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RESEARCH ARTICLE

Collective dynamics of domain structures in liquid crystalline lipid bilayers

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Abstract

Objectives. Numerous studies of biosystems indicate the distinct role of quasi-one-dimensional molecular structures in the transport of energy, charges, and information. Of particular interest are the studies on the collective dynamics of quasi-one-dimensional lateral structures in liquid crystalline membranes and the possibility of local excitation transfer through such structures. In this paper, we developed a model for the collective dynamics of quasi-one-dimensional domain structures in lipid bilayers interacting with the environment. The objective is to study the mechanisms of the directed energy transport in liquid crystalline lipid membranes.

Methods. In this paper, the percolation domain structures formed as a result of phase separation in multicomponent lipid membranes are considered to be quasi-one-dimensional domain structures. The model distinguishes two subsystems interacting with each other and differing in their structural and dynamic properties, i.e., the membrane surface formed by polar groups of lipid molecules and the internal hydrophilic region of the membrane formed by acyl chains of lipids. The acyl chain subsystem is simulated using the Ginzburg–Landau Hamiltonian which considers the dependence of its dynamics on temperature close to the lipid melting phase transition temperature T_c.

Results. Analysis of dynamic states has shown that elastic excitations moving at constant rate in the form of solitons may exist near temperatures T_c in the considered quasi-one-dimensional domain structures. In addition, motion of the elastic excitation region (kink) along domain structures in the acyl chain region causes the formation of acoustic soliton, i.e., the compression region in the polar group subsystem moving in concert with the kink displacement. The soliton localization region covers about 10 molecules and depends significantly on the interaction parameter of the polar group and acyl chain subsystems. Soliton moves at a subsonic speed determined, in particular, by the magnitude of an external force.

Conclusions. The model developed in this paper shows that liquid crystalline domain structures in lipid membranes exhibit properties of active media, wherein the formation and displacement of localized elastic excitations on macroscopic spatial and temporal scales may occur. The proposed molecular mechanism of the soliton transport along quasi-one-dimensional domain structures may be used for describing the directed energy transfer along lateral domain channels in biomembranes and the cooperative functioning of the membrane bioenergetic and receptor complexes.

Keywords: collective dynamics, liquid crystalline domain structures, multicomponent lipid membranes, soliton, directed energy transport

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НАУЧНАЯ СТАТЬЯ

Коллективная динамика доменных структур в жидкокристаллических липидных бислоях

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Резюме

Цели. Многочисленные исследования биосистем указывают на особую роль квазиодномерных (квази-1D) молекулярных структур в процессах транспорта энергии, зарядов и информации. В этой связи особый интерес представляют исследования коллективной динамики квази-1D латеральных структур в жидкокристаллических (ЖК) мембранах и возможности передачи по таким структурам локальных возбуждений. С целью исследования молекулярных механизмов направленного транспорта энергии в ЖК липидных мембранах в настоящей работе разработана модель коллективной динамики квази-1D доменных структур (ДС) в ЖК бислоях, взаимодействующих с окружающей средой.

Методы. В качестве квази-1D ДС рассмотрены перколяционные ДС, формирующиеся при фазовом разделении липидных молекул в многокомпонентных мембранах. В модели выделены две взаимодействующие между собой подсистемы, различающиеся по своим структурным и динамическим свойствам: поверхность мембраны, образованная полярными группами (ПГ) липидных молекул и внутренняя гидрофильная область мембраны, сформированная ацильными цепями (АЦ) липидов. При моделировании подсистемы АЦ использован гамильтониан Гинзбурга – Ландау, учитывающий зависимость ее динамики от температуры вблизи температуры фазового перехода плавления липидов T_c.

Результаты. Анализ динамических состояний модели показал, что вблизи температур T_c в рассматриваемых квази-1D ДС могут существовать перемещающиеся с постоянной скоростью возбуждения в виде солитонов. При этом движение упругого возбуждения (кинка) вдоль ДС в области АЦ вызывает образование акустического солитона – области сжатия в подсистеме ПГ, перемещающейся согласованно с движением кинка. Область локализации солитона охватывает примерно 10 молекул и существенно зависит от параметра взаимодействия подсистем ПГ и АЦ. Движение солитона происходит с дозвуковой скоростью, которая определяется, в частности, величиной внешнего воздействия.

Выводы. В рамках разработанной модели показано, что ЖК ДС в липидных мембранах проявляют свойства активных сред, в которых может происходить формирование и перемещение локализованных упругих возбуждений в виде солитонов на макроскопических пространственных и временных масштабах. Предложенная модель молекулярного транспорта энергии вдоль квази-1D ДС может быть применена к описанию направленной передачи энергии по латеральным доменным каналам в биомембранах и кооперативного функционирования мембранных биоэнергетических и рецепторных комплексов.

Ключевые слова: коллективная динамика, жидкокристаллические доменные структуры, многокомпонентные липидные мембраны, солитоны, направленный транспорт энергии

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INTRODUCTION

The electro-optical and morphological properties of liquid crystal (LC) planar systems determine their high sensitivity to external influences resulting in a fast change in their macroscopic characteristics. The occurrence of a threshold collective response in nematic liquid crystal (NLC) films to external factors is the basis of their high structural mobility. This determines their wide application in various fields of engineering as materials with easily controllable properties. The unique properties of LC are also responsible for the wide distribution of LC structures in living systems and their important biological role [1]. The application of LC physics and condensed matter physics approaches to studying LC states in living cells has led to the development of physics of active LC structures in living systems functioning far from equilibrium states in the presence of pumping and energy dissipation [2].

