,2}\simeq\mathrm{span}\{P_\ell,P_\ell^m\cos m\theta,\ P_\ell^m\sin m\theta\,|\,\ell\ge n+1,\ 1\le m\le\ell\},$$

and the direct sum decomposition

$$\mathcal{A}=E_{n,-\sigma}\oplus E_{n,1}\oplus E_{n,0}\oplus\mathcal{R}\oplus E_{n,\sigma}\oplus E_{n,2}.$$

Furthermore it holds that

$$\mathrm{II}_0=0,\ \mathrm{II}_1<0\quad on\quad E_{n,-\sigma},\quad \mathrm{II}_0<0\quad on\quad E_{n,1},$$

$$\mathrm{II}_0=\mathrm{II}_1=0\quad on\quad E_{n,0},\quad \mathrm{II}=0\quad on\quad \mathcal{R},$$

$$\mathrm{II}_0=0,\ \mathrm{II}_1>0\quad on\quad E_{n,\sigma},\quad \mathrm{II}_0>0\quad on\quad E_{n,2}.$$

Here $\mathrm{II}_1>0$ on $E_{n,-\sigma}$ means that II_1 is positive definite there. Other notation should be understood similarly.

Since the decomposition is not orthogonal one with respect to eigenspaces, we must estimate the cross terms carefully to see the signature of quadratic forms. After these estimations we finally obtain the lower and upper bounds:

$$\dim(E_{n,-\sigma}\oplus E_{n,1})\le\mathrm{Index}(\Sigma_n(\varepsilon))\le\mathrm{codim}\,(\mathcal{R}\oplus E_{n,\sigma}\oplus E_{n,2})$$

$$=\dim(E_{n,-\sigma}\oplus E_{n,1}\oplus E_{n,0}),$$

$$\dim\mathcal{R}\le\mathrm{Nullity}(\Sigma_n(\varepsilon))\le\dim(E_{n,0}\oplus\mathcal{R}).$$

By direct calculations we have $\dim E_{n,1}=(n-2)(n+2)$ and $\dim\mathcal{R}=5$.

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