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RESEARCH ARTICLE

# Lateral proton transport induced by acoustic solitons propagating in lipid membranes

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**Abstract**

**Objectives.** The study of proton transport in membrane structures represents a significant technological task in the development of hydrogen energy as well as a fundamental problem in bioenergetics. Investigation in this field aims at finding out the physical mechanisms of fast proton transport in the meso-porous structures in polymer electrolyte membranes, which serve as electrochemical components of hydrogen fuel cells. The objectives of the research in the field of bioenergetics are to elucidate the molecular mechanisms of effective proton transport in transmembrane channel proteins, as well as along the surface proton-conducting structures in biological membranes. To investigate the molecular mechanisms of the direct proton transport along the water-membrane interface, we developed a model of proton movement along quasi-one-dimensional lateral domain structures in multicomponent lipid membranes.

**Methods.** The developed approach is based on a model of collective excitations spreading along the membranes in the form of acoustic solitons, which represent the regions of local compression of polar groups and structural defects in hydrocarbon chains of lipid molecules.

**Results.** The results of modeling showed that the interaction between an excess proton on the membrane surface and a soliton of membrane compression leads to the proton being trapped by an acoustic soliton, followed by its transport by moving soliton. The developed model was applied to describe effective proton transport along the inner mitochondrial membrane and its role in the local coupling function of molecular complexes in cell bioenergetics.

**Conclusions.** The developed soliton model of proton transport demonstrated that collective excitations within lipid membranes can determine one of the factors affecting the efficiency of proton transport along interphase boundaries. Further development of the theoretical approaches, taking into account dynamic properties of polymer and biological proton-conducting membranes, can contribute to the study of a role of surface proton transport in cell bioenergetics, as well as to the investigation of transport characteristics of the proton-exchange polymer membranes developed for the hydrogen energy industry.

**Keywords:** proton transport, proton-conducting structures, lipid membranes, domain structures, collective dynamics, solitons

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НАУЧНАЯ СТАТЬЯ

# Латеральный протонный транспорт, индуцированный распространением акустических солитонов в липидных мембранах

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**Резюме**

**Цели.** Исследование протонного транспорта в мембранных структурах является важной технологической задачей в области водородной энергетики, а также представляет собой фундаментальную проблему биоэнергетики. Целью этих исследований является выяснение физических механизмов быстрого протонного транспорта в мезо-пористых структурах полимерных электролитных мембран, являющихся электрохимическими компонентами водородных топливных элементов. В области биоэнергетики эти исследования направлены на выяснения молекулярных механизмов эффективного протонного транспорта в трансмембранных белках-каналах и в поверхностных протонпроводящих структурах биологических мембран в системах биоэнергетики клетки. С целью исследования молекулярных механизмов направленного транспорта протонов в работе рассматривается модель движения протонов в квазиодномерных латеральных доменных структурах в многокомпонентных липидных мембранах.

**Методы.** В основе развиваемого подхода лежит модель коллективных возбуждений типа акустических солитонов, которые представляют собой перемещающиеся вдоль мембраны области локального сжатия полярных групп и структурных дефектов в подсистеме углеводородных цепей липидных молекул.

**Результаты.** Показано, что учет в модели взаимодействия избыточного протона на поверхности мембраны с солитоном сжатия мембраны приводит к захвату протона акустическим солитоном с его последующим транспортом. Разработанная модель применяется к описанию механизма эффективного протонного транспорта вдоль внутренней митохондриальной мембраны и его роли в сопряжении функционирования молекулярных комплексов в системе биоэнергетики клетки.

**Выводы.** Развитая солитонная модель протонного транспорта показала, что коллективные возбуждения в липидных мембранах могут определять факторы, влияющие на эффективность протонного транспорта вдоль межфазных границ. Дальнейшее развитие теоретических подходов, учитывающих динамические свойства полимерных и биологических протонпроводящих мембран, может внести вклад в исследование роли поверхностного транспорта протонов в биоэнергетику клетки, а также в исследование транспортных характеристик разрабатываемых протонно-обменных полимерных мембран водородной энергетики.