Active LC structures in cells include lyotropic LC cell membranes as one of their main structural and functional elements. In addition to the functions of cellular compartment formation, they play an active role in the spatial organization of the matrix for embedding signal membrane receptors and bioenergetic protein complexes on the membrane surface, providing optimal conditions for their functioning [1]. Due to the high structural mobility of LC states, membranes may perform a variety of communication functions, providing the transmembrane transport of substances and signal molecules between the cell and the external environment. Furthermore, LC membranes provide the lateral transport of biologically active molecules along the membrane surface. Mitochondrial membranes also play a complex spatial-organizing role in cell bioenergetics, providing cluster organization of nanoscale molecular machines of the respiratory system [3]. It is assumed that the functioning of active LC membranes is realized by the excitation of cooperative molecular processes in complex LC bilayers.

The complex structure of LC lipid membranes is related to their heterogeneous structure resulting from the diverse composition of lipid molecules which differ both in their molecular structure and phase state. The heterogeneous structure of membranes manifests itself in their domain organization by determining many physiological properties of biomembranes [1]. First, the role of membrane domain organization in the formation of specific lipid microenvironment for membrane proteins ensuring their optimal functioning is noted. The destruction of domain structures (DSs) has been shown to result in membrane protein system failure [4]. Secondly, the role of DS in transport and communication processes on the membrane surface is noted [5]. In particular, this study considers the formation of quasi-one-dimensional (quasi-1D) percolation cluster networks formed in the phase separation area of lipid molecules which differ in their structure and phase state [6]. It is assumed that quasi-1D DSs and their networks can act as lateral channels for the directed energy and charge transport along the membrane surface, as well as provide interaction between membrane bioenergetic and receptor complexes [5]. The directed transport and channelling of energy and charges along quasi-1D DSs may surpass the passive transport realized through the two-dimensional diffusion of molecules along the membrane surface in its efficiency.

In the paper, we developed the model for collective dynamics of quasi-1D DSs in lipid bilayers interacting with the environment, in order to study mechanisms of the directed energy transport along LC DSs. It was shown that nonlinear excitations capable of maintaining the interaction and energy transfer between membrane proteins and receptors over considerable distances possibly occur in the DS system. The analytical study has revealed that when considering the interaction of lipid molecules with each other and the environment, excitations like acoustic solitons representing compression (extension) regions moving at constant rate may exist in the considered quasi-1D lateral DSs in lipid bilayers.

1. A DYNAMIC MODEL OF LIPID DOMAIN STRUCTURES

Let us consider the one-dimensional chain of lipid molecules which forms a quasi-1D domain in a flat membrane. The following two subsystems may be distinguished in the lipid membrane structure: the membrane surface formed by the polar groups (PG) of lipid molecules; and the inner hydrophobic region of the membrane formed by the acyl chains (AC) of lipids.

Since the PG and AC regions have different properties and participate in different molecular excitations, the Hamiltonians of non-interacting PG and AC subsystems may be written separately, and then the interaction energy between them may be introduced. The Hamiltonian of interacting PGs of lipid molecules in the harmonic approximation may be written as follows:

$$H_1 = \sum_n \frac{1}{2} m \left[\dot{p}_n^2 + \Omega_0^2 p_n^2 + \Omega_1^2 \left(p_{n+1} - p_n \right)^2 \right], \quad (1)$$

where p_n is the displacements of the nth PG relative to the equilibrium position of the PGs spaced a distance a apart; m is PG mass; Ω_0 and Ω_1 are the characteristic frequencies of vibrations in the PG system. The last term in Eq. (1) takes into account the dispersion of elastic waves in the PG chain. The point stands for differentiation by time t.

The dynamics of the AC subsystem significantly depends on the membrane temperature T. The phase transition, i.e., lipid melting occurring through AC rotational isomerization of lipid molecules (conformational melting) thus resulting in their increased mobility, can be observed in membranes near the phase transition temperature T_c [1]. Therefore, the Ginzburg–Landau Hamiltonian widely used for studying critical phenomena in various structures, including the description of the collective dynamics of lipid membranes, may be most suitable for describing the AC chain dynamics [7, 8]. It is written as follows:

$$H_2 = \sum_n \frac{1}{2} M \left[\dot{u}_n^2 + \omega^2 \left(u_{n+1} - u_n \right)^2 \right] + U_T(u_n) \quad (2)$$

with double-well potential

$$U_T(u_n) = \frac{1}{2} G u_n^2 + \frac{1}{4} B u_n^4, \quad (3)$$

where $G < 0$ and $B > 0$ at $T < T_c$; $G > 0$ and $B > 0$ at $T > T_c$. M is AC mass; $\omega^2 = K/M$, where K is the membrane elastic modulus. The variable u_n characterizes the instantaneous position of the nth AC relative to the equilibrium position corresponding to the top of the potential barrier.

In Eq. (3), the dependence of parameter G on temperature may be written as follows:

$$G(T) = E_0(T/T_c - 1), \quad (4)$$

where E_0 is the height of the potential barrier [9]. The temperature range near T_c spans a few degrees [1]. The symmetric double-well potential (3) has two minima located at a distance from the barrier top:

$$u_0 = \pm \sqrt{\frac{|G|}{B}}. \quad (5)$$

Within the high-temperature range, the following harmonic representation of the AC subsystem Hamiltonian is valid at $T >> T_c$:

$$H_2' = \sum_n \frac{1}{2} M \left[\dot{u}_n^2 + \omega^2 (u_{n+1} - u_n)^2 \right]. \quad (6)$$

The Hamiltonian of the interaction between PG and AC considering the change in the conformation of the closest ACs, when PGs are displaced from the stable equilibrium position may be written as [8]:

$$H_3 = \sum_n \chi p_n (u_n^2 - u_0^2), \quad (7)$$

where χ is the interaction constant generally depending on the lipid molecule structures and the membrane environment.

