

Solitons in quasi-one-dimensional molecular structures

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Theoretical investigations of solitons arising in quasi-one-dimensional molecular structures such as alpha-helical protein molecules are described. The properties of solitons and excitons are discussed. The reasons for the great stability of solitons are investigated. It is noted that the vibrational energy of Amide I vibrations of peptide groups can be transported in the form of solitons along a protein molecule without losses due to creation of phonons. Deceleration of solitons by dissipative forces and the effect of thermal motion and external fields are investigated. A new mechanism for muscle contraction in animals, based on the idea of solitons, is discussed on a molecular level.

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1. INTRODUCTION

The word *soliton*, as a brief designation of solitary waves, corresponding to particular solutions of some nonlinear equations and describing the propagation of excitations in continuous media which are dispersive and nonlinear, was introduced into the scientific literature by Zabusky and Kruskal in 1965.¹ However the first qualitative scientific description of solitary waves on the surface of water in a shallow channel was given by the English marine engineer John Scott-Russell more than 140 years ago.

Writing in the Proceedings of the Royal Society of Edinburgh, Scott-Russell wrote² that he observed a large solitary wave, moving off the bow of a barge, pulled along a channel by a pair of horses, after the barge suddenly stopped. Assuming the shape of a high, solitary, smooth, rounded, distinctly outlined mound of water (height of about one-half meter, length ~10 m), the solitary wave rolled rapidly along the channel. "I galloped after it on a horse," wrote Scott-Russell, "and when I caught up with it, it continued to roll forward without an appreciable decrease in velocity, retaining its initial shape ... Thus my first encounter with this unique and wonderful phenomenon occurred in August 1834."

On the surface of a heavy shallow fluid, solitary waves are isolated rises in the fluid level propagating along a

channel. If the depth of the channel is small, then the equation for the average velocity of the fluid (u) in a given section reduces to the equation for one-dimensional motion

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \beta \frac{\partial^3 u}{\partial x^3} = 0, \quad (1.1)$$

where β is a parameter that characterizes dispersion. In the case of water in a channel with depth h , it is determined by the acceleration of gravity g by the expression $\beta = \sqrt{gh^3}/6$.

This equation was derived by Korteweg and de Vries³ in 1895 and is now called the *Korteweg-de Vries equation* or, briefly the KdV equation.

Based already on the first observations of solitary waves, Scott-Russell noted their extraordinary stability and automatic self-adjustment. It is the great stability of solitons that has stimulated in the last ten years numerous attempts to use them in describing many new phenomena in different areas of physics and other sciences.

The formation of solitons in a continuous medium, described by nonlinear equations, is related to spontaneous breakdown of the local symmetry of a homogeneous system, i.e., with self-localization of excitation energy, electric charge density, or other physical quantities.

Interest in solitons has increased considerably in the last ten years in connection with research in plasma physics. In 1958 Sagdeev^{4,5} showed that solitons, analogous to the solitons on the surface of water, can propagate in a plasma located in a strong magnetic field. In a review paper, Kadomtsev and Karpman⁶ gave a detailed account of the application of the KdV equation to the description of magnetosonic and ionosonic solitons in a plasma. The *nonlinear Schrödinger equation* (NS) is mentioned in the same review (Sec. 4.2). In the simplest one-dimensional case it has the form

$$\left(i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial z^2} - G |\psi|^2 \right) \psi = 0, \quad (1.2)$$

where G is the nonlinearity parameter and $\hbar^2/2m^*$ is a parameter that characterizes dispersion.

The NS equation is used to describe self-focusing phenomena in nonlinear optics, one-dimensional self-modulation of a monochromatic wave in a plasma, stationary two-dimensional self-focusing of plane waves, etc.

Some problems in the theory of superconductivity and ferromagnetism reduce to the *sine-Gordon equation*

$$\frac{\partial^2 \psi}{\partial z^2} - \frac{\partial^2 \psi}{\partial t^2} = \sin \psi. \quad (1.3)$$

The simplest solutions of this equation in a one-dimensional space are typical examples of so-called *topological solitons*, for which the boundary conditions at infinity are not the same: for example, in a one-dimensional system $\psi(\infty) \neq \psi(-\infty)$. The solutions of one-dimensional KdV and NS equations, satisfying the boundary conditions $\psi(\infty) = \psi(-\infty) = 0$, are called *nontopological* or *dynamic solitons*.

Aside from the equations mentioned above, several other nonlinear equations are known that contain dispersion, whose solutions due to the mutual balancing of the effects of nonlinearity and dispersion have particular solutions in the form of stable solitary waves, i.e., *solitons*.

The solutions of Eqs. (1.1)–(1.3) have been studied in greatest detail for one-dimensional systems. In the one-dimensional case, these equations have a remarkable mathematical property. They can be integrated by the so-called method of the inverse scattering problem for the auxiliary linear operator. The inverse problem method originated in the work of Gardner, Green, Kruskal, and Miura.⁷ This method was further developed by Zakharov, Faddeev, Novikov, Cologero, Marchenko, *et al.*⁸⁻¹² The method of the inverse scattering problem is systematically described in the monograph by Zakharov, Manakov, Novikov, and Pitaevskii.¹³

Applications of the soliton concept to different areas of applied sciences are examined in the exhaustive review by Scott, Chu, and McLaughlin.¹⁴ The present review presents the results of theoretical investigations of solitons arising in quasi-one-dimensional molecular structures. In particular, such structures are realized in alpha helix protein molecules of living organisms. In

connection with biological applications, only cases when a single soliton is excited at one time in the system are examined in the review. The object of the study are molecular chains in which molecules (groups of atoms) connected by weak hydrogen bonds are periodically repeated. Such molecular chains are in some approximation models for the alpha-helix protein molecules.

Studies conducted at the Institute of Theoretical Physics of the Academy of Sciences of the Ukrainian SSR have shown that with the help of solitons vibrational intramolecular excitations and electrons can be transported along protein molecules without energy loss. This work opens up a new area for application of the soliton concept.

2. SOLITONS AND EXCITONS IN MOLECULAR CHAINS¹⁾

a) Basic equations describing the interaction of intramolecular excitations with acoustical phonons

The interactions of intramolecular excitations with acoustical phonons in one-dimensional systems were first studied by Rashba.^{15,16} In these papers, as in a number of subsequent papers (Toyazawa, Davydov, *et al.*¹⁷⁻²⁰), the conditions for formation of bound states of the intramolecular excitation and deformation of the chain, neglecting the motion of the excitation, were examined.

In studying the motion, two basic difficulties arise. These are related to separation of the center of mass of the excitation, moving together with the deformation, and to correctly take into account the lag of the deformation as the excitation moves along. These difficulties were overcome most accurately and systematically by Bogolyubov²¹ and Tyablikov.²² In these papers, concerning the analogous problem of the motion of an electron, an adiabatic perturbation theory was developed in which the kinetic energy of the phonon field was viewed as a small perturbation. For this reason, it is convenient to use the theory only in studying excitations moving with low (compared to the velocity of sound velocities in comparatively rigid systems with the parameters of a solid. The problem of the separation of the center of mass of the excitation was also correctly solved in these papers. However, this was achieved by introducing three extra variables and three additional conditions in order to conserve the correct number of degrees of freedom. This circumstance greatly complicated the theory and did not permit calculations beyond the first order terms. Adiabatic perturbation theory was also used in later papers by Mel'nikov, Volovik, and Edel'shtein.^{23,24}

In what follows we present the results of investigations of collective (not transporting electric charge) excitations in one-dimensional "soft" molecular chains without using the adiabatic perturbation theory. The kinetic energy of the phonon field is taken into account exactly. The center of mass is separated by a simple (widely used in the theory of traveling waves) transformation to a system of coordinates moving together

¹⁾ This section was written based on the studies performed by Eremko, Kislukha, Sergienko, and Davydov.²⁵⁻²⁸

with the excitation. It is shown that such excitations are described by nonlinear differential equations that include the time lag.

In order to obtain the basic equations describing excitations in a chain of weakly coupled molecules, we shall assume that molecules of mass M are situated along the z axis at nodes na ($n=0, \pm 1, \dots$). Each molecule can pass into an excited state with energy \mathcal{E}_0 , including the energy of the resonant interaction with neighboring molecules. The electric dipole moment d for the transition is oriented in the excited state either along or perpendicular to the z axis. If B_n^+ and B_n are creation and annihilation operators for the excitation, while u_n is the operator for longitudinal displacements of the equilibrium position of the n -th molecule, then the Hamiltonian operator of an infinite chain of molecules can be written as a sum of three terms

$$H = H_{ex} + H_{ph} - H_{int}, \quad (2.1)$$

where

$$H_{ex} = \sum_n B_n^* [\mathcal{E}_0 B_n - J (B_{n+1} + B_{n-1})], \quad (2.2)$$

$$H_{ph} = \frac{1}{2} \sum_n \left[\frac{1}{M} \hat{p}_n^2 + \kappa (u_n - u_{n-1})^2 \right], \quad (2.3)$$

$$H_{int} = \chi \sum_n B_n^* B_n (u_{n+1} - u_{n-1}). \quad (2.4)$$

In these expressions the parameter κ describes the longitudinal elasticity of the chain, \hat{p}_n is the momentum operator, canonically conjugate to u_n ; χ is the parameter coupling the intramolecular excitations and displacements of the molecules u_n .

H_{ex} is the operator of intramolecular excitations with molecules fixed at the nodes na . The energy of the resonant dipole-dipole interaction ($-J$) between neighboring molecules is expressed in terms of the dipole moment d for the transition by the equalities

$$J = \begin{cases} 2d^2/a^3, & \text{if } d \text{ is parallel to } z \text{ axis,} \\ -d^2/a^3, & \text{if } d \text{ is perpendicular to } z \text{ axis.} \end{cases} \quad (2.5)$$

For strong coupling between intramolecular excitations and molecular displacements, all three terms in (2.1) must be considered on an equal basis. The wave function of collective excitations of the chain described by the Hamiltonian (2.1) can be sought in the form

$$|\psi(t)\rangle = \sum_n A_n(t) B_n^* \exp \sigma(t) |0\rangle, \quad (2.6)$$

where $|0\rangle$ is the vacuum state function,

$$\sigma(t) = -\frac{i}{\hbar} \sum_n [\beta_n(t) \hat{p}_n - \pi_n(t) u_n]. \quad (2.7)$$

The normalization condition for the function (2.6) leads to the equality

$$\sum_n |A_n|^2 = 1. \quad (2.8)$$

Therefore, $|A_n|^2$ characterizes the probability for exciting the n -th molecule in the chain.

The transformation from the displacement operators u_n and the momentum operators conjugate to them \hat{p}_n to the functions $\beta_n(t)$ and $\pi_n(t)$ with the help of a unitary operator for displacements $\exp \sigma(t)$, entering into expression (2.6), corresponds to describing the displacements of equilibrium positions of molecules in

the language of coherent states. As is well known,^{29,30} the temporal evolution of coherent states follows the classical equations of motion (see Eqs. (2.12) and (2.12a) below). However, this does not mean that the quantities $\beta_n(t)$ and $\pi_n(t)$ can be given a strictly classical interpretation. They characterize the average displacement of the equilibrium positions and momenta in the state (2.6):

$$\beta_n(t) = \langle \psi(t) | u_n | \psi(t) \rangle, \quad \pi_n(t) = \langle \psi(t) | \hat{p}_n | \psi(t) \rangle.$$

The coherent states correspond to wave packets both in coordinate and momentum spaces, corresponding to states in which the product of the quadratic deviations from the averages is determined by the minimum value $\hbar^2/4$ permitted by quantum mechanics.

