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SYMMETRY PROPERTIES OF THE MEMBRANE SHAPE EQUATION

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Abstract. Here we consider the Helfrich's membrane shape model from a group-theoretical viewpoint. By making use of the conformal metric on the associated surface the model is represented by a system of four second order nonlinear partial differential equations. In order to construct the determining system for the symmetries of the metric we rely on the previously developed package *LieSymm-PDE* within `Mathematica`®. In this way we have obtained the determining system consisting of 206 equations. Using the above mentioned programs we have solved the equations in a semi-automatic way. As a result we end up with an infinite dimensional symmetry Lie algebra of the Helfrich's model in conformal metric representation which we present here in explicit form.

1. Helfrich's Membrane Shape Model

The Helfrich's model of fluid membranes (biomembranes) is based on the equilibrium shape equation [1, 3]

$$\Delta H + 2(H^2 + \mathbb{h}H - K)(H - \mathbb{h}) - \frac{2\lambda H}{k} + \frac{p}{k} = 0 \qquad (1)$$

often referred to as the general **membrane shape equation** or the **Helfrich's equation**. The Helfrich's equation (1) serves to describe the equilibrium forms of the simplest closed biological membrane structures – lipid vesicles. A lipid vesicle is a small bubble of about 15 μm to 0.5 cm in size and 4-5 nm thickness of its coat. The vesicles are formed in aqueous solution mostly by phospholipid molecules. The phospholipids are substances (chemical compounds) made up of amphiphilic molecules possessing both hydrophilic and hydrophobic properties. In phospholipids, this is due to the well-defined at each end of the molecule hydrophilic head and hydrophobic tails. Placed in aqueous solution the phospholipid molecules arrange themselves into bilayers locating their hydrophilic heads to point outward to the surrounding solution and the tails facing the interior of the layer in order to prevent from direct contact with the water molecules. Having reached a certain critical size, the phospholipid bilayer, initially flat, starts spontaneously bending until a closed cavity filled with fluid is formed – a vesicle has been created.

In the Helfrich's equation (1) the lipid bilayer of the vesicle is regarded as a smooth surface $\mathcal{S}$ with the mean curvature H and the Gaussian curvature K. The physical parameters characterizing the surface are the bending rigidity k, the tensile stress λ, the osmotic pressure p, and the so called spontaneous mean curvature $\mathbb{h}$ and Δ is the Laplace-Beltrami operator on $\mathcal{S}$.

In Mongé representation the Helfrich's equation is a fourth order nonlinear partial differential equation in one dependent and two independent variables. After passing to a conformal metric on S and making an appropriate change of the variables, the order of the derivatives in the Helfich's equation is reduced. At the same time other three differential equations, being the Gauss-Codazzi-Mainardi compatibility conditions, are added. As a result the Helfrich's model (1) in conformal metric representation takes the form of a system of four second order partial differential equations for four functions in two variables [4, 6] (Section 2).

In this paper the conformal metric representation of the Helfrich's membrane shape model is considered in the framework of the Lie group analysis of differential equations [2, 5, 7] (Section 3). By the help of the `Mathematica`® computer program *LieSymm-PDE* [9] the determining system consisting of 206 partial differential equations has been created. For solving of the determining system the program *LieSymm-PDE* has been applied interactively. Based on the general solution of the determining system, an infinite dimensional symmetry Lie algebra of the Helfrich's membrane shape model in conformal metric representation has been obtained (Section 4).

2. Conformal Metric Representation of the Helfrich's Model

Let on S be given, without loss of generality, the curvilinear coordinates (x, y), the **conformal metric**

$$\mathrm{d}s^2 = 4q^2\varphi^2(\mathrm{d}x^2 + \mathrm{d}y^2) \tag{2}$$

and the matrix of the second fundamental form

$$b = \begin{pmatrix} \theta & \omega \\ \omega & 8q^2\varphi(1 + \mathbb{h}\varphi) - \theta \end{pmatrix} \tag{3}$$

where q, φ, θ and ω are functions of x and y. Then, the mean H and the Gaussian K curvatures take the form [4, 6]

