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Orientational Waves in Cell Membranes

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A theoretical analysis of various types of orientational waves in biological membranes is described. In particular, we consider nonlinear solitary waves (solitions) which may result from local membrane disorder in the presence of an electric field across the cell membrane. The non-dispersive waves could provide an efficient mechanism for the lateral spread of local perturbations in the membrane plane for solute transport across the membrane by modifying the orientation of the lipid molecules.

I. INTRODUCTION

It is now generally accepted that the cell membrane is best described as a two-dimensional, liquid-crystalline structure of lipids and proteins.[1] The studies of the dynamic properties of the membrane components[2-4] indicate that the cell membrane has the characteristics of a smectic liquid crystal: the molecules are arranged in apposed monomolecular layers with their long-axes approximately normal to the plane of the resulting bilayer. The molecules are mobile in the plane of the bilayer and are free to rotate about the bilayer normal. The lipid ordering within the layers is strongly influenced by temperature. Many of these liquid-crystalline properties of cell membranes have been intensively studied over the past decade. However, much less attention has been given to another interesting aspect of the liquid crystals, namely the possible existence of propagating mechanical (orientational) waves. In a paper on

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liquid crystals and living systems, Fergason and Brown[5] speculated that a splay wave propagated along the cell membrane could provide a mechanism for solute transport across the membrane by producing reversal of the orientation of the lipid molecules. No further studies have been reported to substantiate this idea. In the present paper, we describe a theoretical analysis of various types of orientational waves that may exist in the cell membrane. In particular, we focus on the nonlinear solitary waves (soliton), which may result from local membrane disorder in the presence of an electric field across the membrane. The latter non-dispersive waves could provide an efficient mechanism for the lateral spread of local perturbations in the membrane plane.

II. THEORETICAL ANALYSIS

We first assume that the cell membrane is similar to a homogeneous smectic liquid crystal. The lipid molecules exhibit a long range order within the plane of the membrane.[6-7] The membrane is viewed as consisting of many small domains.[8-9] We assume each domain contains a sufficiently large number of molecules so that the long-range orientational order is well defined. Such a domain can be characterized by a director $\mathbf{n}$, which is a unit vector representing the mean (or preferred) direction of molecular orientation. The orientational order of a macroscopic sample of membrane can thus be characterized by a local director $\mathbf{n}(\mathbf{r})$ at each domain "point" $\mathbf{r}$. In the following analysis, a one-dimensional splay wave in an infinite plane of membrane is used for model calculations.

In the absence of an external perturbation, the membrane exists in an equilibrium state, and $\mathbf{n}(\mathbf{r})$ is parallel to an axis (Z) normal to the membrane plane. Supposing that a local perturbation of the membrane creates a disorder of the membrane that can be described by a tilt of the director $\mathbf{n}(\mathbf{r})$ with respect to z axis, a splay wave is formed. Ignoring the dissipation of the perturbation, the Lagrangian density of this system is given by

$$L = T - V_{\text{elastic}} - V_{\text{electric}} \tag{1}$$

where

$$T = \tfrac{1}{2} I\dot{\theta}^2 \tag{2}$$

$$V_{\text{elastic}} = \tfrac{1}{2}\{K_{11}[\nabla \cdot \mathbf{n}(\mathbf{r})]^2 + K_{22}[\mathbf{n}(\mathbf{r}) \cdot \nabla \times \mathbf{n}(\mathbf{r})]^2 + K_{33}[\mathbf{n}(\mathbf{r}) \times \nabla \times \mathbf{n}(\mathbf{r})]^2\}$$

$$\approx \tfrac{1}{2} K[\nabla \cdot \mathbf{n}(\mathbf{r})]^2 + [\nabla \times \mathbf{n}(\mathbf{r})]^2 \tag{3}$$

$$V_{\text{elastic}} = -A[\mathbf{n} \cdot \mathbf{Z}_0]^2 \tag{4}$$

I is the average rotational inertia per unit membrane area, $\theta = \partial(x,t)/\partial t$ is the angular velocity for the rotation of director $\mathbf{n}(\mathbf{r})$, T is the average rotational energy per unit area of membrane during the tilting of molecular orientation and V_{elastic} is the Frank's elastic free energy of this system.[10-11] K_{11}, K_{22}, and K_{33} are splay, twist and bend elastic constants, respectively. We may simplify Eq. 3 by setting $K_{11} = K_{22} = K_{33} = K$. This greatly facilitates the mathematics but does not affect the qualitative behavior of the results. The elastic properties of the membrane originate from the molecular interactions among the membrane components. The elastic constants thus reflect various intramembraneous interactions including the dispersive of Van der Waals' forces among the molecules, the effects of hard cores of each atom, the interactions among polar headgroups of the molecules, and the hydrophobic effects on the molecular orientations in the membrane. V_{elastic}, on the other hand, is the contribution of transmembrane electric field to the Lagrangian density in an anisotropic system. The latter attains a minimum value when the director of molecular orientation is aligned with the field axis (normal to the membrane), represented by a unit vector Z_0.