**Ключевые слова:** протонный транспорт, протонпроводящие структуры, липидные мембраны, доменные структуры, коллективная динамика, солитоны

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## INTRODUCTION

Experimental and theoretical studies of proton conductivity of materials and systems are currently carried out in two distinct scientific and technological fields: hydrogen energy and bioenergetics of living systems. The development of proton-conducting materials is of particular interest today for the production of components of electrochemical devices, especially fuel cell membranes for the manufacture of hydrogen power plants, batteries, electric vehicle power units, etc. [1]. With proton batteries already emerging as a competitive alternative to lithium-ion technologies, research in this field is aimed at creating efficient polymeric (e.g., perfluorinated sulfopolymers) and solid-state proton electrolytes. The replacement of lithium ions with protons as charge carriers in hydrogen fuel cells significantly increases the conductivity of the electrolyte due to the high mobility of protons in the electrolyte membrane.

In most polymeric proton-exchange membranes of hydrogen fuel cells, fast proton transport takes place due to hydrate layers of water in the membrane structure—or, more precisely, along the nanoscale structures formed by water molecules in mesoporous structures of polymer materials. The specific proton conductivity of proton exchange membranes can reach values in the range of $10^{-3}$ to $10^{-1}$ S/cm [2], while the proton conductivity of bulk water is in the range of $10^{-6}$ S/cm, i.e., five orders of magnitude lower than the conductivity of polymer membranes. However, the molecular mechanisms of the high proton conductivity of near-surface water in porous polymeric materials, whose properties are anomalously different from those of bulk water, are still not fully understood.

While the study of physicochemical mechanisms of fast proton transport in membrane structures represents an important technological task of hydrogen energetics, it is also a fundamental problem in the field of bioenergetics. Here, studies are aimed at elucidating the molecular mechanisms of proton transport in the system of oxidative phosphorylation in cell mitochondria, in transmembrane channels, and in surface proton-conducting structures of biomembranes.

Artificial polymeric proton-exchange membranes have much in common with biological lipid membranes in terms of their structure and molecular composition: both polymeric membranes and biological membranes consist of amphiphilic molecules with hydrophobic chains and acidic groups. In both systems, the proton-conducting hydrate layer of water molecules forms a hydrogen bonding structure at the interface, along which fast two-dimensional diffusion of protons is assumed to occur. The physical mechanisms of efficient proton transport in hydrophobic channels of protein molecules and the surface layer of mitochondrial membranes are currently the subject of intensive research in cell bioenergetics. However, although Mitchell's chemiosmotic theory gives a general idea of the functioning of the mitochondrial bioenergetic system, it needs further development based on new experimental data on the functioning of individual components of the oxidative phosphorylation system and on the spatial organization of the entire system of adenosine triphosphate (ATP) molecule synthesis in the mitochondrial membrane [3–5]. In particular, new experimental data on the structure of inner mitochondrial membranes have not only demonstrated their structural and organizational function, but also revealed the important coupling and integrating role that they fulfill in the functioning of the whole system of electron transport processes and ATP synthesis [6, 7]. In particular, recent experimental data on fast proton transport across mitochondrial and artificial membranes [8, 9] supported the hypothesis of a local coupling of respiration and phosphorylation due to the near-membrane transport of partially dehydrated protons [10–12].