Using the explicit form of expressions (2.1)–(2.7), we find

$$H = \langle \psi(t) | H | \psi(t) \rangle = \sum_n A_n^* [(\mathcal{E}_0 + W) A_n - J (A_{n+1} + A_{n-1}) + \chi A_n (\beta_{n+1} - \beta_{n-1})], \quad (2.9)$$

where

$$W = \frac{1}{2} \sum_n \left[\frac{1}{M} \pi_n^2 + \kappa (\beta_n - \beta_{n-1})^2 \right] \quad (2.10)$$

is the total deformation energy of the chain. Viewing the expression (2.9) as a Hamiltonian function in the variables A_n and β_n and the generalized momenta conjugate to them, we find the Hamiltonian equations

$$i\hbar \frac{\partial A_n}{\partial t} = [\mathcal{E}_0 + W + \chi (\beta_{n+1} - \beta_{n-1})] A_n - J (A_{n+1} + A_{n-1}), \quad (2.11)$$

$$M \frac{\partial^2 \beta_n}{\partial t^2} + \kappa (2\beta_n - \beta_{n+1} - \beta_{n-1}) = \chi (|A_{n+1}|^2 - |A_{n-1}|^2), \quad (2.12)$$

$$\pi_n = M \frac{\partial \beta_n}{\partial t}. \quad (2.12a)$$

In going over to the continuum approximation, we perform the transformations

$$\begin{aligned} A_n(t) &\rightarrow \Phi(z, t) \exp \left[i \left(kz - \frac{Et}{\hbar} \right) \right], \\ \beta_n(t) &\rightarrow \beta(z, t), \end{aligned} \quad (2.13)$$

where $\Phi(z, t)$ and $\beta(z, t)$ are real smooth functions of the variable z , assuming the values $\Phi_n(t)$ and $\beta_n(t)$ at $z = na$. According to (2.8) and (2.13), the function $\Phi(z, t)$ must satisfy the normalization condition²⁾

$$\frac{1}{a} \int \Phi^2(z, t) dz = 1. \quad (2.14)$$

According to (2.13), in making the transition to the continuum approximation, it is necessary to use the equalities

$$\begin{aligned} A_{n\pm 1}(t) &\rightarrow \exp \left\{ i \left[k(z \pm a) - \frac{Et}{\hbar} \right] \right\} \\ &\quad \times \left(1 \pm a \frac{\partial}{\partial z} + \frac{1}{2} a^2 \frac{\partial^2}{\partial z^2} + \dots \right) \Phi(z, t), \\ \beta_{n\pm 1}(t) &\rightarrow \left(1 \pm a \frac{\partial}{\partial z} + \frac{1}{2} a^2 \frac{\partial^2}{\partial z^2} + \dots \right) \beta(z, t). \end{aligned} \quad (2.15)$$

Performing the transformations (2.13) and (2.15) in expressions (2.10)–(2.12), we obtain a system of equations for the real functions

$$\hbar \frac{\partial \Phi(z, t)}{\partial t} = -2aJ \frac{\partial \Phi}{\partial z} \sin ka, \quad (2.16)$$

²⁾ Here and in the following expressions of this review (unless otherwise mentioned) the integration is performed between infinite limits.

$$\left[\Lambda + a^2 \tilde{J} \frac{\partial^2}{\partial z^2} + 2\chi \rho(z, t) \right] \Phi(z, t) = 0, \quad (2.16a)$$

$$\left(\frac{\partial^2}{\partial t^2} - V_0^2 \frac{\partial^2}{\partial z^2} \right) \rho(z, t) = - \frac{2\chi V_0^2}{\kappa} \frac{\partial^2}{\partial z^2} \Phi^2(z, t), \quad (2.16b)$$

where

$$\tilde{J} = J \cos ka \quad (2.17)$$

is the renormalized resonant interaction energy;

$$V_0 = a \sqrt{\frac{\kappa}{M}} \quad (2.18)$$

is the velocity of longitudinal sound in the unperturbed chain;

$$\rho(z, t) = -a \frac{\partial}{\partial z} \beta(z, t) \quad (2.19)$$

describes the decrease in the distances between neighboring molecules $[a - a - \rho(z, t)]$;

$$E = \Lambda + \mathcal{E}_0 + W - 2\tilde{J} \quad (2.20)$$

is the total energy of the soliton;

$$W = \frac{1}{2a} \int \left[M \left(\frac{\partial \beta}{\partial t} \right)^2 + \kappa \rho^2 \right] dz \quad (2.21)$$

is the kinetic and potential energy owing to displacements of equilibrium positions of the molecules.

Equations (2.16)–(2.16a) determine the energy E and the functions $\Phi(z, t)$ and $\rho(z, t)$ of the states of the chain corresponding to a single intramolecular excitation with energy \mathcal{E}_0 .

Due to the translational invariance of the operator (2.1), stationary solutions of the system of equations (2.16)–(2.16b) can be sought in the form of excitations propagating with constant velocity V . For this, it is sufficient to set

$$\rho(z, t) = \rho(\zeta), \quad \Phi(z, t) = \Phi(\zeta),$$

where

$$\zeta = z - z_0 - Vt. \quad (2.22)$$

For such excitations

$$\frac{\partial \Phi(z, t)}{\partial t} = -V \frac{d\Phi(\zeta)}{d\zeta}, \quad \frac{\partial \rho(z, t)}{\partial t} = -V \frac{d\rho(\zeta)}{d\zeta},$$

$$\frac{\partial \Phi(z, t)}{\partial z} = \frac{d\Phi(\zeta)}{d\zeta}, \dots \quad (2.23)$$

so that the partial differential equations (2.16) transform into the ordinary differential equations

$$(\hbar V - 2aJ \sin ka) \frac{d\Phi}{d\zeta} = 0, \quad (2.24)$$

$$\left[\Lambda + a^2 \tilde{J} \frac{d^2}{d\zeta^2} + 2\chi \rho(\zeta) \right] \Phi(\zeta) = 0, \quad (2.25)$$

$$\frac{d^2}{d\zeta^2} \left[(1 - s^2) \rho(\zeta) - \frac{2\chi}{a\kappa} \Phi^2(\zeta) \right] = 0, \quad (2.26)$$

where

$$s = \frac{V}{V_0}. \quad (2.27)$$

It follows from Eq. (2.26) that the decreases in the equilibrium distances between molecules, caused by the intramolecular excitations, are determined in a system of coordinates moving together with the excitation by the function

$$\rho(\zeta) = \frac{2\chi \Phi^2(\zeta)}{\kappa(1 - s^2)}. \quad (2.28)$$

Substituting this value into Eq. (2.25), we transform it

into the nonlinear Schroedinger equation for stationary states moving with constant velocity $V = sV_0$ along the chain:

$$\left[\Lambda + a^2 \tilde{J} \frac{d^2}{d\zeta^2} + G \Phi^2(\zeta) \right] \Phi(\zeta) = 0, \quad (2.29)$$

where the nonlinearity parameter

$$G = \frac{4\chi^2}{a\kappa(1 - s^2)} \quad (2.30)$$

takes into account the time lag of the deformation displacements. For $V_0 = \infty$, the displacements follow the displacement of the excitation without a lag and G does not depend on V .

For $s^2 \rightarrow 1$, the nonlinearity parameter (2.30) and the decrease in the distances (2.28) between molecules increase sharply. For large displacements of molecules, the harmonic approximation used in (2.3) is not applicable. The theory developed is valid only for $s^2 \ll 1$. In order to enlarge the range of applicability of the theory, it is necessary to include a more rapid, than quadratic, increase in the potential energy of interaction between molecules.

b) Exciton excited states

If the velocity of the excitation exceeds the velocity of longitudinal sound ($s^2 > 1$), then the nonlinearity parameter in Eq. (2.29) is negative. In this case the equation does not have stationary solutions, normalized by the condition (2.14), in an infinite chain. In a sufficiently long chain with length L (when end effects can be neglected), the normalized stationary solutions of Eq. (2.29) correspond to $\Phi(\zeta) = L^{-1/2}$. In this case Eq. (2.24) is satisfied for any value of the wave number k , characterizing the wave function in the form of a plane wave

$$A_k(z, t) = \sqrt{\frac{a}{L}} \exp \left\{ i \left[kz - \frac{E(k)t}{\hbar} \right] \right\}. \quad (2.31)$$

In this case, according to (2.29), the excitation energy is

$$E(k) = \mathcal{E}_0 - \frac{aG}{L} - 2J \cos ka, \quad G < 0. \quad (2.32)$$

In sufficiently long chains ($L \gg a$) the second term in (2.32) can be dropped.

States described by plane waves (2.31) are called excitons. In these states all molecules are excited with equal probability. In addition, according to (2.28), the change in the intermolecular distances is determined by the expression

$$\Delta a = -\rho(\zeta) = \frac{2a\chi}{\kappa L(s^2 - 1)}. \quad (2.33)$$

In long chains this change is very small. However the total length of a chain L , containing L/a molecules, changes by a finite amount

$$\Delta L = \frac{2\chi}{\kappa(s^2 - 1)}. \quad (2.33a)$$

The condition $\Delta L \ll L$ restricts the permissible values of s^2 .

For $J > 0$ (see (2.5)), the minimum in the exciton energy (2.32)

$$E(0) = \varepsilon_0 - 2J - \frac{aG}{L} \quad (L \gg a), \quad (2.34)$$

corresponds to $k=0$. The value $E(0)$ is called the energy of the bottom of the exciton band. All energy states of the exciton energy band are determined by wave numbers satisfying the inequality $|ka| \leq \pi$. Near the bottom of the exciton band, when the inequality $|ka| \ll 1$ is satisfied, expression (2.34) can be put into the form

$$E(V) = E(0) + \frac{1}{2} m_{\text{ex}} V^2, \quad (2.35)$$

where

$$V = \frac{\hbar k}{m_{\text{ex}}}, \quad m_{\text{ex}} = \frac{\hbar^2}{2a^2 J} \quad (2.35a)$$

is the effective mass of the exciton. In order for the condition $s^2 > 1$ to be satisfied, it is necessary that $J > \hbar V_0/2a$.

For $J < 0$, Eqs. (2.35) retain their meaning in the range $|ka| \ll 1$. In this case, the effective mass of the exciton is negative. The value $k=0$ corresponds to the maximum energy of a soliton (top of the band). The energy of the bottom of the exciton band corresponds to $|k| = \pi/a$. Near the bottom of the exciton band, in this case as well, the energy is expressed by Eq. (2.33) with positive effective exciton mass and with the values

$$V = \frac{[k - (\pi/a)\hbar]}{m_{\text{ex}}}, \quad |ak - \pi| \ll 1.$$

The energies (2.32) examined above for the stationary states of excitons are characteristic values of the total energy operator (2.1) excluding the vibrational energy of the molecules. When transforming into such excited states, the length of the chain changes by an amount determined by Eq. (2.33a). It increases for $s^2 > 1$ and decreases for $s^2 < 1$.

Exciton states in the chain can be excited by light with frequency ω (without participation of phonons) with the energy and quasimomentum conservation laws satisfied if the projection of the electric field intensity on the vector d for the transition is not equal to zero. For infrared, visible, and ultraviolet light, $a\omega \ll c$, so that excitons with small ka are excited. In this case, however, it should be kept in mind that at the time of the light-induced transition of the chain into an excited state, the molecules do not have time to move to new equilibrium positions (Franck-Condon principle). For this reason, strictly speaking, the transitions occur not into states corresponding to the complete Hamiltonian (2.1) but into states determined only by the operator (2.2), in which the distances between molecules remain equal to a . The characteristic functions of the operator (2.2) also are plane waves (2.31), corresponding to a definite value of k (excitons). Their energies are determined by the expression

$$E(k) = \varepsilon_0 - 2J \cos ka,$$

which, when the inequality $a \ll L$ is satisfied, practically coincides with (2.32). However these excitons are not stationary. The interaction described by the operator (2.4) leads, with the participation of phonons, to transitions between states with different k . In particular, for $s > 1$, due to the Cherenkov effect, excitons can be retarded (at low temperatures), emitting acousti-

cal phonons. These effects are usually taken into account by perturbation methods.

The exciton states with definite values of k are distributed uniformly over the entire length of the chain. Excitations encompassing a small part of the chain l_0 are not stationary. They are described by a superposition of plane waves, i.e., a wave packet:

$$\Psi(z, t) = \int_{k_0 - \Delta k}^{k_0 + \Delta k} C(k) A_k(z, t) dk, \quad \Delta k = \frac{\pi}{2l_0}, \quad (2.36)$$

made up of the plane waves (2.31) with different values of k . Such an excitation propagates along the chain with group velocity

$$v = \frac{\hbar k_0}{m_{\text{ex}}} = \frac{2k_0 a^2 |J|}{\hbar}, \quad (2.37)$$

where $\hbar k_0$ is the average momentum of an exciton in the quasistationary state (2.36). However, with time the region encompassed by the excitation expands. If at time t it equals l_0 , then at time $t + \tau$ it will equal

$$l_\tau = \sqrt{l_0^2 + \frac{\hbar^2 \tau^2}{(m_{\text{ex}} l_0)^2}}.$$

Spreading of the wave packet (2.36) is an indication of the inexact stationariness of the states in the packet.

The plane waves (2.31) with $\Phi(z, t) = \text{const}$ will be solutions of Eq. (2.29) for $s^2 < 1$ as well. However in this case, as will be shown in what follows, together with excitons with energies in the region of the exciton band $E(k)$, very stable excitations (solitons) with energies lying above the bottom of the exciton band are possible. For this reason, excitons are metastable for $s^2 < 1$.

c) Soliton excited states

For $s^2 < 1$, the nonlinearity parameter in Eq. (2.29) is positive. If $J > 0$, then this equation has a particular solution normalized by condition (2.14) in the form

$$\Phi(\xi) = \frac{\sqrt{aQ}}{\sqrt{2} \operatorname{ch} Q\xi} \quad (2.38)$$

with values

$$Q = \frac{G}{4aJ} = \frac{\chi^2}{2a^2 \kappa J (1-s^2) \cos ka} \quad (2.39)$$

and

$$\Lambda = a^2 Q^2 J \cos ka. \quad (2.40)$$

The value of k is expressed in terms of the velocity V (see below).