Turning from the discrete to the continuum approximation in describing the dynamics of the quasi-1D lateral structure in the membrane, the following expression for the system Hamiltonian may be written:

$$H_M = \frac{1}{a} \int \frac{M}{2} (u_t^2 + c_0^2 u_x^2) + U_T(u) + \\ + \frac{m}{2} (p_t^2 + \Omega_0^2 p^2 + V_0^2 p_x^2) + \chi p (u^2 - u_0^2) dx, \quad (8)$$

where $c_0 = a\omega_1$ is the velocity of sound in the AC subsystem and $V_0 = a\Omega_1$.

At temperatures $T < T_c$, potential function $U_T(u)$ (3) may be written as follows:

$$U_T(u) = \frac{1}{2} |G(T)| u^2 + \frac{1}{4} B u^4. \quad (9)$$

The system of motion equations for the coupled PG and AC system with Hamiltonian H_M (8) may be written as follows:

$$M u_{tt} - M c_0^2 u_{xx} - |G| u + B u^3 + 2\chi p u = f_u, \quad (10)$$

$$M p_{tt} + \Omega_0^2 p - V_0^2 p_{xx} + \chi (u^2 - u_0^2) = 0. \quad (11)$$

When considering the interaction of the two basic PG and AC subsystems with physical fields of the environment, the following terms accounting for viscous friction and external influences should be added to Eqs. (10) and (11):

$$Mu_{tt} - Mc_0^2 u_{xx} - M\Gamma_u u_t - |G|u + Bu^3 + 2\chi pu = f_u, \quad (12)$$

$$Mp_{tt} + \Omega_0^2 p - M\Gamma_p p_t - V_0^2 p_{xx} + \chi(u^2 - u_0^2) = f_p. \quad (13)$$

where $\Gamma_u > 0$ and $\Gamma_p > 0$ are viscous friction coefficients the PG and AC subsystems, while $f_u > 0$ and $f_p > 0$ are are right-hand sides of the equations considering external and internal forces acting upon each subsystem. The elastic stress forces acting at phase interfaces (domains) may act as internal forces. The structures in the quasi-1D DS model under consideration resulting from phase separation are either influenced by compression forces or experience tension depending on the membrane lipid composition and the interface type.

2. DYNAMICS OF QUASI-ONE-DIMENSIONAL DOMAIN STRUCTURES OF LIPID MOLECULES

Let us consider the equations of motion (11) and (12) without taking into account the interaction between PG and AC subsystems and the environment. Then Eq. (11) for the AC dynamics may be transformed into the well-known Ginzburg–Landau equation, as follows:

$$Mu_{tt} - Mc_0^2 u_{xx} - |G|u + Bu^3 = 0. \quad (14)$$

In the low-amplitude limit, $u(x, t)$ describes small displacements $\delta u(x, t)$ of AC near one of the equilibrium positions $u(x, t) = \pm u_0 + \delta u(x, t)$. In a first approximation in $\delta u(x, t)$, these displacements are described by the following equation:

$$M\delta u_{tt} - Mc_0^2 \delta u_{xx} - |G|\delta u = 0, \quad (15)$$

which has the following fundamental solution:

$$\delta u(x,t) \sim e^{i(\omega t - kx)}. \quad (16)$$

The dispersion of elastic waves is defined by the following expression:

$$\omega^2 = \frac{|G|}{M} + c_0^2 k^2 = \omega_0^2 + c_0^2 k^2, \quad (17)$$

where k is a wave vector.

In addition, Eq. (15) has a solution in the form of a soliton wave of non-small finite amplitude:

$$u(x,t) = \mp u_0 \tanh\left(\frac{\omega_0}{\sqrt{c_0^2 - V^2}}(x - Vt)\right). \quad (18)$$

Here, the upper sign corresponds to the soliton (kink) moving with velocity $V < c_0$, while the lower sign corresponds to the antikink. The width of the soliton (kink or antikink) is determined by the following formula:

$$\Delta_0 = \frac{\sqrt{c_0^2 - V^2}}{\omega_0} = \sqrt{\frac{M(c_0^2 - V^2)}{|G|}},$$

where $\omega_0 = (|G|/M)^{1/2}$.

In the absence of interaction between the PG and AC subsystems with each other and with the environment, Eqs. (12) and (13) describe longitudinal (sound) waves with dispersion, as follows:

$$\Omega^2(q) = \Omega_0^2 + V_0^2 q^2, \quad (19)$$

where q is a wave vector.

Let us consider the dynamics of the quasi-1D lateral structure of lipids when taking into account the interaction between the PG and AC subsystems, which is described by Eqs. (12) and (13). In this case, the viscous friction coefficient Γ_u in the PG subsystem is ignored and the external influence on the PG subsystem is assumed to be small, so the PG displacements caused by the external forces may be neglected. Turning to a new spatial variable $\xi = x - Vt$ in Eqs. (12) and (13), the following system of two ordinary differential equations may be written:

$$M(V^2 - c_0^2)u_{\xi\xi} - M\Gamma_u u_\xi - |G|u + Bu^3 + 2\chi pu = f_u, \quad (20)$$

$$M(V^2 - V_0^2)p_{\xi\xi} + m\Omega_0^2 p + \chi(u^2 - u_0^2) = 0. \quad (21)$$

Of particular interest is the excitation moving along the considered structure at constant velocity $V = V_0$. Then Eq. (21) implies the following:

$$p = -\frac{\chi}{m\Omega_0^2}(u^2 - u_0^2). \quad (22)$$

Substituting this relationship into Eq. (20) with the consideration of the expression for u_0 (5), the equation describing the excitation dynamics in the AC subsystem may be written in the following form:

$$M(V^2 - c_0^2)u_{\xi\xi} - M\Gamma_u u_\xi - G_1 u + B_1 u^3 = f_u, \quad (23)$$

where

$$G_1 = \theta|G|, \; B_1 = \theta|B|, \; \theta = 1 - \frac{\chi^2}{m\Omega_0^2 B}, \; 0 < \theta < 1.$$