For a splay wave shown in Figure 1, we have

$$\begin{aligned} n_x &= \sin\theta(x,t) \\ n_y &= 0 \\ n_z &= \cos\theta(x,t) \end{aligned} \tag{5}$$

Substituting Eq. (5) into (1)–(4), we obtain

$$L = \frac{1}{2} I\left(\frac{\partial\theta}{\partial t}\right)^2 - \frac{1}{2} K\left(\frac{\partial\theta}{\partial X}\right)^2 + A\cos^2\theta \tag{6}$$

From the Lagrange–Euler equation, we obtain a basic equation for a one-dimensional splay wave along the membrane:

$$I\frac{\partial^2\theta}{\partial t^2} = K\frac{\partial^2\theta}{\partial X^2} - A\sin 2\theta \tag{7}$$

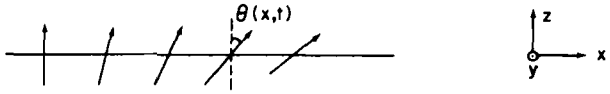

FIGURE 1 A splay wave in a one-dimensional membrane.

In the following, the solution for this equation is described for three different cases.

A. Elastic waves

If we only consider the elastic recovery force in the absence of a transmembrane field, Eq. (7) can be simpified to the following form:

$$\frac{\partial^2\theta}{\partial t^2} = \frac{1}{C_s^2}\frac{\partial^2\theta}{\partial X^2} \tag{8}$$

Where $C_s = \sqrt{K/I}$, is the velocity of the elastic wave propagation.

B. Linear wave

In the case of small perturbations where the amplitude of the splay director is small, we can use a linear approximation of Eq. (7) by taking $\sin 2\theta = 2\theta$. Thus

$$\frac{\partial^2\theta}{\partial X^2} = \frac{1}{C_s^2}\frac{\partial^2\theta}{\partial t^2} + \frac{\omega L^2}{C_s^2}\theta \tag{9}$$

where $\omega_L = \sqrt{2A/I}$, is the characteristic frequency of the membrane. The dispersion relation of the linear wave can be expressed by

$$\omega^2 = \omega_L^2 + C_s^2K^2 \tag{10}$$

where the phase velocity of the wave is

$$v_p = C_s/\sqrt{1 - \omega_L^2/\omega^2} \tag{11}$$

where ω is the angular frequency and k the wave number. When $\omega > \omega_L$, v_p is real, the wave will propagate along the membrane, and $v_p > C_s$. When $\omega < \omega_L$, v_p is imaginary. Assuming $k = i\alpha$ ($i = \sqrt{-1}$, and α is a positive real number), then

$$\theta(x,t) = \theta_0 \exp(-\alpha x) \exp(-i\omega t)$$

This represents an attenuated wave with a characteristic length of attenuation δ given by:

$$\begin{aligned}\delta = 1/\alpha &= C_s/(\omega_L\sqrt{1 - \omega^2/\omega_L^2}) \\ &\approx \sqrt{K/2A} \qquad (\text{if } \omega \geqslant \omega_L)\end{aligned} \tag{12}$$

C. Nonlinear wave

If we introduce $\phi = 2\theta$, $\lambda_0 = \sqrt{K/2A}$ from Eq. (7), we obtain

$$\frac{\partial^2\phi}{\partial x^2} - \frac{1}{C_s^2}\frac{\partial^2\phi}{\partial t^2} = \frac{1}{\lambda_0^2}\sin\phi \tag{13}$$

This is the Sine-Gordon equation in non-normalized form. The limiting or characteristic velocity $C_s = \sqrt{K/I}$ is the velocity of the linear elastic wave in the membrane. λ_0 is the characteristic length of wave propagation. The travelling-wave solution of this nonlinear equation[12-14] has the form of

$$\phi = 4 \tan^{-1}\left[\exp \pm\left(\frac{x - ut}{\lambda_0\sqrt{1 - u^2/C_s^2}}\right)\right] \tag{14}$$

where u is a fixed constant ($|u| < C_s$), i.e. the velocity of this travelling-wave. Solution (14) corresponds to a rotation of the director n, where (+) and (−) signs correspond to a positive and negative rotation, or a "soliton" and antisoliton propagating along the x axis in the positive and negative directions, respectively. The velocity of this nonlinear wave satisfies the condition of $|u| < C_s$, i.e. the nonlinear solitary wave propagates with a velocity smaller than that of the elastic wave.