The excitation described by the amplitude (2.38) of the wave function (2.13) is called a soliton. It is distributed on the segment $\Delta\xi \approx 2\pi/Q$ in the system of coordinates ξ , moving together with the excitation with velocity $V = sV_0$. The condition for applicability of the continuum approximation requires that the inequality

$$aQ \ll 1. \quad (2.41)$$

be satisfied. According to (2.39), this inequality establishes, within the scope of the approximation used, the upper bound for permissible soliton velocities.

In the region of the excitation $d\Phi/d\xi \neq 0$, so that according to (2.24) the inequality

$$\sin ka = -\frac{\hbar V}{2a|J|} \equiv \tau, \quad (2.42)$$

which implicitly relates the value of k and the velocity V of the excitation, must be satisfied. From the condition that the factor $\cos ka = \sqrt{1 - \tau^2}$ entering into (2.17) be real follows the inequality

$$\tau^2 < 1, \quad \text{or} \quad V < \frac{2a|J|}{\hbar} \equiv V_g. \quad (2.43)$$

The velocity V_g in inequality (2.43) corresponds to the maximum group velocity of an exciton in the band.

Inequality (2.43) together with inequalities (2.41) and $s^2 < 1$ limits the permissible velocities of the soliton. From (2.42) and (2.43) it follows that for $J > 0$ the values of k can fall in the range $|ak| \ll \pi/2$, while for $J < 0$ they fall into the range $|ak - \pi| \ll \pi/2$.

We shall proceed to calculate the energy of a soliton moving with constant velocity V . With the help of (2.19) and (2.23), expression (2.21), determining the total deformation energy of the chain, is transformed into the form

$$W = M(V^2 + V_0^2)(2a^2)^{-1} \int \rho^2(\zeta) d\zeta. \quad (2.44)$$

Using the values (2.28) and (2.38), we obtain the final expression

$$W = \frac{2\chi^4(1+s^2)}{3\kappa^2(1-s^2)^2|J|\cos ka}. \quad (2.44a)$$

The total energy of the soliton (2.20), taking (2.40) and (2.44a) into account, is determined by the expression

$$E_{\text{sol}}(V) = \xi_0 - 2|J|V\sqrt{1-\tau^2} + \frac{(5s^2-1)\kappa^4}{3\kappa^2(1-s^2)^2|J|\sqrt{1-\tau^2}}, \quad (2.45)$$

where

$$s \equiv \frac{V}{V_0}, \quad \tau = \frac{V}{V_g}.$$

It follows from (2.44a) and (2.45) that as the velocity of the soliton increases, the energy of deformation of the chain and the total energy of the soliton increase considerably. For this reason, the final values of $E(V)$ correspond to soliton velocities V less than the smaller of the velocities V_0 and V_g .

For low soliton velocities, when $s^2 \ll 1$ and $\tau^2 \ll 1$, the total energy of the soliton (2.45) can be put into the form

$$E_{\text{sol}}(V) = E_{\text{sol}}(0) + \frac{1}{2} m_{\text{sol}} V^2, \quad (2.46)$$

where

$$E_{\text{sol}}(0) = \xi_0 - 2|J| - \frac{\chi^4}{3\kappa^2|J|} \quad (2.47)$$

is the energy of a soliton at rest. It is lower than the energy of the bottom of the energy band of exciton states (2.34a) by an amount

$$\Delta E = \frac{\chi^4}{3\kappa^2|J|} = \frac{a^2\chi^4}{3|J|MV_g^2}, \quad (2.48)$$

which is large when the coupling of intramolecular excitations to displacements of the molecule (parameter χ) is large and the elasticity of the longitudinal deformations (parameter κ) is small.

The effective mass of the soliton is determined by the expression

$$m_{\text{sol}} = m_{\text{ex}} \left[1 + \frac{3\chi^4}{3\kappa^2|J|V_g^2} \left(1 - \frac{V_0}{4V_g} \right) \right]. \quad (2.49)$$

In soft chains (for $V_0 < V_g$) the soliton mass greatly exceeds the exciton mass, since the motion of the soliton is accompanied by motion of the local deformation of the chain. Due to the large soliton mass, it can transport a considerable amount of energy at low velocities as well.

Substituting (2.38) into (2.28), we find the function

$$\rho(\zeta) = \frac{aQ\chi}{\kappa(1-s^2)\text{ch}^2 Q\zeta}, \quad (2.50)$$

which, taking into account the value of (2.39), describes the decrease in the intermolecular distances in the chain in the region of soliton excitation. The qualitative distribution of probabilities of intramolecular excitations and distances between molecules in the region of soliton excitation are indicated in Fig. 1. Figure 2 illustrates the dependence of the soliton and exciton energies on their velocity.

The presence of the energy gap (2.48) in the spectrum of excited states of the molecular chain is one of the reasons for the very high stability of solitons. In order to destroy a soliton, i.e., split it into a free exciton and a uniform deformation, it is necessary to expend the energy ΔE .

Since solitons always move with velocity less than the velocity of longitudinal sound in the chain, they do not emit phonons. In other words, their kinetic energy is not transformed into energy of thermal motion. This is the second important characteristic, which provides for the high stability of solitons in molecular chains.

The bell-shaped form of solitons (2.38) does not depend on the method for exciting them. It is self-consistent. For $s^2 \ll 1$ the shape of the soliton does not change even when its kinetic energy decreases. On the contrary, the shape of the wave packet (2.36) depends on the initial distribution of the amplitudes $C(k)$. With the passage of time, the wave packet "spreads out."

As the resonant interaction energy (J) and the chain rigidity κ increase, the differences between solitons and excitons decrease. The region encompassed by the excitation $\Delta \xi = 2\pi/Q$, according to (2.39), increases in this case. The effective mass of the soliton approaches the effective mass of the exciton at the bottom of the band. The internal energy of the soliton $E(0)$ approaches the energy of the bottom of the exciton band $E_{\text{ex}}(0)$.

Absorption of light by molecular systems is not accompanied by a change in the coordinates of heavy particles at the time of the quantum transition (Franck-Condon principle). Since the formation of solitons is

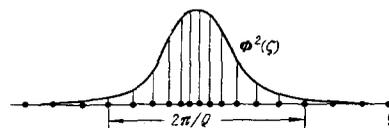


FIG. 1. Qualitative probability distribution of intramolecular excitations (vertical lines) and distances between molecules (points) in the region of a soliton excitation.

accompanied by a displacement of the equilibrium positions of molecules, it cannot be brought about by light. The probability for emission of light by a soliton is small for the same reason. The theory of this problem was developed in a paper by Erenko and Davydov.²⁶

Solitons corresponding to positive values of J can be excited by local external actions, for example, chemical reactions. The probability for excitation of solitons is highest when such local action takes place at the end of the molecular chain. If the bottom of the exciton band corresponds to the value $k=\pi/a$ (for $J < 0$), then in the soliton state the excitations of neighboring molecules have opposite phases. Excitation of such solitons requires very specific and difficult to realize conditions.

3. SOLITONS IN BIOLOGICAL MOLECULES

It is well known that many biological phenomena are related to spatial displacement of energy along protein molecules. As has now been established, the universal unit of energy transported by protein molecules is the energy (about 0.43 eV) liberated with the hydrolysis of adenosine triphosphate (ATP) molecules. This energy is only 20 times greater than the average thermal energy under physiological temperatures. This energy is insufficient for exciting electron states. For this reason, vibrational excitation of some groups of atoms in protein molecules must play the basic role in transporting the energy of hydrolysis of ATP molecules.

It has been proposed repeatedly that vibrational oscillations C=O in peptide groups play the greatest role in energy transport in proteins (see Sec. 3a below). These vibrations are called Amide I. They have an energy of about 0.21 eV and a comparatively large electric dipole transition moment $d \approx 0.3$ Debye, ensuring a large resonant interaction between peptide groups leading to collectivization of the excitation.

Isolated vibrations of this type in a condensed medium have a short lifetime of about 10^{-12} s. With a probable velocity of 10^4 cm/s they could move over a distance of the order of 10^{-8} cm. As a result, many researchers doubted the possibility of participation of these vibrations in energy transport along protein molecules having dimensions of 10^{-5} cm. Thus, for example, in 1973 in discussing the problem of energy transport in biological systems, some participants at the conference of the New York Academy of Sciences spoke of a "crisis" in bioenergetics and of the necessity of establishing special laws of bioenergetics by an a priori method.^{31, 32}

It was shown by Davydov³³⁻³⁵ that the difficulty noted above is removed if the fact is taken into account that the energy of hydrolysis of ATP molecules is transported along alpha-helical molecules as solitons moving without loss of energy to phonon emission. In what follows, we shall present the basic results of this work. But, we shall first in Sec. 3a generalize some of the elementary information on the structure of proteins.

a) Alpha-helix structure of proteins

The specific structure of protein molecules plays a key role in the stabilization and increase in the lifetime

of the vibrational states of these molecules. In what follows we shall present only some information concerning the structure of proteins, necessary to understand the mathematical models that we use. More complete information is contained in the monographs by Vol'kenshtein³⁶ and by Davydov.³⁷

Proteins are polymer molecules with very high molecular weight. These are the largest and most complicated molecules entering into the composition of cells of living organisms. All proteins are constructed from a small number (about 20) of structural units, the aminoacid residues.

Figure 3 illustrates the structure of an aminoacid. Polymerization of aminoacids (in the presence of the appropriate catalyzers and energy) is accompanied by the formation of water molecules with the detachments of hydrogen from the aminogroup NH_2 of one of the aminoacids and hydroxyl OH from the carboxyl group COOH from another. At the same time, the nitrogen and carbon of the aminoacid residues join with one another forming a chemical peptide bond. This polymerization process can continue repeatedly, forming long polypeptide chains (proteins) with repeating groups of four atoms



called peptide groups. Figure 4 shows a section of the protein chain containing two peptide groups. The sequence of the position of different residues of aminoacids in the molecule is called the primary structure of the protein.

The atoms making up each peptide group lie in a single plane. However, the entire protein molecule is a very flexible structure due to the possibility of rotation around single bonds. Such rotations are indicated in Fig. 4 by arrows. The flexible protein molecule can form different spatial configurations (secondary structure of the protein).

In particular, the protein chain can curl into a helix. This helical structure of protein molecules was first established by Pauling and Curie in 1953 (see Ref. 38). They called it the alpha helix and showed that it arises with the formation of three chains of hydrogen bonds between the peptide groups of the protein molecule. In Fig. 5 the peptide groups are indicated by ellipses and the hydrogen bonds are indicated by the lines connecting these groups.

The equilibrium position of peptide groups in a mole-

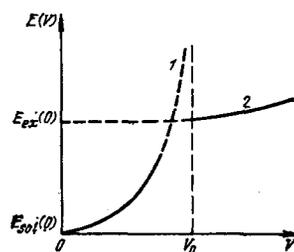


FIG. 2. Qualitative dependence of the excitation energy on velocity V . a) Solitons; 2) Excitons. V_0 is the velocity of longitudinal sound.

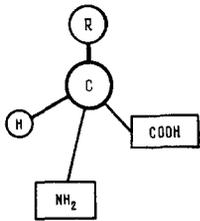


FIG. 3. Structural diagram of an amino acid molecule. NH_2 is an amino group; COOH is a carboxyl group; R is a group of atoms distinguishing one amino acid from another.

cule, whose axis coincides with the z axis, can be represented by the position vectors

$$R_{n\alpha} = R \left[e_x \cos \frac{2\pi}{p} (3n + \alpha) + e_y \sin \frac{2\pi}{p} (3n + \alpha) \right] + e_z \frac{a}{p} (3n + \alpha), \quad (3.1)$$

where e_x , e_y , and e_z are mutually orthogonal unit vectors and the index $\alpha = \text{I, II, and III}$ corresponds to the three chains of peptide bonds; a is the pitch of the helix (5.4 \AA); R is its radius (2.8 \AA) along the center of the peptide groups; $p = 3.6$ is the number of peptide groups per single loop of the helix; and, $n = 0, 1, 2, \dots$ is the number of the cells of the three nearest peptide groups with different indices α . One such cell would coincide with the elementary crystallographic cell for $p = 3$.

b) Solitons in alpha-helical proteins

We shall examine the collective excited states of an alpha-helical protein, corresponding to the characteristic Amide I vibration with energy $\mathcal{E}_0 = 0.21 \text{ eV}$ and electric dipole transition moment $d \approx 0.3 \text{ Debye}$,³⁾ oriented at a small angle to the axis of the helix. According to estimates by Nevskaya and Chirgadze,³⁹ the energy of the resonant interaction between neighboring peptide groups in a single chain is $-J = 7.8 \text{ cm}^{-1}$. The energy of the same interaction between neighboring peptide groups in different chains is $L = 12.4 \text{ cm}^{-1}$.