$$H = \frac{1}{\varphi} + \mathbb{h}$$

$$K = \frac{1}{4q^4\varphi^4}[\varphi^2(q_x^2 + q_y^2) + q^2(\varphi_x^2 + \varphi_y^2) - q\varphi^2(q_{xx} + q_{yy}) - q^2\varphi(\varphi_{xx} + \varphi_{yy})]$$

where $\varphi_x = \partial\varphi/\partial x$, etc. Note that the Gaussian curvature is obtained by the use of the **Brioschi formula**

$$K = -\Delta \log(2q\varphi)$$

where

$$\Delta = \frac{1}{4q^2\varphi^2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)$$

is the **Laplace-Beltrami operator**. It is straightforward that in regard to the above conformal metric coordinates the Helfrich's equation (1) is recast into a second order differential equation with respect to the functions $q(x, y)$ and $\varphi(x, y)$.

The existence of an embedded surface $\mathcal{S}$ in the Euclidean space $\mathbb{R}^3$, with the first and the second fundamental forms given by (2) and (3), is ensured by the so called Gauss-Codazzi-Mainardi equations [8]. After adding these equations to the Helfich's equation, a system of four second order partial differential equations for the four unknown functions $q = q(x, y)$, $\varphi = \varphi(x, y)$, $\theta = \theta(x, y)$ and $\omega = \omega(x, y)$ are obtained. This system is the conformal metric representation of the Helfrich's membrane shape model. By introducing the phenomenological constants $\alpha_2 = 24\mathbb{h}$, $\alpha_3 = 8(2\mathbb{h}^2 - \frac{\lambda}{k})$, $\alpha_4 = \frac{4p}{k} - \frac{8\lambda\mathbb{h}}{k}$, the system takes the form

$$\begin{aligned} q^2(\varphi_{xx} + \varphi_{yy}) &+ 2q\varphi(q_{xx} + q_{yy}) \\ &- 2\varphi(q_x^2 + q_y^2) + q^4(8\varphi + \alpha_2\varphi^2 + \alpha_3\varphi^3 + \alpha_4\varphi^4) = 0 \end{aligned}$$

$$\begin{aligned} \theta_y - \omega_x - (8 + \frac{\alpha_2}{3}\varphi)q(\varphi q_y + q\varphi_y) &= 0 \\ \omega_y + \theta_x - \frac{\alpha_2}{3}q\varphi(\varphi q_x + q\varphi_x) - 8q\varphi q_x &= 0 \end{aligned} \tag{4}$$

$$\begin{aligned} 4q^2\varphi(\varphi_{xx} + \varphi_{yy}) &+ 4q\varphi^2(q_{xx} + q_{yy}) \\ &- 4\varphi^2(q_x^2 + q_y^2) - 4q^2(\varphi_x^2 + \varphi_y^2) - \omega^2 - \theta^2 + (8 + \frac{\alpha_2}{3}\varphi)q^2\varphi\theta = 0. \end{aligned}$$

3. Lie Group Analysis of Differential Equations

The Lie group analysis of differential equations is based on the natural symmetries of the differential equations. A symmetry of a given system of differential equations is a transformation of the independent and dependent variables with the property to transform each solution of the system to solution as well. For the system under consideration (4) a one-parameter group of symmetry transformations is determined by

$$\begin{aligned} x'^i &= \Phi^i(\vec{x},\vec{u},a), \qquad & \Phi^i|_{a=0} &= x^i, \qquad & i &= 1,2 \\ u'^\alpha &= \Psi^\alpha(\vec{x},\vec{u},a), \qquad & \Psi^\alpha|_{a=0} &= u^\alpha, \qquad & \alpha &= 1,2,3,4 \end{aligned} \tag{5}$$

where $a\,(a \in I \subset \mathbb{R}, 0 \in I)$ is the group parameter. The two vectors $\vec{x} = (x^1, x^2)$ and $\vec{u} = (u^1, u^2, u^3, u^4)$ denote the respective independent and dependent variables: $x^1 = x$, $x^2 = y$, $u^1 = q$, $u^2 = \varphi$, $u^3 = \theta$ and $u^4 = \omega$.