Several possible molecular mechanisms for the fast lateral transport of protons along the membrane interface through bound water molecules over long distances are currently under consideration. The first of these is the Grotthuss mechanism of proton transport along the hydrogen bond chain (structural diffusion) [13]. A second potential mechanism is based on the diffusion of protons within the hydroxonium ion $H_3O^+$ (vesicular diffusion) [14]. A third approach describes the process of co-diffusion of a lipid molecule with a strongly bound proton. Effective proton transport along the membrane-bound water interface can also be envisaged in terms of a combination of structural and vesicular diffusion [15]. To date, no conclusive experimental evidence can be adduced in favor of one or another mechanism of proton transport. However, all proposed mechanisms are based on experimental data confirming proton retention at the membrane-water interface that ensure the efficient two-dimensional diffusion of protons with limited release into the bulk phase [7, 16, 17]. The retention of protons at the membrane surface has been studied in experiments on bilayer membranes [18, 19] and liposomes [20]. Moreover, part of the energy stored in the form of partially dehydrated proton has been shown to be incorporated into ATP synthesis [21]. The causes of proton affinity to interfaces and surface proton transport have also been studied theoretically [22–24]. The results of these studies showed that the mechanism of proton retention at the membrane surface is determined by electrostatic interaction and the entropic barrier. The polar groups (PG) of lipid molecules have also been found to significantly affect the rate of proton surface transport [25]. Here, the PG composition is assumed to influence the formation of one-dimensional

proton-conducting structures of hydrogen bonds of water molecules bound to the membrane [9].

In work [5], proton-conducting lateral structures, representing quasi-one-dimensional domain structures (DS) in the cristae of inner mitochondrial membranes enriched with cardiolipin molecules were considered. Based on the Grotthuss mechanism, the authors have developed a model of proton transport along hydrogen-bonded chains of water molecules interacting with cardiolipin PGs in proton-conducting membrane structures. The interaction of the proton subsystem and the lipid PG subsystem has been shown to lead to the formation of a two-component soliton, whose motion corresponds to the coordinated movement of the proton and soliton of compression along the lipid membrane [5].

A similar theoretical approach to modeling the soliton transport of protons has also been developed for polymer membranes [26]. In the proposed model, proton transport as part of the hydroxonium ion $H_3O^+$ occurs due to collective excitations of the soliton-like type spreading in ordered chains of hydrogen bonds formed by water molecules on the membrane with sulfide surface groups. The model establishes the relationship between the soliton mobility and the parameters of the spatial structure of the surface sulfide groups.

The present work considers a model of alternative proton transport realized by proton trapping by an acoustic soliton moving along proton-conducting structures in lipid membranes. This mechanism is closer to the vesicular mechanism, where an acoustic soliton rather than a hydroxonium ion acts as a proton carrier (vesicle). The work is based on the model of acoustic soliton formation and propagation in quasilinear DSs proposed in our previous study [27]. Nonlinear excitations of the soliton-like type represent regions of local compression of lipid PGs and structural defects in the subsystem of hydrocarbon chains (HC) moving along the membrane molecular structures.

The experimental observation of soliton-like excitations in lipid monolayers and bilayers has been carried out in a number of experiments using different excitation and registration methods. The excitation of acoustic soliton-like pulses and their dissipationless motion were observed in experiments with optical generation of solitary waves in lipid monolayers [28]. Excitation of elastic soliton-like pulses was also found in liposomes in the temperature range of the lipid phase transition. Acoustic waves accompanying the propagation of a nerve impulse in an axon were shown to have one of the characteristic properties of solitons, i.e. two colliding nerve impulses pass through each other without changing their shape [29].

The present work considers a model of proton trapping by an acoustic soliton and its subsequent transport. The possibility of such trapping and the resulting mechanism of charge transport by acoustic solitons through one-dimensional nonlinear molecular structures has been discussed in [30, 31]. It is assumed that lateral proton transport in lipid membranes can occur in a similar way as a result of proton trapping by a soliton, and that quasi-one-dimensional DSs in multi-component membranes may represent proton-conducting channels on the membrane surface.

## 1. MODEL OF THE LATERAL TRANSPORT OF A PROTON TRAPPED BY A SOLITON IN A QUASI-ONE-DIMENSIONAL DS OF A LIPID MEMBRANE

We consider the model of a one-dimensional chain of lipid molecules forming a quasi-one-dimensional DS in mixed lipid bilayers. In the model, two subsystems are distinguished: the membrane surface formed by PGs of lipid molecules and the inner hydrophobic region of the membrane formed by lipid HCs [32]. In [27], we developed a model of soliton-type collective excitations representing the regions of local displacements of lipid PGs $\rho(x, t)$ from equilibrium positions and structural defects of the kink type in the lipid HC subsystem, which is described by the HC deviation from the normal to the membrane surface $u(x, t)$:

$$\rho(x,t) = -\rho_0 \operatorname{sech}^2 \frac{x - Vt}{\Delta}, \quad (1)$$

$$u(x,t) = u_0 \tanh \frac{x - Vt}{\Delta}, \quad (2)$$

where $V$ is the soliton velocity and the lipid PG equilibrium position $\rho_0$ is determined by the following equation:

$$\rho_0 = \frac{\chi u_0^2}{M\Omega_0^2}.$$

Here, $M$ is the mass of the PG of lipid molecule; $\chi$ is the constant of interaction between lipid PGs and HCs, which accounts for the change in HC conformation upon PG displacement from the equilibrium position; $\Omega_0$ is the characteristic frequency of a chain of the lipid PG; $\Delta$ is the kink width. $u_0 = \pm(|G|/B)^{1/2}$ is the HC equilibrium state in the Ginzburg–Landau double-well potential:

$$U_T(u) = -\frac{1}{2}|G(T)|u^2 + \frac{1}{4}Bu^4,$$

where $G(T) = E_0(T/T_c - 1)$ and $B$ are potential parameters; $E_0$ is the potential barrier height; $T_c$ is the temperature of the main phase transition of the membrane, at which lipid melting occurs [27, 32].

The soliton solution for the PG displacement $\rho(x, t) < 0$ (1) describes the compression strain in the lipid PG subsystem associated with the defect in the lipid HC system. For protons in the near-membrane layer, which are trapped in such a structure, the presence of a soliton appears as an additional interaction energy. The solution $u(x, t)$ (2) in the form of a kink in the region of coordinate $x = Vt$ describes the deviations of lipid molecule HCs in opposite directions, which is characteristic of structural defects like dislocations in liquid crystals.

In the proposed model, the motion of a proton trapped by soliton of compression in a lipid PG chain is described by the wave function $\psi(x, t)$ which satisfies the time-dependent Schrödinger equation:

$$i\hbar\frac{\partial\psi(x,t)}{\partial t}+\frac{\hbar^2}{2m}\cdot\frac{\partial^2\psi(x,t)}{\partial x^2}-U(x,t)\psi(x,t)=0, \quad (3)$$

where $U(x, t) = \sigma\rho(x, t)$ is the potential well generated by negatively charged PGs of lipid molecules in the soliton region; $\sigma$ is the parameter of the electrostatic interaction between the proton and the PGs of lipid molecules in the soliton region; $m$ is the mass of the proton; $\hbar$ is the Planck constant.

The solution of the time-dependent Schrödinger equation Eq. (3) was sought in the following form:

$$\psi(x,t)=\varphi(\xi)e^{-\frac{i}{\hbar}Et}, \quad (4)$$

where the spatial coordinate $\xi = x - Vt$ associated with the soliton motion at velocity $V$ is introduced.

Substituting (4) into (3), we obtained the stationary Schrödinger equation for the real part of the amplitude $\varphi(\xi)$ of the proton in the potential well $U(\xi)$:

$$\frac{\hbar^2}{2m}\cdot\frac{\partial^2\varphi}{\partial\xi^2}+[E-U(\xi)]\varphi=0, \quad (5)$$

where $U(\xi)=-\sigma\rho_0\,\mathrm{sech}^2\left(\frac{\xi}{\Delta}\right)$.

Equation (5) can be transformed into the equation for generalized Lagrangian functions, as follows:

$$\frac{d}{dz}\left[1-z^2\frac{d\varphi}{dz}\right]+\left[s(s+1)-\frac{\varepsilon^2}{1-\varepsilon^2}\right]\varphi=0, \quad (6)$$

where the variable $z = \tanh(\Delta^{-1}\xi)$ and the following notations were introduced:

$$\varepsilon=\frac{\Delta\sqrt{-2mE}}{\hbar};\ s=\frac{1}{2}\left(-1+\sqrt{1+8m\sigma\rho_0\Delta^2\hbar^{-2}}\right). \quad (7)$$