When studying collective excitations corresponding to intrapeptide oscillations Amide I, we shall examine as a model of the protein a system of three parallel chains of peptide groups (in what follows we shall simply call them molecules), occupying equilibrium positions (3.1). We shall restrict our analysis to only the resonant interactions J and L and two types of displacements of molecules, determined by the change in the pitch of the helix $a - a + u_{n\alpha}$ and a change in its radius $R - R + r_{n\alpha}$.

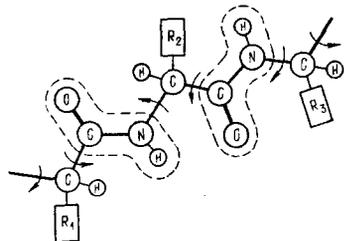


FIG. 4. Section of a protein molecule containing two peptide groups (surrounded by the dashed line).

³⁾One Debye equals the product of the proton charge and 10^{-8} cm .

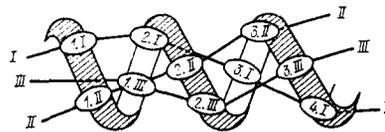


FIG. 5. Three chains of hydrogen bonds between peptide groups (shown by ellipses) in an alpha-helical protein molecule.

With these simplifications, the previously examined Hamiltonian function (2.9) of a single molecular chain will be replaced by the function

$$\mathcal{H} = \sum_{n\alpha} A_{n\alpha} \left\{ \left[\mathcal{E}_0 + W + \chi (\beta_{n+1, \alpha} - \beta_{n-1, \alpha}) + \frac{1}{2} \eta (2\gamma_{n\alpha} + \gamma_{n, \alpha+1} + \gamma_{n, \alpha-1}) \right] A_{n\alpha} - J (A_{n+1, \alpha} + A_{n-1, \alpha}) + L (A_{n, \alpha+1} + A_{n, \alpha-1}) \right\}, \quad (3.2)$$

where

$$W = \frac{1}{2} \sum_{n\alpha} \left\{ M \left[\left(\frac{\partial \beta_{n\alpha}}{\partial t} \right)^2 + \left(\frac{\partial \gamma_{n\alpha}}{\partial t} \right)^2 \right] + \kappa (\beta_{n\alpha} - \beta_{n-1, \alpha})^2 - \frac{1}{4} w (\gamma_{n\alpha} + \gamma_{n, \alpha-1})^2 \right\}. \quad (3.3)$$

In these expressions the quantity $|A_{n\alpha}(t)|^2$, normalized by the condition

$$\sum_{n\alpha} |A_{n\alpha}(t)|^2 = 1, \quad (3.3a)$$

determines the probability for exciting the molecule $n\alpha$ in the state sought $|\psi(t)\rangle$. The functions $\beta_{n\alpha}(t)$ and $\gamma_{n\alpha}(t)$ characterize the average values of $u_{n\alpha}$ and $r_{n\alpha}$, respectively, in the same state. Compared to (2.9), expressions (3.2) and (3.3) contain new quantities: η is the coupling parameter for intramolecular excitations and displacements γ , and w is the coefficient of elasticity relative to the change in radius of the helix. Since w is determined by chemical forces acting between atoms of the main protein chain, while κ is determined by the weaker hydrogen bonds only, the inequality

$$w \gg \kappa \quad (3.4)$$

is satisfied.

The function (3.2) determines the Hamiltonian equations, which in the continuum approximation with respect to n and for small velocities of excitations along the protein can be written in the form

$$\left[i\hbar \frac{\partial}{\partial t} - (\mathcal{E}_0 + W - 2J) + a^2 J \frac{\partial^2}{\partial z^2} + 2\chi \rho_\alpha - \frac{1}{2} \eta (2\gamma_\alpha + \gamma_{\alpha+1} + \gamma_{\alpha-1}) \right] A_\alpha = L (A_{\alpha+1} + A_{\alpha-1}), \quad A_\alpha \equiv A_\alpha(z, t); \quad (3.5)$$

$$\left(\frac{\partial^2}{\partial t^2} - V_0^2 \frac{\partial^2}{\partial z^2} \right) \rho_\alpha = - \frac{2\chi V_0^2}{\kappa} \frac{\partial^2}{\partial z^2} |A_\alpha|^2, \quad (3.6)$$

$$\rho_\alpha \equiv \rho_\alpha(z, t) = -a \frac{\partial \beta_\alpha(z, t)}{\partial z}, \quad (3.6a)$$

$$\frac{2M}{a^2} \frac{\partial^2 \gamma_\alpha}{\partial t^2} + w (2\gamma_\alpha + \gamma_{\alpha+1} + \gamma_{\alpha-1}) = \eta (2|A_\alpha|^2 + |A_{\alpha+1}|^2 + |A_{\alpha-1}|^2). \quad (3.7)$$

The normalization condition (3.3a) now assumes the form

$$\frac{1}{a} \int |A_\alpha(z, t)|^2 dz = 1. \quad (3.8)$$

By taking into account the translational symmetry of Eqs. (3.5)–(3.7), we can seek their solution in the form of excitations propagating with constant velocity V lower

than the velocity of longitudinal sound waves $V_0 = a\sqrt{\kappa/m}$ and the maximum group velocity of excitons $V_g = 2aJ/\hbar$ in the form

$$A_\alpha(z, t) = C_\alpha \Phi(\zeta) \exp \left\{ i \left[k(z - z_0) - \frac{Et}{\hbar} \right] \right\}, \quad (3.9)$$

$$\rho_\alpha(z, t) = \rho_\alpha(\zeta), \quad \gamma_\alpha(z, t) = \gamma_\alpha(\zeta), \quad (3.9a)$$

where

$$\zeta = z - z_0 - Vt. \quad (3.10)$$

The real function $\Phi(\zeta)$ is defined by the expression

$$\Phi(\zeta) = \sqrt{\frac{aQ}{2}} \operatorname{sech} Q\zeta \quad (3.11)$$

with the parameter Q to be determined.

From the normalization condition (3.8) follows the equality

$$\sum_\alpha |C_\alpha|^2 = 1. \quad (3.12)$$

Taking (3.9) into account we find from Eq. (3.6)

$$\rho_\alpha(\zeta) = \frac{2\chi |C_\alpha|^2}{\kappa(1-s^2)} \Phi^2(\zeta). \quad (3.13)$$

Using the inequality (3.4), the first term in (3.7), which is of the order of $\kappa V/mV_0 \ll 1$, can be neglected. Then we obtain

$$\gamma_\alpha(\zeta) = \frac{\Phi^2(\zeta) |C_\alpha|^2 \eta}{w}. \quad (3.14)$$

Substituting the values of (3.9), (3.13), and (3.14) into Eq. (3.5) and expressing the resonant interaction parameter J with the help of (2.35a) in terms of the effective mass of the exciton, we obtain a system of equations⁴⁾ for the unknown coefficients C_α and the parameter Q :

$$\left[E - (\xi_0 + W - 2J) + \frac{\hbar^2}{2m_{\text{ex}}} (Q^2 - k^2) \right] C_\alpha = L (C_{\alpha+1} + C_{\alpha-1}), \quad (3.15)$$

$$\left[\frac{2\chi^2 |C_\alpha|^2}{\kappa(1-s^2)} + \frac{\eta^2}{4w} (2|C_\alpha|^2 + |C_{\alpha+1}|^2 + |C_{\alpha-1}|^2) - \frac{\hbar^2 Q^2}{2m_{\text{ex}}} \right] C_\alpha = 0. \quad (3.16)$$

This system of equations together with condition (3.12) determines three types of solitons with values Q_i , ρ_α^i , and γ_α^i , $i = 1, 2, 3$. They correspond to energies

$$E_i(V) = \xi_0 + W_i - 2J + \Delta_i + \frac{m_{\text{ex}} V^2}{2} - \frac{\hbar^2 Q_i^2}{2m_{\text{ex}}}, \quad (3.17)$$

$$\Delta_i = -L, \quad 2L, \quad -L.$$

The deformation energies of the molecule W_i entering into this expression are determined by expression (3.3). Neglecting the small derivative $d\gamma_i/dt$ and going over to the continuum approximation, we transform (3.3) into the form

$$W_i = \frac{1}{2a} \sum_\alpha \int \left[M(V^2 + V_\alpha^2) \frac{(\rho_\alpha^i)^2}{a^2} + \frac{w}{4} (\gamma_\alpha^i + \gamma_{\alpha-1}^i)^2 \right] dz. \quad (3.18)$$

Finally, substituting the values (3.13) and (3.14) and calculating the integral, we find, using inequality (3.4), the final expression

$$W_i = \frac{1}{3} a Q_i \left[\frac{2(s^2+1)\chi^2}{\kappa(1-s^2)} \sum_\alpha |C_\alpha^i|^4 + \frac{\eta^2}{4w} \sum_\alpha (|C_\alpha^i|^2 + |C_{\alpha-1}^i|^2) \right] \\ \approx \frac{2aQ_i(s^2+1)\chi^2}{3\kappa(1-s^2)} \sum_\alpha |C_\alpha^i|^4. \quad (3.19)$$

⁴⁾ The system of equations (3.15) and (3.16) was obtained by Eremko and Sergienko.⁴⁰ For $\eta = 0$ they coincide with the equations obtained by Eremko, Sergienko, and Davydov.⁴¹ The case of solitons at rest was examined by Suprun and Davydov.⁴²

For the first type of solitons, called in Ref. 41 unsymmetrical solitons, the solution of the system of equations (3.15) and (3.16) has the form

$$C_\alpha^1 = 0, \quad C_{\alpha+1}^1 = -C_{\alpha-1}^1 = \frac{1}{1+s^2}, \quad (3.20)$$

$$Q_1 = \frac{am_{\text{ex}}}{\hbar^2} \left[\frac{\chi^2}{\kappa(1-s^2)} + \frac{3\eta^2}{8w} \right] \approx \frac{am_{\text{ex}}\chi^2}{\kappa(1-s^2)\hbar^2}. \quad (3.21)$$

In the case that $s^2 \ll 1$ the energy (3.17) can be written in the form

$$E_1(V) = E_1(0) + \frac{1}{2} m_{\text{sol}}^1 V^2, \quad (3.22)$$

where

$$E_1(0) = \xi_0 - 2J - L - \frac{a^2 m_{\text{ex}} \chi^4}{6\kappa^2 \hbar^2} \quad (3.23)$$

is the energy of a soliton at rest;

$$m_{\text{sol}}^1 = m_{\text{ex}} \left(1 + \frac{a^2 \chi^4}{6\kappa^2 \hbar^2 V_g^2} \right) \quad (3.24)$$

is the effective mass of the soliton.

The motion of an unsymmetrical soliton is accompanied by local deformation of the protein molecule. In the region of excitation the distances between molecules in the two chains decrease. According to (3.13) and (3.20) these changes are determined by the quantities

$$\rho_\alpha^1(\zeta) = 0, \quad \rho_{\alpha\pm 1}^1(\zeta) = \frac{a\chi Q_1}{2\kappa(1-s^2)\hbar^2 \zeta Q}. \quad (3.25)$$

The diameter of the helix in the region of excitation increases, but, also nonuniformly. As follows from (3.14), the increase in the distances between chains and the center of the helix is determined by the expression

$$\gamma_\alpha^1(\zeta) = 0, \quad \gamma_{\alpha\pm 1}^1(\zeta) = \frac{a\eta Q_1}{2w \hbar^2 \zeta Q_1}. \quad (3.26)$$

Thus the helical molecule bends in the region encompassed by the unsymmetrical type soliton excitation (see Fig. 6c).

The examined solutions (3.20) with constant values of the coefficients C_α are approximate. They separate out the α -th chain. Due to the resonant interaction L between peptide groups, entering into the makeup of different chains, there is an exchange of excitations between chains, so that the coefficients C_α must depend on time. The period of the exchange is approximately determined by the quantity $T = 2\pi\hbar/L \approx 2.7 \cdot 10^{-12}$ s. Thus the motion of an unsymmetrical soliton along the molecule must have a helical character.

The exchange of excitations between chains was first examined by Scott,⁴³⁻⁴⁵ who used it to interpret the experimental investigations by Webb,⁴⁶ who was studying the scattering of laser radiation by metabolically active bacteria (see Sec. 3c).

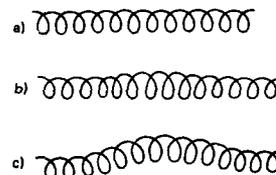


FIG. 6. a) Unperturbed helical protein molecule; b) excitation of a symmetrical soliton in the molecule; c) excitation of an unsymmetrical soliton.