We shall turn to the new variables in Eq. (23)

$$z = \frac{\xi}{L} = \frac{\sqrt{2}\xi}{\Delta} \text{ and } \eta = \frac{u}{u_0},$$

where Δ is the width of the excitation localization region. Then the equation describing the excitation state in AC subsystem of lipid molecules is written in the following form:

$$\eta_{zz} + \mu\eta_z - \eta + \eta^3 - \lambda = 0, \quad (24)$$

where

$$\mu = V\Gamma_u\sqrt{\frac{M}{(c_0^2 - V^2)G_1}}, \quad (25)$$

$$\lambda = f_u\sqrt{\frac{B_1}{G^3}}. \quad (26)$$

The solution of Eq. (24) may be written using the roots of a polynomial [9]:

$$\Phi(\eta) = -\eta + \eta^3 - \lambda = (\eta - \eta_1)(\eta - \eta_2)(\eta - \eta_3). \quad (27)$$

Here, values $\eta_1 < \eta_2 < \eta_3$ satisfy the following relations:

$$\eta_1 + \eta_2 + \eta_3 = 0,\ \eta_1\eta_2 + \eta_2\eta_3 + \eta_1\eta_3 = -1,\ \eta_1\eta_2\eta_3 = \lambda$$

and define the stationary states of the system:

$$u_1(x,t) = \eta_1 u_0,\ \ u_2(x,t) = \eta_2 u_0,\ u_3(x,t) = \eta_3 u_0. \quad (28)$$

In addition, Eq. (24) has a solution describing excitation moving at constant velocity in the form of a soliton wave (of non-small finite amplitude), provided that

$$\mu = \pm\frac{3\eta_3}{\sqrt{2}}. \quad (29)$$

The specified solution in variables u, x, and t may be written in the following form [9]:

$$u(x,t) = \pm u_0\left(\eta_1 + \frac{\eta_2 - \eta_1}{1 + \exp\dfrac{x - Vt}{\Delta}}\right), \quad (30)$$

where

$$\Delta = \frac{\sqrt{2M(c_0^2 - V^2)}}{\sqrt{G_1(\eta_3 - \eta_1)}}. \quad (31)$$

The minus sign in Eq. (30) corresponds to the kink ($\eta < 0$), while the plus sign stands for the anti-kink. Eqs. (25) and (26) define the relation between the soliton velocity and the external field in the following form:

$$V^2 = \frac{9c_0^2 G_1\eta_3^2}{2M\Gamma_1^2 + 9G_1\eta_3^2} = V_0 < c_0^2. \quad (32)$$

The soliton velocity V is always less than c_0 because the soliton radiates waves when accelerating under external influence. This results in the additional energy loss (dissipation) not considered in Eqs. (23) and (32), according to which $V \to c_0$ with decreasing f_u (at $f_u \to 0$). The propagation direction of excitation (soliton) is determined by the f_u sign.

The excitation (kink) motion in the AC subsystem causes the formation of the compression (extension) region in the PG subsystem moving in concert with the kink motion in the AC subsystem. The spatiotemporal structure of the deformation region in the PG system is determined by the equation following from relations (22) and (30):

$$p(x,t) = \frac{\chi u_0^2}{m\Omega_0^2}\left[\left(\frac{\eta_1\exp\dfrac{x - Vt}{\Delta} + \eta_2}{1 + \exp\dfrac{x - Vt}{\Delta}}\right)^2 - 1\right]. \quad (33)$$

At the fixed value of parameter $V = V_0$, the solutions for Eqs. (10) and (11) have the following forms:

$$u(x,t) = \mp u_0\tanh\frac{x - Vt}{\Delta}, \quad (34)$$

$$p(x,t) = \frac{\chi u_0^2}{m\Omega_0^2}\operatorname{sech}^2\frac{x - Vt}{\Delta}. \quad (35)$$

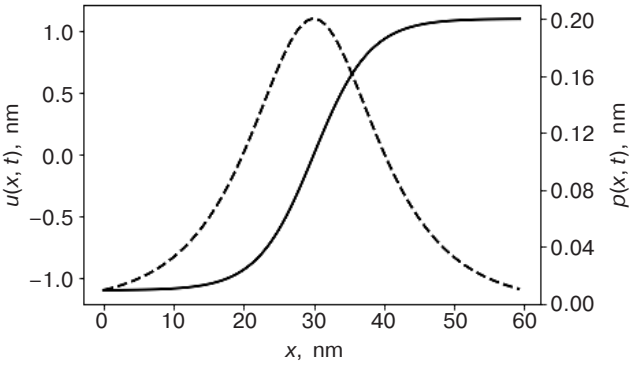

Figure. Displacements of AC $u(x, t)$ (34) (solid curve) and PG $p(x, t)$ (35) (dashed curve) of lipid molecules in quasi-1D DS of the membranes