The group of transformations (5) is a Lie group of point symmetry transformations (also called an **admissible group**) for the system (4), provided that, the **group generator** [2, 5, 7]

$$X = \sum_{i=1}^{2} \xi^i(\vec{x},\vec{u}) \frac{\partial}{\partial x^i} + \sum_{\alpha=1}^{4} \eta^\alpha(\vec{x},\vec{u}) \frac{\partial}{\partial u^\alpha}$$

satisfies the infinitesimal criterion

$$\mathrm{pr}^{(2)} X[F_\nu] = 0, \qquad \text{for} \qquad F_\nu = 0, \qquad \nu = 1,\ldots,4 \tag{6}$$

where

$$\mathrm{pr}^{(2)} X = X + \sum_{\alpha=1}^{4} \eta^x_\alpha \frac{\partial}{\partial u^\alpha_x} + \sum_{\alpha=1}^{4} \eta^y_\alpha \frac{\partial}{\partial u^\alpha_y} + \sum_{\alpha=1}^{4} \eta^{xx}_\alpha \frac{\partial}{\partial u^\alpha_{xx}} + \sum_{\alpha=1}^{4} \eta^{xy}_\alpha \frac{\partial}{\partial u^\alpha_{xy}} + \sum_{\alpha=1}^{4} \eta^{yy}_\alpha \frac{\partial}{\partial u^\alpha_{yy}}$$

is the **second prolongation** of the operator X with respect to the first and the second order derivatives $u^\alpha_x, \ldots, u^\alpha_{yy}$ and F_ν are the left-hand sides of the equations of the system (4). The coefficients $\eta^x_\alpha, \ldots, \eta^{yy}_\alpha$ are expressed by the first and the second order derivatives of the functions $u^\alpha(\vec{x})$, $\xi^i(\vec{x},\vec{u})$ and $\eta^\alpha(\vec{x},\vec{u})$.

The one-parameter groups, admissible for the given system of differential equations (4), can be found by solving the **Lie equations**

$$\begin{aligned} \frac{\mathrm{d}\Phi^i}{\mathrm{d}a} &= \xi^i(\vec{\Phi},\vec{\Psi}), 7 \qquad & \Phi^i|_{a=0} &= x^i, \qquad & i &= 1,2 \\ \frac{\mathrm{d}\Psi^\alpha}{\mathrm{d}a} &= \eta^\alpha(\vec{\Phi},\vec{\Psi}), \qquad & \Psi^\alpha|_{a=0} &= u^\alpha, \qquad & \alpha &= 1,2,3,4 \end{aligned}$$

where the functions $\xi^i(\vec{x}, \vec{u})$ and $\eta^\alpha(\vec{x}, \vec{u})$ satisfy the infinitesimal criterion (6) and $\vec{\Phi}$ and $\vec{\Psi}$ are vectors with coordinates Φ^i and Ψ^α.

4. Determining System and Symmetries

The infinitesimal criterion (6) results in a linear homogeneous system of partial differential equations – the so called **determining system of equations** for the coefficient functions $\xi^i(\vec{x}, \vec{u})$, $\eta^\alpha(\vec{x}, \vec{u})$ of the symmetry group generator. For most of the important physical applications the determining system consists of hundreds of equations. Creating and solving of such a large system of differential equations, though overdetermined, cause serious technical difficulties. These difficulties can be, at least partially, overcome by the use of the contemporary computer algebra systems, such as `Mathematica`®, *Maple*®, etc.

Concretely we take advantage of the specially developed `Mathematica`® package **LieSymm-PDE** [9]. By applying the package we obtained the determining system of equations for the Helfrich's membrane shape model in conformal metric representation (4), consisting of 206 first and second order partial differential equations. Each one of the equations is a sum of expressions of the form

$$\mu(u^1)^j(u^2)^l(u^3)^m(u^4)^n f(\vec{x}, \vec{u}), \qquad j, l, m, n = 0, 1, \ldots, 7$$

where μ is some real constant and $f(\vec{x}, \vec{u})$ is either one of the functions $\xi^i(\vec{x}, \vec{u})$, $\eta^\alpha(\vec{x}, \vec{u})$ or any of their first or second order derivatives. Thirty five equations consist of more than ten addends (expressions of the above form), six of them are with more than twenty addends, the largest of which are two equations with 43 and 44 addends. Many of these equations are equivalent to each other or functionally dependent, which means that the determining system is overdetermined. Nevertheless, manipulating of so many equations without making errors is quite boring and time consuming. With the aid of the *LieSymm-PDE* facilities for solving determining systems we managed to perform all the symbolic calculations automatically, eluding the tedious substitutions, transformations and other technicalities, which otherwise we should had made by hand.