In the case of the second type of excitation (symmetrical solitons), the solutions of the system of equations (3.15) and (3.16) have the form

$$C_{\alpha\pm 1}^{(2)} = C_{\alpha\pm 1}^{(2)} = \frac{1}{\sqrt{3}}, \quad (3.27)$$

$$Q_2 = \frac{am_{ex}}{3\hbar^2} \left[\frac{2\chi^2}{\alpha(1-s^2)} + \frac{\eta^2}{w} \right] \approx \frac{2m_{ex}a^2\chi^2}{3\alpha\hbar^2(1-s^2)}. \quad (3.28)$$

For $s^2 \ll 1$ the energy of such solitons is determined by the expression

$$E_2(V) = E_2(0) + \frac{1}{2} m_{sol}^{(2)} V^2, \quad (3.29)$$

where

$$E_2(0) = \xi_0 - 2J - 2L - \frac{2m_{ex}a^2\chi^4}{27\alpha^2\hbar^2}, \quad (3.30)$$

$$m_{sol}^{(2)} = m_{ex} \left(1 - \frac{2a^2\chi^4}{27\alpha^2\hbar^2 V_0^2} \right). \quad (3.31)$$

In this case in the region of excitations the distances between molecules in the three chains decrease symmetrically:

$$r_{\alpha\pm 1}^{(2)}(\xi) = r_{\alpha\pm 1}^{(2)}(\xi) = \frac{a\gamma Q_2}{3\alpha(1-s^2)\hbar^2 \xi Q_2}, \quad (3.32)$$

while the diameter of the helix increases (see Fig. 6b)

$$r_{\alpha}^{(2)}(\xi) = r_{\alpha\pm 1}^{(2)}(\xi) = \frac{a\eta Q_2}{6w\hbar^2 \xi Q_2}. \quad (3.33)$$

Finally, the third type of solution of the system of equations (3.15) and (3.16) can be written in the form

$$C_{\alpha}^{(3)} = 3^{-1/2} \exp\left(\frac{i2\pi\alpha}{3}\right), \quad \alpha = 1, 2, 3, \quad (3.34)$$

$$Q_3 = \frac{am_{ex}}{3\hbar^2} \left[\frac{2\chi^2}{\alpha(1-s^2)} + \frac{\eta^2}{w} \right] \approx \frac{2m_{ex}a^2\chi^2}{3\alpha\hbar^2(1-s^2)}. \quad (3.35)$$

In this case, for $s^2 \ll 1$, the energy of the soliton is determined by the expression

$$E_3(V) = E_3(0) + \frac{1}{2} m_{sol}^{(3)} V^2, \quad m_{sol}^{(3)} = m_{sol}^{(3)}, \quad (3.36)$$

where

$$E_3(0) = \xi_0 - 2J - L - \frac{2m_{ex}a^2\chi^4}{27\alpha^2\hbar^2}. \quad (3.37)$$

Thus the effective masses and spatial extent of solitons of the second and third types coincide. However the excitations of separate chains are shifted in phase for solitons of the third type (see (3.34)). As a result, their energy is less than the energy of symmetrical solitons by an amount $3L$.

Unsymmetrical solitons are more compact ($Q_1 > Q_2 = Q_3$). They have a much lower energy and a higher effective mass. Thus, of the three possible types of solitons transporting the energy of the Amide I vibrational excitation through the protein molecules, the unsymmetrical solitons are the most stable ones. They can transport the vibrational energy of Amide I without losses.

c) Numerical calculations of soliton excitations in discrete protein molecules

In all the preceding calculations, a continuum model of an infinite chain was used in order to obtain analytical results. In studying more realistic discrete finite chains, the corresponding systems of equations must be integrated numerically on modern computers. In the case of helical protein molecules, modeled by three

discrete chains of peptide groups held together by hydrogen bonds, these equations follow directly from the Hamiltonian function (3.2). For $\eta=0$ the corresponding equations were first obtained by Eremko, Sergienko, and Davydov.⁴¹ They have the form

$$i\hbar \frac{dA_{n\alpha}}{dt} = [\xi_0 + W + \chi(\beta_{n+1, \alpha} - \beta_{n-1, \alpha})] A_{n\alpha} - J(A_{n-1, \alpha} + A_{n+1, \alpha}) + L(A_{n, \alpha+1} + A_{n, \alpha-1}), \quad (3.38)$$

$$M \frac{d^2\beta_{n\alpha}}{dt^2} - \kappa(\beta_{n+1, \alpha} - 2\beta_{n, \alpha} + \beta_{n-1, \alpha}) = \chi(|A_{n+1, \alpha}|^2 - |A_{n-1, \alpha}|^2), \quad \alpha = 1, 2, 3. \quad (3.39)$$

The quantity W entering into (3.38) is determined by the expression

$$W = \frac{1}{2} \sum_{n\alpha} \left[M \left(\frac{d\beta_{n\alpha}}{dt} \right)^2 + \kappa(\beta_{n, \alpha} - \beta_{n-1, \alpha})^2 \right].$$

Equations (3.38) and (3.39) were integrated numerically by Hyman, McLaughlin, and Scott⁴⁷ with the help of the computer at the Los Alamos Scientific Laboratory in 1979. They studied excited states of three chains of helical protein molecules. Each chain contained 200 peptide groups. The molecule was characterized by the following quantities: $E_0 = 0.205$ eV; $M = 70$ proton masses; $V_0 \approx 10^6$ cm/s; $J = 1.55 \cdot 10^{-22}$ J, $L = 2.46 \cdot 10^{-22}$ J. The initial conditions at $t=0$ were taken as

$$A_{n\alpha} = \begin{cases} 1 & \text{for } n=1, \\ 0 & \text{for } n \neq 1, \end{cases} \quad \beta_{n\alpha} = 0. \quad (3.40)$$

The calculations were performed for different values of the coupling parameter χ of intrapeptide Amide I excitations with displacements of their equilibrium positions. It was shown that for the initial conditions (3.40) distinct solitons are formed and propagate in the molecule with $\chi \geq 3 \cdot 10^{-11}$ N.⁵⁾

Solitons with χ close to the critical value propagate with velocity $\sim 1.26 \cdot 10^3$ m/s. Therefore, the distance 1700 Å, corresponding to the length of the alpha-helical myosine molecule in muscle fibers (see Sec. 4), could be traversed by solitons (neglecting friction forces and the work performed by them) within 130 ps.

Hyman *et al.*⁴⁷ arrived at the conclusion that "numerical studies of Davydov's nonlinear dynamic model of alpha-helical proteins confirm his prediction of the formation of solitons."

Reference 47 is interesting in that the process of formation of solitons from a definite initial state is investigated and the role of the discreteness of the chain, which, apparently reduces to the fact that solitons are formed in the chain only with supercritical values of the coupling parameter χ , determining the nonlinearity of the system, is clarified.

In 1979, Eilbeck, in consultation with Scott, made a computer film⁴⁸ that demonstrates the propagation of

⁵⁾The values of the velocity V_0 used in the calculation are too high. The velocity of longitudinal sound in helical protein molecules is determined by weak hydrogen bonds between peptide groups. For this reason V_0 must be of the order of 10^4 cm/s. Therefore, the critical value of χ for formation of solitons will be lower.

an internal vibrational excitation of an edge group along a PG (peptide groups) chain. This film clearly shows that for an above threshold value of the coupling parameter χ between the vibrational excitation and displacements of PG along the molecule, the excitation propagates in the form of a soliton, i.e., in the form of a local pulse, whose shape and width remain constant during the motion. Eilbeck's film is important for two reasons: first, it confirms the previous calculations performed at the Los Alamos Laboratory and, second, it clearly demonstrates the stability of solitons relative to interactions with sound waves. The sound wave was excited together with the soliton. Moving faster than the soliton, it reflected several times from the ends of the chain passing through the soliton and not causing any changes in it.

Eilbeck's film and the numerical calculations in Ref. 47 show that the soliton forms at the very beginning of the peptide chain. Therefore, solitons can arise within comparatively short sections of alpha-helical proteins.

The necessity of exceeding some threshold value of the coupling parameter χ for exciting a soliton, discovered in the numerical calculations, as shown by Brizhik and Davydov⁴⁷ (see Sec. 6 of this review) is due to the conditions for excitation of a soliton. In the continuum approximation slow solitons can exist in an infinite chain for any values of χ . As χ decreases the properties of the solitons continuously approach the properties of excitons.

In the continuum description, the role of short wavelength displacements is not taken into account. Such displacements lead to an effective decrease in the resonant dipole-dipole interaction between PG. In the paper by Davydov⁵⁰ the displacement of peptide groups was described in the language of quantum theory taking into account short-wavelength displacements. It was shown that a smooth change in the magnitude of the coupling of an exciton (electron) with acoustical phonons can lead to a jump-like change in the parameters of the nonlinear equation: the magnitude of the resonant interaction (effective exciton mass) and the nonlinearity coefficient. In easily deformed systems, considerable self-localization is realized in a jump-like manner, if the coupling parameter exceeds a critical value. The problem of the jump-like transition into the self-localized state was examined by Toyazawa back in 1961.

In recent years, indications of solitons in some biological phenomena have appeared. Thus, for example, Scott⁴³⁻⁴⁵ used the theory of solitons to explain interesting experimental results obtained by Webb⁴⁶ in studying Raman scattering of laser radiation by the rod-shaped intestinal bacteria (*E. Coli*). Anti-Stokes frequencies appeared in the scattered spectrum in the range 40-200 cm^{-1} only in the case when the bacteria were in a metabolically active state. Scott asserts that these frequencies are due to vibrational states of solitons arising in live bacteria as a result of chemical reactions.

According to numerical estimates made by Scott⁴³⁻⁴⁵ the motion of a soliton along an alpha-helical protein

is characterized by two internal periods: the period $T_1 = 2 \cdot 10^{-16}$ s, corresponding to the time for a soliton to jump from one chain of hydrogen bonds to another, and the period $T_2 = 8/3 \times 10^{-13}$ s, corresponding to the discreteness of these chains. These periods correspond to the frequencies $E_1 = 17 \text{ cm}^{-1}$ and $E_2 = 125 \text{ cm}^{-1}$. The sums and differences of these frequencies coincide in a surprising manner with the values found experimentally by Webb. On this basis Scott comes to the conclusion⁴⁵ that "Raman spectroscopy can give a direct experimental indication of the functional role of Davydov solitons in metabolic processes."

Solitons were used in work by Italian scientists⁵¹ to explain the changes, in a certain temperature range, in the Raman spectrum of laser radiation scattered by green algae (*Chlorella pyrenoidosa*).

4. SOLITONS AND THE MOLECULAR MECHANISM FOR MUSCLE CONTRACTION

One of the most interesting problems in biophysics is the explanation of the molecular foundations of the transformation of the chemical energy of hydrolysis of ATP molecules into mechanical energy of motion. At the present time, striated muscles, which form the entire skeletal muscular structure and the heart muscle of vertebrate animals, man, and some nonvertebrate animals, have been studied in greatest detail. The present author has used the idea of the motion of solitons in helical protein molecules to explain the mechanism for contraction of striated muscles on a molecular level. In order to understand the idea on which the explanation is based, we shall first recall the basic information on the structure of such muscles.

a) Structure of striated muscles

The principal contracting element of muscle is the muscle fiber. This muscle fiber is an independent, very long and thin (diameter 20-80 μm) cell with many nuclei. The internal part of this cell forms a bunch of several thousand densely packed, filaments or myofibrils with diameter 1-2 μm , situated parallel to one another. Each myofibril consists of regularly alternating sections or sarcomers (Fig. 7a). The sarcomer is the smallest elementary section of a muscle capable of contraction.

Sarcomers are separated from one another by transverse membranes called z plates. Thin protein strands (Fig. 7b), consisting of the proteins actin, tropomyosine, and troponine, extend inside the sarcomer on both sides of the z plates. They partially penetrate into the space between the thick strands, situated in the interior region of a sarcomer (see Fig. 7b). The thin and thick strands are surrounded by a fluid medium, the sarcoplasm, which contains ATP molecules, Mg^{2+} ions, and some other particles.

b) Current models of the mechanism of muscle contraction

Contraction of sarcomers and, therefore, of the muscle fiber, occurs at a time when under the influence of the nerve pulse calcium ions enter the sarcoplasm from

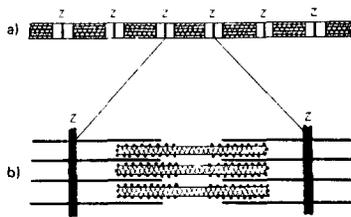


FIG. 7. a) Myofibril of a muscle fiber, separated by membranes z into sarcomers; b) diagram of the structure of a single sarcomer.

special microtubes. The calcium ions stimulate the process of hydrolysis of ATP molecules at locations where the thick and thin protein strands touch.

With the help of electron microscopic studies, Hanson and Huxley⁵² and Huxley and Niedergerke⁵³ established in 1954 that contraction of a sarcomer is associated with the penetration of thin filaments into the space between the thick filaments without contraction of the filaments themselves (Fig. 8). This model of slipping of thin protein strands relative to the thick strands received rapid general recognition. The experimentally established model of contraction of sarcomers raised a very important problem for researchers: to explain the mechanism of slipping on a molecular level. What forces cause the slipping of thin strands relative to thick strands? How does the energy of hydrolysis of the ATP molecule transform into slipping energy?