Figure shows calculation results of the displacement of AC $u(x, t)$ (34) and PG $p(x, t)$ (35) of lipid molecules

in a quasi-1D DS of the membrane. Calculations have been performed with the parameters derived from the following experimental data. The characteristic frequency $\Omega_0 = 10^{11}$ Hz is estimated on the basis of experimental data for PG dipole oscillations [8]. The value $c_0 = 200$ m/s as an estimate of sound velocity was taken from the interval of values obtained in experiments on measuring of the sound velocity in lipid monolayers [7]. The value $u_0 = 1.1$ nm is estimated on the basis of experimental data for the AC average angle of inclination (34°–41°) in $L_{\beta'}$ phase in lecithin liposomes [10]. The kink width value $\Delta = 8.0$ nm is estimated from the data on the size of defect area formed in the AC subsystem of the lipid membranes at temperatures close to the main phase transition temperature (pre-transition temperature range) [10]. At the calculated value of width Δ, the soliton region covers approximately 10 lipid molecules. The kink solution for the AC displacement $u(x, t)$ describes a dislocation-type defect forming in AC subsystem. Negative and positive values $u(x, t)$ correspond to deviations of AC of lipid molecules in opposite directions. The soliton solution for the PG displacement $p(x, t)$ describes the compression deformation in PG subsystem caused by the defect in AC.

Comparing the equations for the soliton width Δ (18) and (31) derived without considering the PG and AC interaction, it may be seen that the interaction of the PG and AC subsystems results in increasing excitation region (kink or antikink width) by $\sqrt{\theta}$ times. Thus, with increasing interaction parameter χ, the potential barrier height $E = \theta E_0$ decreases and the excitation autolocalization region increases.

With increasing temperature in the temperature range below T_c, the value of parameter $G(T)$ (4), determining the barrier height of the potential $U_T(u_n)$ (3), decreases that leads to a single minimum potential $T > T_c$ and disappearing of bistability in the system. A decrease in $G(T)$ results in the soliton spatial size reduction.

Thus, the degree of excitation localization in the one-dimensional membrane lipid structure increases as the temperature approaches T_c. This is due to the increase in the effective force λ (26) in Eq. (24), which increases with increasing temperature as $|T - T_c|^{-1.5}$ up to the maximum value determined by Eq. (26). At the same time, as noted above, the sign of the external force determines the propagation direction of excitation along quasi-linear DCs in the membrane. In addition, the soliton becomes asymmetric under the impact of the external field.

With increasing temperature T and, consequently, effective force λ (26), the soliton velocity along the lipid chain also increases. At temperatures close to $\lambda = \lambda_{max}$, the localized state begins to collapse, and a periodic spatiotemporal structure of cnoidal wave type is formed.

3. DISCUSSION

Numerous theoretical studies in biophysics indicate the distinct role of quasi-1D regular molecular structures in biosystems including the transport of energy, matter, and information over considerable molecular distances [11–13]. This research area covers mainly the transport of energy and charges along linear molecules such as DNA, polypeptides, and linear polymers [14–16]. Of particular interest in this regard are studies of the collective dynamics of quasi-1D lateral structures in multicomponent biological membranes and the possibility of transferring local excitations through such structures, which are caused by physical and chemical influences on selected membrane components. This interest is determined by the crucial role of biological membranes in living cells. It is assumed that the nature of the cooperative properties of biological membranes is determined by the interaction of its subunits (receptors and ion channels) carried out through such quasi-1D structures in lipid bilayers [5].

This paper undertakes a theoretical study on the collective dynamics of quasi-1D domain structures in liquid crystalline lipid membranes. Here, quasi-1D structures of lipid molecules formed as a result of lateral domain organization of the bilayer are considered as quasi-1D DS in the membranes. The existence of these structures in cellular membranes is confirmed by various experimental methods: X-ray diffraction, neutron scattering, electron paramagnetic resonance (EPR), and electron microscopy in multicomponent lipid bilayers [6, 17, and 18], as well as by numerical simulation of DSs in lipid membranes. Computer simulations showed that the self-organization of percolation DSs may result from phase separation in two-component membranes formed by lipid molecules differing in their structural and physical properties [19, 20].

In the developed model of quasi-1D DS dynamics, we considered two interacting subsystems in lipid bilayers: the membrane surface formed by PG of lipid molecules; and the inner hydrophobic region of the membrane consisting of lipid ACs. The model took into account the significant dependence of the AC subsystem dynamics on temperature T in temperature range T_c of the lipid melting phase transition [1]. Therefore, the Ginzburg–Landau Hamiltonian, widely used in the study of critical phenomena, is chosen for describing the hydrophobic region dynamics of lipid ACs. The results of an analytical study in the paper showed that elastic excitations moving at constant velocity in the form of soliton waves (of non-small finite amplitude) may exist in the quasi-1D lateral structures of lipids when taking into account the interaction of two subsystems with each other and the environment. The formation and displacement of a defect (dislocation) in the AC

subsystem causes the formation of the acoustic soliton as the compression region in the lipid PG subsystem moving in concert with the displacement of the defect (kink) in the AC subsystem. Thus, the soliton-type excitations formed in quasi-1D DS are local regions of of lipid PG displacements and structural defects in the AC subsystem moving along the molecular structure. When increasing temperature T (with the external influence unchanged), the soliton velocity along the chain of lipid molecules and its localization degree increase. However, at a certain temperature value close to melting temperature T_c, the localized state begins to collapse, and the periodic spatial structure of cnoidal wave type is formed. We suggested that this periodic structure may be correlated with the $P_{\beta'}$ phase observed in lipid bilayers in the temperature range below the main phase transition temperature [10]. It should also be noted that disturbances in the form of small amplitude waves (small-amplitude phonons) whose frequency decreases with increasing temperature up to zero at $T = T_c$ ("soft mode") may exist in the considered quasi-1D DS at $T < T_c$ [21].