In order to start up the solving process we invoked a *LieSymm-PDE* iterative function for solving some predetermined types of equations with known solutions [9]. If *LieSymm-PDE* identifies such an equation, its solution is substituted for the respective variable in the remainder part of the equations. In this way the determining system of the Helfrich's model has been reduced to 29 partial differential equations for six unknown functions of the form

$$\xi^1 = h(x, y), \qquad \eta^1 = v(x, y, q, \varphi), \qquad \eta^3 = g(x, y, q, \varphi, \theta, \omega)$$

$$\xi^2 = r(x, y), \qquad \eta^2 = w(x, y, q, \varphi), \qquad \eta^4 = \rho(x, y, q, \varphi, \theta, \omega)$$

where $h(x, y)$ and $r(x, y)$ satisfy the **Cauchy-Riemann conditions**

$$\frac{\partial h}{\partial y} = -\frac{\partial r}{\partial x}, \qquad \frac{\partial h}{\partial x} = \frac{\partial r}{\partial y}. \tag{7}$$

The equations that remained unsolved are not handled by the *LieSymm-PDE* solving modules. In order to solve them we proceeded with applying the package in an interactive mode. Once we had found a solution for at least one of the equations, we fed back this solution as initial data to the program. By rerunning the program successively in seven interactive cycles two of the coefficient functions has changed their form to

$$\eta^1 = q\sigma(x, y), \qquad \eta^2 = -C\varphi$$

($C \in \mathbb{R}$) and the determining system has been reduced to 10 equations

$$\begin{aligned}
q\varphi(24 + \alpha_2\varphi)\rho_\theta + 3\rho_q &= 0 \\
24q^2 r_x + \alpha_2 q^2 \varphi\rho_\theta + 3\rho_\varphi &= 0 \\
q^2\varphi(24 + \alpha_2\varphi)\sigma_x - 3g_x - 3\rho_y &= 0 \\
q^2\varphi(24 + \alpha_2\varphi)\sigma_y - 3g_y + 3\rho_x &= 0 \\
24q^2 r_x - q^2(24 + \alpha_2\varphi)\rho_\theta - 3\rho_\varphi &= 0 \\
3g_\varphi + \alpha_2 q^2\varphi\rho_\omega - 2\alpha_2 q^2\varphi\sigma + 2\alpha_2 C q^2\varphi &= 0 \\
3g_\varphi + q^2(24 + \alpha_2\varphi)\rho_\omega - 2q^2(24 + \alpha_2\varphi)\sigma + 2Cq^2(12 + \alpha_2\varphi) &= 0 \\
3g_q + q\varphi(24 + \alpha_2\varphi)\rho_\omega - 2q\varphi(24 + \alpha_2\varphi)\sigma + 2Cq\varphi(12 + \alpha_2\varphi) &= 0
\end{aligned}$$

$$\begin{aligned}
&2\sigma_{xx} + 2\sigma_{yy} + 2q^2(8 + \alpha_2\varphi + \alpha_3\varphi^2 + \alpha_4\varphi^3)r_y \\
&\quad + 2q^2(8 + \alpha_2\varphi + \alpha_3\varphi^2 + \alpha_4\varphi^3)\sigma - Cq^2\varphi(\alpha_2 + 2\alpha_3\varphi + 3\alpha_4\varphi^2) = 0
\end{aligned}$$

$$\begin{aligned}
&2(\alpha_2 q^2\varphi^2\theta - 6\alpha_2 q^4\varphi^3 - 6\alpha_3 q^4\varphi^4 - 6\alpha_4 q^4\varphi^5 - 48q^4\varphi^2 \\
&\quad + 24q^2\varphi\theta - 3\theta^2 - 3\omega^2)r_y + (\alpha_2 q^2\varphi^2 + 24q^2\varphi - 6\theta)g - 6\omega\rho \\
&\quad - 6(2\alpha_2 q^4\varphi^3 + 2\alpha_3 q^4\varphi^4 + 2\alpha_4 q^4\varphi^5 + 16q^4\varphi^2 - \theta^2 - \omega^2)\sigma \\
&\quad + 6Cq^4\varphi^3(\alpha_2 + 2\alpha_3\varphi + 3\alpha_4\varphi^2) + 6C(4q^2\varphi\theta - \theta^2 - \omega^2) = 0.
\end{aligned}$$