At the present time biologists widely believe that the slipping of thin strands relative to thick strands is due to the active motion of the "heads" of the myosine molecules, which makes up the thick strands.

The myosine molecule with molecular weight of about 500,000 resembles a thin rod with diameter $\sim 40 \text{ \AA}$ and length $\sim 1700 \text{ \AA}$ with a thickening at one end called the "head" of the molecule. The main part of the molecule is called the "tail." The molecule is formed by two polypeptide chains, having the conformation of an alpha helix over a large distance. The thick strand, shaped like a long cigar, contains about 400 myosine molecules. They are arranged in such a manner that the molecular heads are oriented toward both ends of the thick strand, extending to its surface, while the tails are oriented toward the center (see Fig. 7).

It is proposed that with hydrolysis of an ATP molecule, attached to the head of the myosine molecule, the latter stretches, forming a bond ("bridge") with the

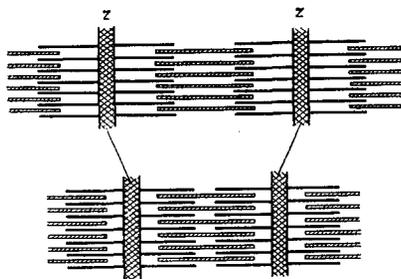


FIG. 8. Illustration of the model of slipping of thin strands relative to thick strands in a sarcomer.

globular actine molecule, which is contained in the thin strand; then, the head rotates, moving the thin strand toward the center of the sarcomer and, finally, separates from the active molecule, returning to the previous size and position in the thick strand. Attaching a new ATP molecule, it repeats this cycle, if calcium ions are present in the sarcomer. These motions of the head of the myosine molecule are illustrated in Fig. 9, which we took from the review by Murray and Weber.⁵⁴

According to this model, the slipping of the thin strands relative to the thick ones is reminiscent of the motion of water near a boat with oarsmen, sitting at the ends of the boat facing one another. The heads of the myosine molecules play the role of oars. For this reason, this model can be called the "oar model."

The idea of bridges between the thick and thin strands, which close, pull the fibers, causing their displacement, and then rupture, does not describe the molecular nature of the phenomenon. Many questions remain unanswered. How is the energy of hydrolysis of ATP expended on elongation, formation of bonds, pulling forces, and rupture of bridges? What is the molecular mechanism for the changes in the head of the myosine molecule, leading to these phenomena? And, finally, why does only the head of the enormous myosine molecular take an active part in the contraction mechanism?

c) New hypothesis concerning the mechanism of muscle contraction

Based on theoretical studies of solitons in helical proteins (see Sec. 3b), Davydov proposed a new hypothesis to explain the mechanism of contraction of sarcomers in muscle fibers.^{35, 37, 55-59} According to this hypothesis, calcium ions entering the sarcomer near the z plates diffuse toward the center of the sarcomer and, reaching the first row of myosine molecule heads at the ends of the thick strands, cause hydrolysis of the ATP molecules perpendicular to them. The energy liberated creates unsymmetrical solitons, which move from the

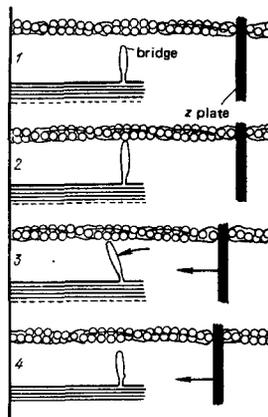


FIG. 9. Phenomenological model of contraction of sarcomers of striated muscle. The motion of a single head of a myosine molecule, leading to displacement of z plates, is shown. The figure is taken from Ref. 54.

heads of the molecules to their tails. As shown in Sec. 3b, the motion of the unsymmetrical soliton is accompanied by local expansion and bending of molecules. For this reason, in the region of excitations, moving along the bunch of myosine molecules, the thick strand expands (Fig. 10). As a result of the expansion of the thick strands the heads of the myosine molecules, located on their surface, are pressed against the thin strands. As the "swelled" regions of the thick strands move toward the center of the sarcomer, they carry the thin strands with them. The hydrolysis of ATP molecules in the second row of myosine molecule heads gives rise to new solitons. Their motion inside the thick strands gives rise to motion of new swelled regions of thick strands, which also displace the thin strands toward the center of the sarcomer. Hydrolysis of other ATP molecules leads to additional displacement, etc.

According to the model that we have proposed, the heads of the myosine molecules press against the thin strands, push them over a small distance, and move away from them (as in the model of formation and rupture of bridges). However this motion is due not to elongation, rotation, and contraction of the heads themselves, but to the penetration of an excitation and deformation wave in the form of solitons into the thick strand. In this case the kinetic energy of solitons transforms into contraction energy or leads to stretching, if the muscle has a load on it. In this model, the active elements of contraction are all parts of the myosine molecule and not only its head.

Expending their kinetic energy on the work necessary to contract the muscle fiber, the solitons are slowed down and, stopping near the centers of the thick strands, are annihilated, giving up their rest energy to thermal motion. Thus, only the kinetic energy of solitons is used in contraction of muscle fibers.

If we take into account the fact that with hydrolysis of ATP molecules ~ 0.43 eV is liberated, while the internal energy of a soliton is ~ 0.20 eV, then the maximum efficiency of muscle contraction is about 50%.

A good macroscopic illustration of the mechanism of displacement of thin sarcomer strands due to the motion of the swelled region of thick strands, in which solitons are excited, are the vibromotors of Ragulskis and his coworkers at the Vibration Technology Scientific Research Institute at the Kaunas Polytechnical Institute.^{60,61} In these motors, elastic oscillations excited in piezoelectric films in the form of pulses move along

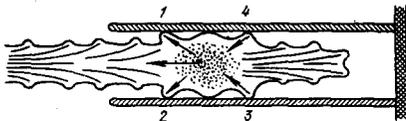


FIG. 10. Motion of solitons arising at the heads of myosine molecules along the tails of molecules inside a thick strand causes the thick strand to swell and displaces the swelled part toward the center of the sarcomer. The arrows 1-4 indicate the direction of motion of the heads of myosine molecules on displacement of the swelled region.

their surface and give rise under the action of friction to rotation or displacement of the bodies next to them. Figure 11 shows a functional diagram of the simplest vibromotor. Elastic pulses are excited at the input unit A. The bulges that arise, moving along the film toward the absorbing outlet unit B, cause the cylinder to rotate due to sliding friction forces.

5. DYNAMIC PROPERTIES OF SOLITONS

The possibility of using the soliton concept to explain some phenomena in physics, biology, and other sciences necessarily involves the investigation of dynamic properties of solitons and the reasons for the nonlinearity and dispersion. The dynamic properties of solitons are manifested when they interact with external fields and other degrees of freedom of the system, leading to their relaxation. The mathematical analysis of such interactions is usually conducted using perturbation theory.

Different variants of the perturbation theory for solitons in one dimensional systems were developed by Karpman and Maslov,⁶² Bishop *et al.*,⁶³ Keener and McLaughlin,⁶⁴ and other researchers. In this section we shall present the results of investigations by Eremko and Davydov,⁶⁵ who studied the effect of external actions on solitons, arising in the case of local excitations in molecular quasi-one-dimensional chains.

a) Free solitons with low velocities

As shown in Sec. 2, the properties of free solitons in a molecular chain are determined by the system of equations (2.11) and (2.12) with the normalization condition (2.8). When the condition $V_0 < 2aJ/\hbar$ is satisfied, which characterizes the soft chains with strong resonant dipole-dipole interaction, this system in the continuum approximation takes the form

$$\left\{ i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m_{ex}} \frac{\partial^2}{\partial z^2} - [E_{ex}(0) + W] - 2\chi a \frac{\partial \beta(z, t)}{\partial z} \right\} A(z, t) = 0, \quad (5.1)$$

$$\left(\frac{\partial^2}{\partial t^2} - V_0^2 \frac{\partial^2}{\partial z^2} \right) \beta(z, t) - \frac{2a\chi}{M} \frac{\partial}{\partial z} |A(z, t)|^2 = 0. \quad (5.2)$$

$$W = \frac{1}{2a} \int \left[M \left(\frac{\partial \beta}{\partial t} \right)^2 + \kappa a^2 \left(\frac{\partial \beta}{\partial z} \right)^2 \right] dz; \quad (5.3)$$

here m_{ex} is the effective mass of the exciton and $E_{ex}(0)$ is the energy of the bottom of the exciton band.

If we introduce the transformation

$$A(z, t) = \sqrt{a} \tilde{B}(z, t) \exp \left\{ -\frac{i}{\hbar} [E_{ex}(0) + W] \right\}$$

and the function

$$\rho(z, t) = -a \frac{\partial \beta(z, t)}{\partial z}, \quad (5.4)$$

which characterizes the decrease in the intermolecular

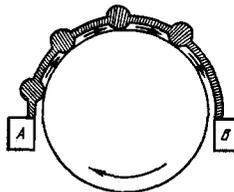


FIG. 11. Functional diagram of the simplest Ragulskis vibromotor.

distances, then the system of equations (5.1) and (5.2) takes the form

$$\left[i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m_{ex}} \frac{\partial^2}{\partial z^2} + 2\chi\rho(z, t) \right] B(z, t) = 0, \quad (5.5)$$

$$\left(\frac{\partial^2}{\partial t^2} - V_0^2 \frac{\partial^2}{\partial z^2} \right) \rho(z, t) + \frac{2\chi a}{\kappa} V_0^2 \frac{\partial^2}{\partial z^2} |B(z, t)|^2 = 0. \quad (5.6)$$

Here, in accordance with (2.8), the condition

$$\int |B(z, t)|^2 dz = 1. \quad (5.7)$$

is satisfied. In the case of excitations moving with constant velocities V , much lower than the velocity of longitudinal sound V_0 , we obtain from Eq. (5.6)

$$\rho(z, t) = \frac{2a\chi |B(z, t)|^2}{\kappa}, \quad V \ll V_0. \quad (5.8)$$

Substituting (5.8) into Eq. (5.5), we obtain the nonlinear Schrodinger equation

$$\left(i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m_{ex}} \frac{\partial^2}{\partial z^2} + g |B(z, t)|^2 \right) B(z, t) = 0, \quad (5.9)$$

where the nonlinearity parameter is given by

$$g = \frac{4\chi^2 a}{\kappa}. \quad (5.10)$$

The solution of this equation normalized by condition (5.7) has the form

$$B_0(z, t) = \frac{\sqrt{q} \exp\{i[k(z-\zeta) + \Theta]\}}{\sqrt{2 \operatorname{ch}[q(z-\zeta)]}}, \quad (5.11)$$

in which

$$\zeta = z_0 + \frac{\hbar k t}{m_{ex}}, \quad \Theta = \frac{\hbar(k^2 + q^2)t}{2m_{ex}}, \quad q = \frac{2a\chi^2 m_{ex}}{\kappa \hbar^2}. \quad (5.12)$$

The function (5.11) describes a solitary wave (soliton) with maximum of the envelope at $z = \zeta$ and phase Θ moving along the z axis with constant velocity

$$V = \frac{\hbar k}{m_{ex}}. \quad (5.13)$$

b) Motion of solitons in the presence of friction

If the molecular chain is located in some medium, then friction will act on the moving soliton and the soliton will slow down. This deceleration can be included by introducing on the right side of Eq. (5.2), which determines the shift in the equilibrium positions of the molecules, dissipative terms. In the presence of friction forces, proportional to the displacement velocity ($\epsilon \gamma \partial \beta / \partial t$), Eq. (5.6) assumes the form

$$\left(\frac{\partial^2}{\partial t^2} - V_0^2 \frac{\partial^2}{\partial z^2} \right) \rho(z, t) + \frac{2a\chi^2 \kappa}{\kappa} \frac{\partial^2}{\partial z^2} |B|^2 = -\epsilon \gamma \frac{\partial \rho}{\partial t}, \quad (5.14)$$

where ϵ is a small positive parameter. Therefore, in the presence of friction the motion of a soliton is determined by the system of equations (5.9) and (5.14).