Experimental data on the observation of soliton-type excitations in lipid bilayers have been obtained in a number of experiments using different methods for excitation and registration of elastic pulses. In the experiment with optical generation of elastic waves in lipid monolayers, excitation of acoustic soliton-like pulses forming and propagating with shape preservation has been observed at surface pressure above a certain threshold value [22]. Elastic excitations of the soliton type have been also observed in lipid liposomes in the lipid melting temperature range [23]. Soliton formation and motion have been also detected and studied in nematic and cholesteric LC planar structures using methods of nonlinear optics under various experimental conditions [24, 25]. It has been shown experimentally that formation of solitons (small-width domain walls) occurs in the magnetic field or under the action of shear stresses within a certain range of values. Soliton formation and motion in nematic LC planar structures have been described theoretically within the framework of the Ericksen–Leslie theory for the nematic state [24]. It was shown in our paper that similar soliton-type excitations may occur in lyotropic LC DSs in lipid membranes.

The described mechanism of local region formation of elastic deformation and its motion in the form of a soliton is considered to be a possible molecular mechanism of directed transport of elastic energy along the LC membrane surfaces. The soliton capture by membrane protein complexes (receptors, ion channels) results in the elastic energy transfer to the protein molecule, which may be a trigger for their conformational transitions and their activation [26]. It is also assumed that excitation and propagation of the elastic deformation pulse in the form of a soliton may accompany the nerve impulse propagation in the axon [23].

The formation and displacement of the local deformation region in the membrane may also result in the charge capture by the soliton and the charge motion together with it. The capture mechanism and the resulting charge transport process by the acoustic soliton along one-dimensional molecular structures are discussed in [13, 27, and 28]. Similarly, the capture of charges and their transport by solitons in quasi-1D DS of lipid membranes may result in lateral transport in cell membranes. The possibility of particle transport by solitons has been confirmed in experimental studies of solitons in planar cholesteric LC structures [25]. It was established in the paper that the soliton corresponding to the local defect in LC structure is an attraction region for impurity particles, resulting in the capture of particles and their transport by the moving soliton. Further progress and application of the developed model to the description of soliton transport of particles in LC membranes will be discussed in the next paper.

CONCLUSIONS

The simulation of dynamic properties of LC domain structures of lipid membranes, carried out in the paper, showed that these structures exhibit the properties of active media, wherein the formation of localized coherent excitations on macroscopic spatial and temporal scales occurs. The formation process of localized soliton-type excitations in quasi-linear domain structures represents the formation of the local deformation region in the PG system and the formation of topological defects in the AC system of lipid molecules. The simulation results revealed the possibility of a soliton motion along quasi-1D DSs as the non-dissipative motion of the local deformation region in the chain of lipid PGs, accompanied by the cooperative motion of the defect (kink) in the region of acyl chains of lipid molecules. The molecular mechanism herein proposed may be used for describing the elastic energy directed transfer along LC membranes and the cooperative behaviour of membrane bioenergetic complexes. Further development of the model will be targeted at describing the molecular mechanisms of particle capture by moving solitons and directed transport of charged particles (protons and electrons) along quasi-linear domain structures in biological and artificial polymeric membranes.

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REFERENCES

1. Gennis R. *Biomembrany: molekulyarnaya struktura i funktsii* (*Biomembranes: molecular structure and function*). Moscow: Mir; 1997. 624 p. (in Russ.). ISBN 5-03-002419-0
[Gennis R. *Biomembranes: Molecular Structure and Function.* New York: Springer; 1989. 533 p.]
2. Zhao J., Gulan U., Horie T., et al. Advances in biological liquid crystals. *Small.* 2019;15(18):1900019. https://doi.org/10.1002/smll.201900019
3. Nesterov S.V., Chesnokov Y.M., Kamyshinsky R.A., Yaguzhinsky L.S., Vasilov R.G. Determining the structure and location of the ATP synthase in the membranes of rat's heart mitochondria using cryoelectron tomography. *Nanotechnol. Russia.* 2020;15(1):83–89 (in Russ.) https://doi.org/10.1134/S1995078020010139
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4. Zhou Y., Prakash P., Liang H., Cho K.J., Gorfe A.A., Hancock J.F. Lipid-sorting specificity encoded in K-ras membrane anchor regulates signal output. *Cell.* 2017;168(1–2):239–251.e16. https://doi.org/10.1016/j.cell.2016.11.059
5. Marsh D. Connectivity of membrane domains. *Biophys. J.* 1993;64(2):299–300. https://doi.org/10.1016/S0006-3495(93)81368-7
6. Vaz W.L.C. Percolation properties of two-component, two-phase phospholipid bilayers. *Mol. Membr. Biol.* 1995;12(1):39–43. https://doi.org/10.3109/09687689509038493
7. Griesbauer J., Wixforth A., Schneider M.F. Wave propagation in lipid monolayers. *Biophy. J.* 2009;97(10):2710–2716. https://doi.org/10.1016/j.bpj.2009.07.049
8. Bolterauer H., Tuszyński J.A., Satarić M.V. Fröhlich and Davydov regimes in the dynamics of dipolar oscillations of biological membranes. *Phys. Rev. A.* 1991;44(2):1366–1381. https://doi.org/10.1103/PhysRevA.44.1366
9. Collins M.A. Solitons in chemical physics. In: *Advances in Chemical Physics*. 2007;53:225–339. https://doi.org/10.1002/9780470142776.ch3
10. Wack D.C., Webb W.W. Synchrotron x-ray study of the modulated lamellar phase P_{β} in the lecithin-water system. *Phys. Rev. A.* 1989;40(5):2712–2730. https://doi.org/10.1103/PhysRevA.40.2712
11. Davydov A.S. *Solitons in Molecular Systems*. Dordrecht: Springer Netherlands; 1985. 317 p. https://doi.org/10.1007/978-94-017-3025-9
12. Scott A.C. Dynamics of Davydov solitons. *Phys. Rev. A.* 1982;26(1):578. https://doi.org/10.1103/PhysRevA.26.578
13. Lupichev L.N., Savin A.V., Kadantsev V.N. *Synergetics of Molecular Systems*. Springer Series in Synergetics. Springer International Publishing; 2015. https://doi.org/10.1007/978-3-319-08195-3