In order to obtain a physical picture of the propagation of the nonlinear solitary wave, we imagine a coordinate system moving with the same velocity as the wave. In this coordinate system, the orientation angle θ of the director varies with distance x from the center of the wave, as described by

$$\theta = 2 \tan^{-1}[\exp \pm (x/\lambda_0)]$$

Figure 2 plots the orientation angle θ with distance x in units of the characteristic length λ_0. (a) and (b) correspond to a soliton and an antisoliton propagating in the positive and negative directions of the axis, respectively. It is clear that (1) at the arrival of the soliton wave, the average molecular orientation in the membrane undergoes drastic splay or even inversion, and (2) the orientation change is limited within a narrow domain defined by the characteristic length λ_0 of the wave, which in turn reflects the liquid crystalline properties of the membrane molecules.

III. DISCUSSION

The above theoretical analysis points out the possible existence of several kinds of orientation waves in a liquid-crystalline structure of a cell membrane. We now make numerical estimates of some of the characteristic constants associated with these waves. Due to the lack of quantitative data on the physical properties of the cell membranes, these estimates are based on those for liquid bilayer model systems. We expect the properties of cell membranes to be qualitatively similar. First, we

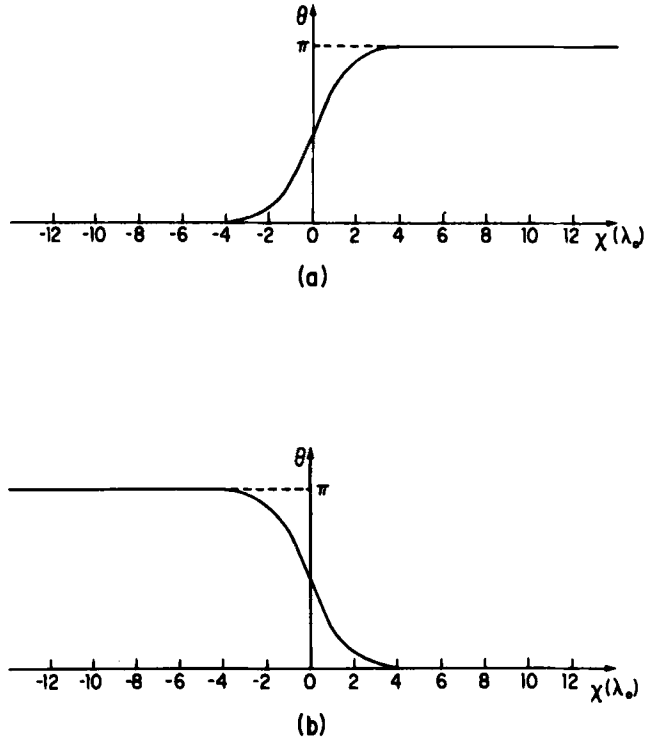

FIGURE 2 The average molecular orientational angle θ with distance x in the unit of the characteristic length λ_0. (a) and (b) correspond to a soliton and an antisoliton propagating in the positive and negative directions along the axis, respectively.

consider the Frank's elastic constant (K_1) of a lipid-bilayer membrane. From dimensional analysis, we expect the value of K_1's to be in the order of U/a, where U is a typical interaction energy between the molecules, and a is the average intermolecular distance.[10-11] The intermolecular interaction energy within the lipid bilayer can be estimated from the latent heat of the phase transition. Taking an average number of carbon atoms in the lipid hydrocarbon chains to be 12, the experimental data on lecithin bilayers[15] indicate that U is about 6.2 Kcal/mol, or 4.3×10^{-13} ergs/molecule. Taking an intermolecular distance of 5 Å, we obtain an elastic constant $K_1 \sim 8.6 \times 10^{-6}$ dynes, so $K = K_1 d = 5.1 \times 10^{-12}$ ergs†, where d is the thickness of the bilayer (60Å). Our

† In the theory of liquid crystals, V_{elastic} has units of ergs per unit volume. For the membrane situation we consider V_{elastic} in ergs per unit membrane area. Thus, the elastic constant K used in the present study is equal to the usual Frank's elastic constant K_1 times the membrane thickness d (see also Ref. 17).