In order to solve this system of equations, A. Eremko and Davydov⁶⁵ used the method of "slowly varying coefficients," introduced by Van der Pol and developed in detail by N. N. Bogolyubov and Yu. A. Mitropol'skii.⁶⁶

Let us assume that at $t=0$ the soliton is described by the function (5.11) with $k=k_0$. In order to determine how this function changes under the action of friction forces we shall seek the solution of the system of equa-

tions (5.9) and (5.14) in the form

$$B(z, t) = B_0(z, t) + \epsilon B_1(z, t), \quad (5.15)$$

$$\rho(z, t) = \rho_0(z, t) + \epsilon \rho_1(z, t), \quad (5.16)$$

where

$$\rho_0(z, t) = \frac{2\chi a |B_0(z, t)|^2}{\kappa}, \quad (5.17)$$

while the function $B_0(z, t)$ coincides with expression (5.11), in which the time dependent quantities k , ζ , and Θ are determined by the equations

$$\frac{dk}{dt} = \epsilon f(k), \quad (5.18)$$

$$\frac{d\zeta}{dt} = \frac{\hbar k}{m_{ex}}, \quad \frac{d^2\zeta}{dt^2} = \frac{\epsilon \hbar f(k)}{m_{ex}}, \quad (5.19)$$

$$\frac{d\Theta}{dt} = \frac{\hbar(k^2 + q^2)}{2m_{ex}} + \epsilon \varphi(k). \quad (5.20)$$

Thus the problem reduces to determining the unknown functions $f(k)$, $\varphi(k)$, and $B_1(z, t)$ with the additional requirement that the function $B_1(z, t)$ not include terms containing the derivatives $\partial B_0 / \partial \zeta$ and $\partial B_0 / \partial \Theta$. These terms increase quadratically with time and are called secular terms.⁶⁶

Substituting expression (5.16) with values (5.17) and (5.11) into Eq. (5.14) and retaining terms of the first order with respect to ϵ , we obtain in the case of a weak time dependence of $\rho_1(z, t)$

$$\rho_1(z, t) = -\frac{a\hbar\chi \operatorname{sh}^2[q(z-\zeta)]}{\kappa V_0^2 m_{ex} \operatorname{ch}^3[q(z-\zeta)]} [\gamma k + f(k)]. \quad (5.21)$$

As the next step, we substitute expression (5.15) and (5.16) into Eq. (5.9). Taking into account (5.21) and (5.18), we obtain an equation determining the function $B_1(z, t)$:

$$\left[i\hbar \frac{\partial}{\partial t} - \frac{\hbar^2}{2m_{ex}} \frac{\partial^2}{\partial z^2} + \frac{8a\chi^2}{\kappa} |B_0(z, t)|^2 \right] B_1(z, t) + \frac{4a\chi^2 B_0^* B_1^*}{\kappa} = F(B_0), \quad (5.22)$$

where

$$F(B_0) = [f(k)(z-\zeta) + \varphi(k) - 2\chi\rho_1(z, t)] B_0(z, t). \quad (5.23)$$

The conditions for the absence of secular terms in $B_1(z, t)$ reduce to the requirement that the function $F(B_0)$ be orthogonal to the functions $\partial B_0 / \partial \zeta$ and $\partial B_0 / \partial \Theta$. Satisfaction of these conditions leads to equations determining together with (5.21) the unknown functions

$$f(k) \int \operatorname{th}[q(z-\zeta)](z-\zeta) |B_0(z, t)|^2 dz = \frac{2\chi}{\hbar} \int |B_0(z, t)|^2 \rho_1(z, t) \operatorname{th}[q(z-\zeta)] dz, \quad (5.24)$$

$$\varphi(k) = \frac{2\chi}{\hbar} \int |B_0(z, t)|^2 \rho_1(z, t) dz. \quad (5.25)$$

After calculating the integrals we find

$$\varphi(k) = 0, \quad f(k) = \frac{k\gamma D}{1+D}, \quad (5.26)$$

where

$$D = \frac{m_{sol} - m_{ex}}{m_{ex}}. \quad (5.27)$$

Substituting (5.26) into (5.18), we obtain after integrating and using the equality (5.13) the law for the decrease of the soliton velocity in the presence of friction forces proportional to velocity

$$V(t) = V_0 \exp(-\alpha t), \quad (5.28)$$

where

$$\alpha = \frac{\varepsilon \gamma (m_{\text{sol}} - m_{\text{ex}})}{m_{\text{sol}}} \quad (5.29)$$

If the friction force is proportional to the square of the velocity ($-\varepsilon \lambda (\partial \beta / \partial t)^2$) and is directed opposite to it, then Eq. (5.14) is replaced by the equation

$$\left(\frac{\partial^2}{\partial t^2} - V_0^2 \frac{\partial^2}{\partial z^2} \right) \rho(z, t) + \frac{2\alpha \gamma V_0^2}{\kappa} \frac{\partial^2}{\partial z^2} |B(z, t)|^2 = -\varepsilon \lambda \frac{V}{a} \frac{\partial \rho^2(z, t)}{\partial t}.$$

In this case, with analogous calculations, we find that the decrease in the soliton velocity is determined by the expression

$$V(t) = \frac{V_0}{1 + \beta V_0 t} \approx V_0 (1 - \beta V_0 t), \quad (5.30)$$

where

$$\beta = \frac{\varepsilon \lambda 16 \gamma^2 a q^2}{15 m_{\text{sol}} \kappa^2 V_0^2}. \quad (5.31)$$

Thus the decrease in velocity is nearly linear with a coefficient of proportionality βV_0^2 .

c) Motion of solitons under the action of external inhomogeneous coefficient of proportionality βV_0^2

The effect of external inhomogeneous fields or local inhomogeneities in the distribution of molecules can be taken into account by introducing into Eq. (5.1), together with the energy $E_{\text{ex}}(0)$, the additional term $\varepsilon U(z)$, depending on the z coordinate. In this case the system of equations for the soliton moving along the chain of molecules with velocity $V \ll V_0$, has the form

$$\left[i \hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + 2\chi \rho(z, t) \right] B(z, t) = \varepsilon U(z) B(z, t), \quad (5.32)$$

$$\left(\frac{\partial^2}{\partial t^2} - V_0^2 \frac{\partial^2}{\partial z^2} \right) \rho(z, t) + \frac{2\chi a}{\kappa} V_0^2 \frac{\partial^2}{\partial z^2} |B(z, t)|^2 = 0. \quad (5.33)$$

The solution of this system in the first approximation can also be sought in the form (5.15)–(5.17). In this case from (5.32) and (5.33) follow the equations

$$\left(i \hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m_{\text{ex}}} \frac{\partial^2}{\partial z^2} + \frac{4a\chi^2}{\kappa} |B(z, t)|^2 \right) \chi B(z, t) = \varepsilon [U(z) + \rho_1(z, t)] B(z, t), \quad (5.34)$$

$$\left(\frac{\partial^2}{\partial t^2} - V_0^2 \frac{\partial^2}{\partial z^2} \right) \rho_1 = -\frac{1}{\varepsilon} \frac{d^2 \xi}{dt^2} \frac{\partial \rho_0}{\partial z}. \quad (5.35)$$

Using the weak dependence of the function $\rho_1(z, t)$ on time, the explicit form of (5.11), and the value $d^2 \xi / dt^2$ from (5.19), we obtain after integrating (5.35),

$$\rho_1(z, t) = -\frac{\hbar a \chi}{\kappa m_{\text{ex}} V_0^2} f(k) \text{th} [q(z - \xi)]. \quad (5.36)$$

Substituting (5.15) and (5.36) into (5.34), we transform Eq. (5.34) into the form

$$\left(i \hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m_{\text{ex}}} \frac{\partial^2}{\partial z^2} + \frac{8a\chi^2}{\kappa} |B_0|^2 \right) B_1 + \frac{4a\chi^2}{\kappa} B_0^* B_1 = \tilde{F}(B_0),$$

where

$$\tilde{F}(B_0) = [U(z) - 2\chi \rho_1 + (z - \xi) f(k) + \varphi(k)] B_0(z, t). \quad (5.37)$$

From the conditions that terms increasing with time are absent in $B_1(z, t)$, we obtain two equations:

$$\varphi(k) = -\frac{1}{\hbar} \int |B_0(z, t)|^2 U(z) dz, \quad (5.38)$$

$$f(k) = -\frac{2q}{\hbar(1+D)} \int |B_0(z, t)|^2 U(z) \text{th} [q(z - \xi)] dz, \quad (5.39)$$

where D is determined by expression (5.27). Substituting this value into Eq. (5.19) and including the in-

equality $m_{\text{ex}}(1+D) = m_{\text{sol}}$, we obtain an equation determining the motion of the center of the soliton, i.e., the maximum of the envelope of the solitary wave:

$$m_{\text{sol}} \frac{d^2 \xi}{dt^2} = F(\xi), \quad (5.40)$$

where

$$F(\xi) = -2eq \int |B_0(z, t)|^2 U(z) \text{th} [q(z - \xi)] dz. \quad (5.41)$$

Equation (5.40) is reminiscent of Newton's equation for particles with the soliton mass. The soliton is affected by the potential field $U(z)$ from the entire region where $|B_0|^2 \neq 0$. At the same time, from the region $z > \xi$, the potential $U(z)$ makes a contribution with negative sign, while from the region $z < \xi$ it contributes with a positive sign. It is very significant that Eq. (5.40) contains the effective mass of the soliton and not the effective mass of an exciton, entering directly into Eq. (5.32). This is due to the fact that the nonlinearity of the collective excitation being examined is determined by the interaction of the exciton with the local deformation of the chain, created by the exciton itself and whose inertial properties change the effective mass of the free exciton.

In a number of papers,^{67,68} the effect of a perturbation on the nonlinear Schrodinger equation is studied by solving the equation

$$\left(i \hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m_{\text{ex}}} \frac{\partial^2}{\partial z^2} + G |B(z, t)|^2 \right) B(z, t) = \varepsilon U(z) B(z, t). \quad (5.42)$$

This equation corresponds to the problem in which the nonlinearity is due to the self-action of the field B or its interaction with another inertia-less field, for example, in a plasma neglecting the inertia of ions. In this case it can be shown that the function $f(k)$, entering into Eq. (5.19), has the form

$$f(k) = -\frac{2q}{\hbar} \int |B_0(z, t)|^2 U(z) \text{th} [q(z - \xi)] dz,$$

and the equation of motion of the maximum of the envelope reduces to the equation

$$m_{\text{ex}} \frac{d^2 \xi}{dt^2} = F(\xi), \quad (5.43)$$

where $F(\xi)$ is determined by expression (5.41), while the mass m_{ex} coincides with the mass directly entering into Eq. (5.42).

d) Motion of solitons in molecular chains in the presence of thermal motion

In all preceding sections of this review it was assumed that the temperature of the molecular chain is absolute zero, so that only the forced displacement of equilibrium positions of molecules was examined. It is interesting to clarify the effect of thermal motion of molecules on the properties of solitons. In what follows we describe the results obtained in Ref. 69.

We shall assume that the chain contains a large number N of molecules; therefore, end effects can be neglected.

Phonons with all N possible values of the wave number q , satisfying the inequality

$$-\frac{\pi}{a} < q \leq \frac{\pi}{a}, \quad (5.44)$$

participate in the thermal motion. For this reason, the displacements u_n the equilibrium position of molecules entering into the operators (2.3) and (2.4) must be expressed in terms of the creation b_q^+ and annihilation b_q operators for phonons with wave numbers q ,

$$u_n = \sum_q \sqrt{\frac{\hbar}{2MN\Omega_q}} (b_q + b_{-q}^+) \exp(iqna), \quad (5.45)$$

where the phonon frequency is

$$\Omega_q \approx 2\sqrt{\chi/M} \sin\left(\frac{1}{2}|q|a\right) \approx |q|V_0, \quad (5.45a)$$

V_0 is the velocity of longitudinal sound in the chain.

In this case the energy operator of the acoustical phonons is determined by the expression

$$H_{ph} = \sum_q \hbar\Omega_q b_q^+ b_q, \quad (5.46)$$

while the operator describing the interaction of displacements with intramolecular excitations (2.4) assumes the form

$$H_{int} = \frac{1}{\sqrt{N}} \sum_{n,q} F(q) B_n^+ B_n \exp(ikna) (b_q + b_{-q}^+), \quad (5.47)$$

$$F(q) = i\sigma \sqrt{\frac{\hbar|q|}{2MV_0}} \frac{q}{|q|}, \quad \sigma = 2\chi a. \quad (5.48)$$

We shall define the collective states of the chain by the functions

$$|\psi_v(t)\rangle = \sum_n \varphi_n(t) B_n^+ |0\rangle U_n(t) |v\rangle, \quad (5.49)$$

where

$$|v\rangle = | \{v_q\} \rangle = \prod_q |v_q\rangle, \quad |v_q\rangle = |v_q\rangle^{1/2} (b_q^+)^{v_q} |0\rangle \quad (5.50)$$

is the phonon function;

$$U_n(t) = \exp \sum_q [\tilde{\beta}_{qn}(t) b_q - \tilde{\beta}_{qn}^*(t) b_q^+] \quad (5.51)$$

is the unitary operator of displacements of equilibrium positions of peptide groups, in which the unknown functions are chosen in the form of modulated plane waves

$$\tilde{\beta}_{qn}(t) = \beta_{qn}(t) \exp(iqna). \quad (5.52)$$

The squares of the moduli of the unknown wave functions $\varphi_n(t)$ characterize the probability distribution of the intramolecular excitation. They satisfy the normalization conditions

$$\sum_n |\varphi_n(t)|^2 = 1. \quad (5.53)$$

We shall calculate the unknown functions $\varphi_n(t)$ and $\beta_{qn}(t)$, characterizing the excited state of the chain, which is in thermal equilibrium with a thermostat having a temperature T . For this we form the function

$$\mathcal{H} = \sum_{\{v_q\}} \rho_{vv} H_{vv}, \quad (5.54)$$

where

$$\rho_{vv} = \frac{\langle v | \exp(-H_{ph}/\Theta) | v \rangle}{\sum_{\{v_q\}} \langle \{v_q\} | \exp(-H_{ph}/\Theta) | \{v_q\} \rangle} \quad (5.54a)$$

are the diagonal elements of the density matrix of phonon states, $\Theta = kT$;

$$H_{vv} = \sum_n \left[\left(\mathcal{E}_0 + \frac{\hbar^2}{m_{ex} a^2} \right) \varphi_n^* \varphi_n - \frac{\hbar^2 e^{-W_n}}{2m_{ex} a^2} \times \varphi_n^* (\varphi_{n+1} + \varphi_{n-1}) - \frac{1}{\sqrt{N}} \sum_q F(q) |\varphi_n|^2 (\beta_{qn}^* + \beta_{q, n}) \right] + \sum_{n,q} \hbar\Omega_q (|\beta_{qn}|^2 + \nu_q); \quad (5.54b)$$

here, \mathcal{E}_0 is the energy of the bottom of the energy band of free excitons and m_{ex} is their effective mass.