СПИСОК ЛИТЕРАТУРЫ

1. Геннис Р. Биомембраны*: молекулярная структура и функции*. М.: Мир; 1997. 624 с. ISBN 5-03-002419-0
2. Zhao J., Gulan U., Horie T., et al. Advances in biological liquid crystals. *Small.* 2019;15(18):1900019. https://doi.org/10.1002/smll.201900019
3. Нестеров С.В., Чесноков Ю.М., Камышинский Р.А., Ягужинский Л.С., Василов Р.Г. Определение расположения и структуры АТФ-синтетазы в мембранах митохондрий сердца крыс с помощью криоэлектронной томографии. *Российские нанотехнологии*. 2020;15(1):93–100. https://doi.org/10.1134/S1992722320010136
4. Zhou Y., Prakash P., Liang H., Cho K.J., Gorfe A.A., Hancock J.F. Lipid-sorting specificity encoded in K-ras membrane anchor regulates signal output. *Cell.* 2017;168(1–2):239–251.e16. https://doi.org/10.1016/j.cell.2016.11.059
5. Marsh D. Connectivity of membrane domains. *Biophys. J.* 1993;64(2):299–300. https://doi.org/10.1016/S0006-3495(93)81368-7
6. Vaz W.L.C. Percolation properties of two-component, two-phase phospholipid bilayers. *Mol. Membr. Biol.* 1995;12(1):39–43. https://doi.org/10.3109/09687689509038493
7. Griesbauer J., Wixforth A., Schneider M.F. Wave propagation in lipid monolayers. *Biophy. J.* 2009;97(10):2710–2716. https://doi.org/10.1016/j.bpj.2009.07.049
8. Bolterauer H., Tuszyński J.A., Satarić M.V. Fröhlich and Davydov regimes in the dynamics of dipolar oscillations of biological membranes. *Phys. Rev. A.* 1991;44(2):1366–1381. https://doi.org/10.1103/PhysRevA.44.1366
9. Collins M.A. Solitons in chemical physics. In: *Advances in Chemical Physics*. 2007;53:225–339. https://doi.org/10.1002/9780470142776.ch3
10. Wack D.C., Webb W.W. Synchrotron x-ray study of the modulated lamellar phase P_{β} in the lecithin-water system. *Phys. Rev. A.* 1989;40(5):2712–2730. https://doi.org/10.1103/PhysRevA.40.2712
11. Davydov A.S. *Solitons in Molecular Systems*. Dordrecht: Springer Netherlands; 1985. 317 p. https://doi.org/10.1007/978-94-017-3025-9
12. Scott A.C. Dynamics of Davydov solitons. *Phys. Rev. A.* 1982;26(1):578. https://doi.org/10.1103/PhysRevA.26.578
13. Lupichev L.N., Savin A.V., Kadantsev V.N. *Synergetics of Molecular Systems*. Springer Series in Synergetics. Springer International Publishing; 2015. https://doi.org/10.1007/978-3-319-08195-3
14. Yakushevich L.V., Savin A.V., Manevitch L.I. Nonlinear dynamics of topological solitons in DNA. *Phys. Rev. E.* 2002;66(1):016614. https://doi.org/10.1103/PhysRevE.66.016614
15. Каданцев В.Н., Гольцов А.Н. Коллективные возбуждения в альфа-спиральной молекуле белка. *Российский технологический журнал*. 2018;6(2):32–45. https://doi.org/10.32362/2500-316X-2018-6-2-32-45
16. Kadantsev V.N., Goltsov A. Collective excitations in **α**-helical protein structures interacting with the water environment. *Electromagn. Biol. Med.* 2020;39(4):419–432. https://doi.org/10.1080/15368378.2020.1826961