In this case, Eq. (6) has a solution in the following form:

$$\varphi_n(\xi)=A_n\,\mathrm{sech}^{\varepsilon}\left(\frac{\xi}{\Delta}\right)\times$$
$$\times F\left(\varepsilon-s,\ \varepsilon+s+1,\ \varepsilon+1,\ \frac{1}{2}\left(1-\tanh(\Delta^{-1}\xi)\right)\right), \quad (8)$$

where $A_n$ is the normalization factor of the wave function; $F$ is a hypergeometric function representing a polynomial of degree $n$ under the condition $\varepsilon - s = -n$ ($n = 0, 1, 2, \ldots$) [33].

This condition gives the following expression for the proton energy levels in the potential well $U(\xi)$:

$$E_n=-\frac{\hbar}{8m\Delta^2}\left(-(1+2n)+\sqrt{1+8m\sigma\rho_0\Delta^2\hbar^{-2}}\right)^2.$$

Thus, the potential well $U(\xi)$ contains a finite number of stationary energy levels for a proton trapped by a soliton in the PG chain of lipid molecules. For the ground level at $n = 0$, the wave function (8) has the following form:

$$\varphi_0(\xi)=A_0\,\mathrm{sech}^{\varepsilon}\left(\frac{\xi}{\Delta}\right). \quad (9)$$

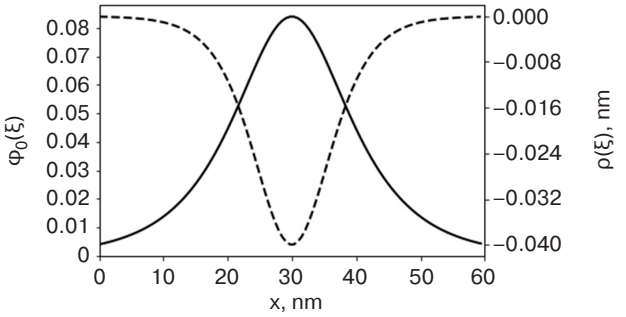


**Figure.** Wave function of the ground state of proton $\varphi_0(\xi)$ (solid line) in the potential well $U(\xi)$ generated by soliton of compression $\rho(\xi)$ (dashed line) of lipid molecule PGs in a quasi-one-dimensional lipid DS

The figure shows the proton wave function $\varphi_0(\xi)$ (9) calculated for $\varepsilon = 1$ with the normalization factor $A_0 = 0.42$. The calculation was performed for the soliton parameters obtained based on the following experimental data. The characteristic frequency $\Omega_0 = 10^{11}$ Hz was estimated according to the experimental data for the oscillation frequency of the lipid membrane [32]. The velocity of the trapped proton was determined by soliton propagation velocity $V$ (Eqs. (1) and (2)), which was estimated by us to be in the range of 50–100 m/s [5]. The kink width $\Delta \approx 8$ nm was estimated on the basis

of experimental data on the size of the defect region in the HC subsystem formed in membrane structures at the temperature near the main phase transition temperature [34]. In this case, the soliton region includes about 10 lipid molecules located along the one-dimensional DS. The kink solution for the HC displacement $u(x, t)$ describes a dislocation-type defect. Negative and positive values of $u(x, t)$ correspond to the deviations of lipid molecule HCs in opposite directions. The soliton solution for the PG displacement $\rho(x, t)$ describes the compressive deformation in the PG subsystem caused by a defect in the HC subsystem.

## 2. DISCUSSION

In the present work, we developed a model of proton motion in quasi-one-dimensional lateral DSs, which are assumed to play the role of proton conducting structures in multi-component cell membranes [27, 35]. The proposed approach is based on the model of collective excitations in lipid membranes such as acoustic solitons which represent regions of local PG compression and structural defects of lipid molecule HCs coordinately moving along the membrane.