Continuing in the same manner of solving, we have obtained the solution of the above system. Finally, we arrived at the symmetry group generator for the Helfrich's model in conformal metric representation, in the most general form, for two cases of interest (compare with the results in [4, 10, 11])

Case 1. $|\alpha_2| + |\alpha_3| + |\alpha_4| \neq 0$

$$X^{\mathrm{I}}(\xi^1, \xi^2) = \xi^1 \frac{\partial}{\partial x} + \xi^2 \frac{\partial}{\partial y} - q\xi^1_x \frac{\partial}{\partial q} - 2(\theta\xi^1_x + \omega\xi^2_x)\frac{\partial}{\partial \theta} - 2\left[\omega\xi^1_x - \left(\theta - 4q^2\varphi - \frac{\alpha_2}{6}q^2\varphi^2\right)\xi^2_x\right]\frac{\partial}{\partial \omega}$$

Case 2. $\alpha_2 = \alpha_3 = \alpha_4 = 0$

$$X^{\mathrm{II}}(\xi^1, \xi^2) = X_1(\xi^1, \xi^2) + cX_2, \qquad c \in \mathbb{R}$$

with

$$X_1(\xi^1, \xi^2) = \xi^1 \frac{\partial}{\partial x} + \xi^2 \frac{\partial}{\partial y} - q\xi^1_x \frac{\partial}{\partial q} - 2(\theta\xi^1_x + \omega\xi^2_x)\frac{\partial}{\partial \theta} - 2\left[\omega\xi^1_x - \left(\theta - 4q^2\varphi\right)\xi^2_x\right]\frac{\partial}{\partial \omega}$$

$$X_2 = \varphi\frac{\partial}{\partial \varphi} + \theta\frac{\partial}{\partial \theta} + \omega\frac{\partial}{\partial \omega}$$

and $\xi^1 = h(x, y)$, $\xi^2 = r(x, y)$ – arbitrary real-valued harmonic functions satisfying the Cauchy-Riemann conditions (7).

The full sets of group generators $X^{\mathrm{I}}(\xi^1, \xi^2)$ and $X^{\mathrm{II}}(\xi^1, \xi^2)$ constitute two symmetry Lie algebras L^{I} and L^{II} for each one of the considered cases. The Lie algebras L^{I} and L^{II} are infinite dimensional with the commutator operator defined by

$$[X(\xi^1, \xi^2), X(\widehat{\xi^1}, \widehat{\xi^2})] = X(\Xi^1, \Xi^2)$$

where

$$\Xi^1 = \xi^1\widehat{\xi^1_x} - \xi^2\widehat{\xi^2_x} - \widehat{\xi^1}\xi^1_x + \widehat{\xi^2}\xi^2_x, \qquad \Xi^2 = \xi^2\widehat{\xi^1_x} + \xi^1\widehat{\xi^2_x} - \widehat{\xi^2}\xi^1_x - \widehat{\xi^1}\xi^2_x$$

(X equals X^{I} or X^{II} respectively).

5. Conclusion

The results presented here are obtained by an application of the Lie group analysis to a system of differential equations – the Helfrich's shape model of biological membranes. The Helfrich's model has been considered in conformal metric representation. The Lie group analysis has been carried out by the help of the program *LieSymm-PDE* within the computer system `Mathematica`®. The determining system of equations for the admissible group of point symmetry transformations has been created. The determining system consists of 206 second order partial differential equations. With the help of the program *LieSymm-PDE* the determining system has been solved in full explicit form. Its solution constitutes an infinite dimensional symmetry Lie algebra of the Helfrich's model.

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