14. Yakushevich L.V., Savin A.V., Manevitch L.I. Nonlinear dynamics of topological solitons in DNA. *Phys. Rev. E.* 2002;66(1):016614. https://doi.org/10.1103/PhysRevE.66.016614
15. Kadantsev V.N., Goltsov A.N. Collective excitations in alpha-helical protein molecule. *Russian Technological Journal.* 2018;6(2):32–45 (in Russ.). https://doi.org/10.32362/2500-316X-2018-6-2-32-45
16. Kadantsev V.N., Goltsov A. Collective excitations in **α**-helical protein structures interacting with the water environment. *Electromagn. Biol. Med.* 2020;39(4):419–432. https://doi.org/10.1080/15368378.2020.1826961
17. Meder D., Moreno M.J., Verkade P., Vaz W.L.C., Simons K. Phase coexistence and connectivity in the apical membrane of polarized epithelial cells. *Proc. Natl. Acad. Sci. USA.* 2006;103(2):329–334. https://doi.org/10.1073/pnas.0509885103
18. Risović D., Frka S., Kozarac Z. The structure of percolating lipid monolayers. *J. Colloid Interface Sci.* 2012;373(1):116–121. https://doi.org/10.1016/j.jcis.2011.12.009
19. Jørgensen K., Mouritsen O.G. Phase separation dynamics and lateral organization of two-component lipid membranes. *Biophys. J.* 1995;69(3):942–954. https://doi.org/10.1016/S0006-3495(95)79968-4
20. Goltsov A.N. Electromagnetic-field-induced oscillations of the lipid domain structures in the mixed membranes. *Bioelectrochem. Bioenerg.* 1999;48(2):311–316. https://doi.org/10.1016/S0302-4598(99)00040-9
21. Salari V., Tuszynski J., Rahnama M., Bernroider G. Plausibility of quantum coherent states in biological systems. *J. Phys.: Conf. Ser.* 2011;306(1):012075. https://doi.org/10.1088/1742-6596/306/1/012075
22. Shrivastava S., Schneider M.F. Evidence for two-dimensional solitary sound waves in a lipid controlled interface and its implications for biological signalling. *J. R. Soc. Interface.* 2014;11(97):20140098. https://doi.org/10.1098/rsif.2014.0098
23. Heimburg T., Jackson A.D. On soliton propagation in biomembranes and nerves. *Proc. Natl. Acad. Sci. USA.* 2005;102(28):9790–9795. https://doi.org/10.1073/pnas.0503823102
24. Lei L., Changqing S., Juelian S., Lam P.M., Yun H. Soliton propagation in liquid crystals. *Phys. Rev. Lett.* 1982;49(18):1335. https://doi.org/10.1103/PhysRevLett.49.1335
25. Shen Y., Dierking I. Dynamics of electrically driven solitons in nematic and cholesteric liquid crystals. *Commun. Phys.* 2020;3(1):14. https://doi.org/10.1038/s42005-020-0288-4
26. Cavallo F., De Giovanni C., Nanni P., Forni G., Lollini P.-L. 2011: the immune hallmarks of cancer. *Cancer Immunol. Immunother.* 2011;60(3):319–326. https://doi.org/10.1007/s00262-010-0968-0
27. Žmuidzinas J.S. Electron trapping and transport by supersonic solitons in one-dimensional systems. *Phys. Rev. B.* 1978;17(10):3919. https://doi.org/10.1103/PhysRevB.17.3919
28. Kadantsev V.N., Goltsov A.N., Kondakov M.A. Electrosoliton dynamics in a thermalized molecular chain. *Russian Technological Journal.* 2020;8(1):43–57 (in Russ.). https://doi.org/10.32362/2500-316X-2020-8-1-43-57

17. Meder D., Moreno M.J., Verkade P., Vaz W.L.C., Simons K. Phase coexistence and connectivity in the apical membrane of polarized epithelial cells. *Proc. Natl. Acad. Sci. USA.* 2006;103(2):329–334. https://doi.org/10.1073/pnas.0509885103
18. Risović D., Frka S., Kozarac Z. The structure of percolating lipid monolayers. *J. Colloid Interface Sci.* 2012;373(1):116–121. https://doi.org/10.1016/j.jcis.2011.12.009
19. Jørgensen K., Mouritsen O.G. Phase separation dynamics and lateral organization of two-component lipid membranes. *Biophys. J.* 1995;69(3):942–954. https://doi.org/10.1016/S0006-3495(95)79968-4
20. Goltsov A.N. Electromagnetic-field-induced oscillations of the lipid domain structures in the mixed membranes. *Bioelectrochem. Bioenerg.* 1999;48(2):311–316. https://doi.org/10.1016/S0302-4598(99)00040-9
21. Salari V., Tuszynski J., Rahnama M., Bernroider G. Plausibility of quantum coherent states in biological systems. *J. Phys.: Conf. Ser.* 2011;306(1):012075. https://doi.org/10.1088/1742-6596/306/1/012075
22. Shrivastava S., Schneider M.F. Evidence for two-dimensional solitary sound waves in a lipid controlled interface and its implications for biological signalling. *J. R. Soc. Interface.* 2014;11(97):20140098. https://doi.org/10.1098/rsif.2014.0098
23. Heimburg T., Jackson A.D. On soliton propagation in biomembranes and nerves. *Proc. Natl. Acad. Sci. USA.* 2005;102(28):9790–9795. https://doi.org/10.1073/pnas.0503823102
24. Lei L., Changqing S., Juelian S., Lam P.M., Yun H. Soliton propagation in liquid crystals. *Phys. Rev. Lett.* 1982;49(18):1335. https://doi.org/10.1103/PhysRevLett.49.1335
25. Shen Y., Dierking I. Dynamics of electrically driven solitons in nematic and cholesteric liquid crystals. *Commun. Phys.* 2020;3(1):14. https://doi.org/10.1038/s42005-020-0288-4
26. Cavallo F., De Giovanni C., Nanni P., Forni G., Lollini P.-L. 2011: the immune hallmarks of cancer. *Cancer Immunol. Immunother.* 2011;60(3):319–326. https://doi.org/10.1007/s00262-010-0968-0
27. Žmuidzinas J.S. Electron trapping and transport by supersonic solitons in one-dimensional systems. *Phys. Rev. B.* 1978;17(10):3919. https://doi.org/10.1103/PhysRevB.17.3919
28. Каданцев В.Н., Гольцов А.Н., Кондаков М.А. Динамика электросолитона в термализованной молекулярной цепи. *Российский технологический журнал.* 2020;8(1):43–57. https://doi.org/10.32362/2500-316X-2020-8-1-43-57

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