The model takes into account the electrostatic interaction of a membrane-bound proton with soliton of compression. This interaction leads to the proton trapping by a moving acoustic soliton and its subsequent transport. In contrast to the model of proton soliton transport previously developed by us on the basis of the structural proton diffusion mechanism (Grotthuss mechanism) [5], in this work, we considered an alternative model of proton transport. The proposed model overcomes two problems of the structural proton diffusion model. Firstly, in contrast to the Grotthuss mechanism, a proton trapped by the soliton does not undergo a large number of jumps along the hydrogen bond chain over a short distance of 2.5 Å, which significantly increases the velocity of its movement. Secondly, the described approach provides proton transport that is strongly coupled to the region of local compression of PGs moving along the membrane surface in the form of a soliton. The experimentally observed effect of proton retention at the membrane surface implies the strong local interaction of the proton with lipid PGs that is inconsistent with the data on proton delocalization and its movement along the membrane surface.

The developed model can be applied to describe proton transport along the surface of the inner mitochondrial membrane in the oxidative phosphorylation coupling system, which has been experimentally established to possess a unique spatial organization. The cryo-electron tomography method has revealed an ordered cluster oligomeric structure formed by parallel rows of respiratory complexes and ATP synthase dimers located on the folds of the cristae of mitochondrial inner membranes [7]. The formation, morphology, and dynamics of mitochondrial cristae are determined by structural rearrangements of lipid membranes, which are highly sensitive to the physiological state of mitochondria [36]. The small distance (~50 Å) between the rows of proton pumps and ATP synthase molecules provides conditions for direct and fast proton transport to ATP synthases along the cristae membrane. Currently, considerable interest is shown in investigating the molecular mechanisms of proton transport in mitochondrial membranes and determining the factors that influence its efficiency [16, 17, 37]. Based on the developed approach, we proposed that this research should not only consider the influence of the membrane surface structure on proton transport, but should also take into account the dynamic properties of biomembranes, in particular the formation of collective excitations in lipid bilayers. Through the consideration of elastic excitations of the membrane in the proposed model, proton transport is accompanied by the transfer of membrane deformation energy stored by the acoustic soliton. This approach links lateral proton motion to the non-equilibrium dynamics of mitochondrial cristae by coupling transport and dynamic processes at the biomembrane surface [38]. The energy of the local membrane elastic oscillations transferred together with the charge may additionally be hypothesized to contribute to functioning and synchronizing membrane proteins, receptors, and ion channels [39, 40] in particular, those involved in synchronizing the functioning of oligomeric protein complexes making up the mitochondrial oxidative phosphorylation system. The experimental detection of proton transport, accompanied by the propagation of elastic excitations along membrane surfaces, may confirm the contribution of collective excitations to the effective proton transport in the inner mitochondrial membranes, as well as to the coupling mechanism in the oxidative phosphorylation system.

## CONCLUSIONS

The results of theoretical and experimental studies in the fields of bioenergetics of mitochondrial membranes and polymeric proton-exchange membrane technology of hydrogen fuel cells allowed the elucidation of many common features of surface proton transport in biological and artificial membranes. Two primary mechanisms of efficient proton transport—structural diffusion (Grotthuss mechanism) and vesicular transport—are considered in the study of both systems to confirm the role of a membrane bounded layer of structured water, in which proton transport is localized. In polymer membranes, this was demonstrated by the detection of fast proton transport at low membrane

hydration. In mitochondrial membranes, the same effect was confirmed in the experiments that showed the localization of protons in the surface layer of the inner mitochondrial membrane in the oxidative phosphorylation system. In both artificial and biological membranes, a significant influence of membrane composition and structure (surface acidic groups) on proton conductance was discovered. The soliton model of proton transport developed in this paper showed that the collective excitations of lipid membranes together with their structural properties can determine the factors that influence the proton transport efficiency. The further development of theoretical approaches that take into account both structural and dynamic properties of polymeric and biological proton-conducting membranes can contribute to the study of the role of surface proton transport in cell bioenergetics, as well as to the investigation of transport characteristics of polymeric proton-exchange membranes developed for hydrogen energetics.

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**Authors' contribution.** All authors equally contributed to the research work.

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