value of the elastic constant is the same order of magnitude as Helfrich and Marcelja's $K_{11}(\sim 2 \times 10^{-12}$ ergs)[16] which was used by Gebhardt *et al.*[8] in their calculation for a mixture of dipalmitoyl lecithin (DPL) and dipalmitoyl phosphatidic acid (DPA). For a first order approximation, the lipid molecule can be considered as a rigid rod of an average length of 25 Å. The rotational inertia of a lipid molecule with respect to an axis lying in the plane of the membrane and the center of rotation at one end of the molecule is given by $I_{\text{molecule}} = \frac{1}{3} ml^2 = \frac{1}{3} (G/A_0)l^2$, where m is the mass and l is the length of the molecule. G and A_0 are molecular weight and Avogadro's constant, respectively. The rotational inertia per unit area of the membrane is thus given by $I \sim I_{\text{molecule}} N_0 = \frac{1}{3}\rho l^2 d$ where $N_0 = (\rho/G)A_0 d$ is the number of molecules per unit area and ρ is the specific density of the lipids. Taking $\rho \sim 1$ gm/cm^3 and $l = 25$ Å, we obtain $I \sim 1.3 \times 10^{-20}$ gms. Thus, the velocity of the elastic wave (and the upper limit of that of the nonlinear soliton wave) is given by

$$C_s = \sqrt{K/I} \sim 200 \text{ m/sec}$$

In the presence of an electric field across the membrane, the electric field contribution to the free-energy density (per unit membrane area), similar to the treatment in the elastic continuum theory of liquid crystals,[10,11] is given by

$$-\frac{\Delta\epsilon}{8\pi} [\mathbf{E} \cdot \mathbf{n}(\mathbf{r})]^2 d$$

where $\Delta\epsilon = \epsilon_{\parallel} - \epsilon_{\perp}$ is the difference between the local dielectric constants in directions parallel and perpendicular to the local director $\mathbf{n}(\mathbf{r})$; $\mathbf{E} = E\mathbf{Z}_0$ is the transmembrane electric field and $\mathbf{Z}_0$ is the unit vector normal to the membrane plane. Comparing to Eq. (4), we obtain the constant $A = (\Delta\epsilon E^2/8\pi)d$. From experimental data on black lecithin films,[18] we take $\Delta\epsilon = \epsilon_{\parallel} - \epsilon_{\perp} = (n_{\parallel})^2 - (n_{\perp})^2 \sim 0.06$, where $n_{\parallel}$ and $n_{\perp}$ are refractive indices parallel and perpendicular to the normal of the membrane plane, $E = \Delta V/d$, where ΔV is the transmembrane potential (taken to be 80 mV) and d is the thickness of the bilayer (~60 Å). We thus obtain an A value of about 2.6×10^{-4} ergs/cm^2. The characteristic frequency of the membrane is given by

$$\omega_L = \sqrt{2A/I} \sim 2 \times 10^8 \text{ sec}^{-1}$$

and the characteristic length for the splay spread in an attenuated nonpropagating linear wave and for that of a propagating non-linear wave (soliton) is

$$\delta \sim \lambda_0 = \sqrt{K/2A} \sim 1 \ \mu\text{m}$$

To sum up, we note that in the absence of a membrane potential (transmembrane electric field), the only possible wave in a cell membrane is a conventional elastic wave, having a propagating velocity of about 200 m/sec. In the presence of membrane potential, we have two possible situations: (a) with small perturbations we have an attenuated, nonpropagating linear wave with a characteristic decay distance of about 1 μm. A propagating linear wave is unlikely to occur, since the characteristic frequency of biologically relevant perturbations is unlikely to exceed that of the cell membrane (2×10^8 sec^{-1}). (b) When the perturbation exceeds a threshold value, a non-dispersive, non-linear solitary wave (soliton) could be produced. This wave could propagate over long distances along the cell membrane.

As mentioned above, Fergason and Brown[5] speculated that a splay wave propagated along the cell membrane could provide a mechanism for ion transport across the membrane by producing a reversal of the orientation of the lipid molecules. This idea is consistent with a change in the average molecular orientation in the membrane upon the arrival of a non-linear splay wave (soliton). A complete lipid inversion, however, seems unlikely. Nevertheless, splay waves could have significant effects on transport proteins in bilayers or on a bilayer's permeability to a variety of solutes. Due to the lack of experimental data so far, the existence of these orientational waves in biological membranes is unconfirmed. If they exist, they could be related to some cooperative phenomena in the membrane.

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