The statistical averaging (5.54) of the operator H_{vv} reduces to replacing ν by the average value

$$\bar{\nu}_q = \left[\exp\left(\frac{\hbar\Omega_q}{\Theta}\right) - 1 \right]^{-1}$$

and replacing the function W_n by the function

$$\bar{W}_n = \frac{1}{2} a^2 \sum_q q^2 (2\bar{\nu}_q + 1) |\beta_{qn}|^2. \quad (5.55)$$

Now, using the function (5.54), it is possible to obtain the equations of motion

$$i\hbar \frac{\partial \varphi_n}{\partial t} = \left(\mathcal{E}_0 + \frac{\hbar^2}{m_{ex} a^2} \right) \varphi_n - \frac{\hbar^2 e^{-\bar{W}_n}}{2m_{ex} a^2} (\varphi_{n+1} + \varphi_{n-1}) - \frac{1}{\sqrt{N}} \sum_q F(q) \varphi_n |\beta_{qn}^*(t) + \beta_{-q, n}(t)|, \quad (5.56)$$

$$\hbar \sqrt{N} \left(i \frac{\partial}{\partial t} - \Omega_q - \frac{\hbar q^2 e^{-\bar{W}_n}}{4m_{ex}} |\varphi_n|^2 \right) \beta_{qn} = F(q) |\varphi_n|^2. \quad (5.57)$$

We shall choose periodic boundary conditions. Due to the translational symmetry of the system, the velocity V is conserved together with the energy and the total momentum. In order to include translational symmetry from the very beginning, we shall choose the unknown functions $\beta_{qn}(t)$ in the form

$$\beta_{qn}(t) = \beta_{qn}(0) \exp(-iqVt). \quad (5.58)$$

Then it follows from (5.57) that

$$\beta_{qn}(t) = - \frac{F(q) |\varphi_n|^2}{|q| \hbar V_0 \sqrt{N} (1 + |q| \alpha_n + s)}. \quad (5.59)$$

In writing (5.59) we used the abbreviated notation

$$s = \frac{V}{V_0}, \quad \alpha_n = \frac{\hbar |\varphi_n|^2 \exp(-\bar{W}_n)}{4m_{ex} V_0}. \quad (5.60)$$

In the region where $|\varphi_n|^2 \neq 0$, there is a change in the equilibrium distances between neighboring molecules by an amount determined by the function

$$\delta_n(t) = \langle 0 | U_n^*(t) (u_n - u_{n-1}) U_n(t) | 0 \rangle = - \frac{\sigma \sum_q |\varphi_n(t)|^2}{MN\sqrt{\hbar}} \sum_q \frac{1 + |q| \alpha_n}{(1 + |q| \alpha_n)^2 - s^2}. \quad (5.61)$$

Substituting (5.58) into (5.56), we obtain the nonlinear equation

$$\left(i\hbar \frac{\partial}{\partial t} - \mathcal{E} - \frac{\hbar^2}{m_{ex} a^2} \right) \varphi_n + G_n |\varphi_n|^2 \varphi_n + \frac{\hbar^2 \exp(-\bar{W}_n) (\varphi_{n+1} + \varphi_{n-1})}{2m_{ex} a^2} = 0, \quad (5.62)$$

in which the quantity

$$G_n = \frac{\sigma^2}{M\sqrt{\hbar} N} \sum_q \frac{1 + |q| \alpha_n}{(1 + |q| \alpha_n)^2 - s^2}, \quad (5.63)$$

in its turn, depends in a complicated manner on $\varphi_n(t)$. The sums over q entering into (5.61) and (5.63) can be replaced by integrals according to the equality

$$\frac{1}{N} \sum_q f(|q|) = \frac{1}{q_0} \int_0^{q_0} f(q) dq, \quad q_0 = \frac{\pi}{2a};$$

then

$$\frac{1}{N} \sum_q \frac{1+|q| \alpha_n}{(1+|q| \alpha_n)^2 - s^2} = \frac{1}{q_0 \alpha_n} \ln \left[1 + \frac{q_0 \alpha_n (2+q_0 \alpha_n)}{1-s^2} \right]. \quad (5.63')$$

We shall further assume that the inequality

$$q_0 \alpha_n \ll 1. \quad (5.64)$$

is satisfied. In this case, taking into account (5.63'), expressions (5.61) and (5.63) assume the simpler form

$$\delta_n(t) \approx -\frac{a\sigma |\varphi_n|^2}{MV_0^2(1-s^2)}, \quad (5.65)$$

$$G_n \approx \frac{\sigma^2}{MV_0^2(1-s^2)}. \quad (5.66)$$

In the same approximation expression (5.55) assumes the form

$$\bar{W}_n = |\varphi_n|^4 B f(\Theta), \quad (5.67)$$

where

$$B \equiv \frac{a^2 q_0 \sigma^2}{4M\hbar V_0^2(1-s^2)} \ll 1. \quad (5.67a)$$

$$f(\Theta) \equiv \frac{1}{q_0} \int_0^{q_0} q(1+\bar{v}_q) dq = \begin{cases} \frac{1}{2} + \frac{2\theta}{\hbar\Omega_0}, & \text{if } \hbar\Omega_0 \ll \Theta, \\ \frac{1}{2} + \frac{\pi^2\Theta^2}{6\hbar^2\Omega_0^2}, & \text{if } \hbar\Omega_0 \gg \Theta, \end{cases} \quad (5.67b)$$

with $\Omega_0 = q_0 V_0$.

The energy of phonons (neglecting the zero-point energy), entering into expression (5.54b), assumes the form

$$E_{ph} \equiv \sum_{n,q} \hbar\Omega_q (\bar{v}_q + |\beta_{qn}|^2) = N\hbar\Omega_0 [f(\Theta(-)1/2)] + \frac{\sigma^2}{2MV_0^2(1-s^2)} \sum_n |\varphi_n|^4. \quad (5.68)$$

In this expression the first term determines the energy of deformation of the chain (virtual phonons).

The nonlinear equation (5.62) in the continuum approximation reduces to the equation

$$\left(i\hbar \frac{\partial}{\partial t} - \mathcal{E}_0 - \frac{\hbar^2(1-e^{-\bar{W}})}{a^2 m_{ex}} + \frac{\hbar^2 e^{-\bar{W}}}{2m_{ex}} \frac{\partial^2}{\partial z^2} + G|\varphi(z,t)|^2 \right) \varphi(z,t) = 0 \quad (5.69)$$

with the normalization condition

$$\frac{1}{a} \int |\varphi(z,t)|^2 dz = 1. \quad (5.70)$$

Equation (5.70) is still too complicated, since the function \bar{W} according to (5.67), depends on $|\varphi(z,t)|^4$. Equation (5.69) can be simplified due to the small value of B and satisfaction of the inequality $|\varphi(z,t)|^4 < 1$. We introduce the quantity g equal to the average value of the function $|\varphi(z,t)|^2$ in the region where it differs greatly from zero. We shall then determine this number from the requirement of consistency with the solution obtained below. Then, in Eq. (5.67) we can make the substitution

$$(1-e^{-\bar{W}}) \varphi(z,t) \approx g |\varphi(z,t)|^2 B f(\Theta) \varphi(z,t), \quad (5.71a)$$

and, taking into account the smoothness of the function $\varphi(z,t)$, in the next term of Eq. (5.67) we can use the rougher approximation

$$\exp(-\bar{W}) \frac{\partial^2 \varphi}{\partial z^2} \approx \exp[-g^2 B f(\Theta)] \frac{\partial^2 \varphi}{\partial z^2}. \quad (5.71b)$$

With these simplifications Eq. (5.69) reduces to the

nonlinear Schroedinger equation

$$\left(i\hbar \frac{\partial}{\partial t} + \mathcal{E}_0 + \frac{\hbar^2}{2m_{ex}(\Theta)} \frac{\partial^2}{\partial z^2} + G(\Theta) |\varphi(z,t)|^2 \right) \varphi(z,t) = 0, \quad (5.72)$$

in which the parameters

$$G(\Theta) = G - \frac{g\hbar^2 B f(\Theta)}{m_{ex} a^2}, \quad (5.73)$$

$$m_{ex}(\Theta) = m_{ex} \exp[g^2 B f(\Theta)] \quad (5.74)$$

depend on the temperature.

Solving Eq. (5.72) we find that the probability distribution of the excitation along the chain is determined by the function

$$|\varphi(z,t)|^2 = \frac{aQ(\Theta)}{2\text{ch}^2 [Q(\Theta)(z-z_0-Vt)]}, \quad (5.75)$$

where

$$Q(\Theta) = \frac{am_{ex}(\Theta)G(\Theta)}{2\hbar^2}. \quad (5.76)$$

The average value of (5.75) in the interval $\Delta z = \pi/Q(\Theta)$ equals

$$g \approx \frac{aQ(\Theta)}{\pi} = \frac{a^2 m_{ex}(\Theta)G(\Theta)}{2\pi\hbar^2}.$$

Substituting this value into (5.73) and (5.74), we obtain the explicit values

$$G(\Theta) = \frac{\sigma^2}{MV_0^2 [1 + f(\Theta)(Bm_{ex}(\Theta)/m_{ex})]}, \quad (5.77)$$

$$m_{ex}(\Theta) = m_{ex} \exp \left[\frac{m_{ex} a^2 G(\Theta)}{2\hbar^2} \right]. \quad (5.78)$$

The decrease in the nonlinearity parameter (5.77) in Eq. (5.72) with increasing temperature is related to the effective decrease in the coupling between the excitons and the deformation of the chain. The increase in the exciton mass (5.78) is due to the effective decrease in the resonant interaction between molecules, caused by breakdown of phase coherence due to thermal motion.

Transforming in (5.65) to the continuum approximation and using (5.75), we shall find the function characterizing the change in the equilibrium distances between the neighboring molecules

$$\delta(z,t) = -\frac{a^2 Q(\Theta) \sigma}{2M V_0^2 \text{ch}^2 [Q(\Theta)(z-z_0-Vt)]}. \quad (5.79)$$

Using the same approximations, from (5.68) we find the energy of deformation of the chain

$$E_{def} = \frac{a^2 \sigma^2 m_{ex}(\Theta) G(\Theta)}{6V_0^2 M \hbar^2 (1-s^2)}. \quad (5.80)$$

The energy of a soliton moving in the chain with constant velocity V_0 including the energy of deformation (5.80) is determined by the expression

$$E_{sol}(V) = \mathcal{E} + \frac{1}{2} m_{ex}(\Theta) V^2 - \frac{a^2 \sigma^2 m_{ex}(\Theta)}{24 \hbar^2 M^2 V_0^2 (1-s^2) \Xi(\Theta)}, \quad (5.81)$$

where

$$\Xi(\Theta) = 1 + \frac{m_{ex}(\Theta) f(\Theta) B}{2\pi m_{ex}} \approx 1.$$

An approximate expression follows from (5.81) for low exciton velocities

$$E_{sol}(V) = E_{sol}(0) + \frac{1}{2} m_{sol}(\Theta) V^2, \quad (5.82)$$

where

$$E_{sol}(0) = \mathcal{E}_0 - \frac{a^2 \sigma^2 m_{ex}(\Theta)}{24 M^2 V_0^2 \hbar^2 \Xi(\Theta)} \quad (5.83)$$

is the energy of a soliton at rest, and

$$m_{\text{sol}}(\Theta) = \frac{a^2 \sigma^2 m(\Theta)}{6M^2 V^2 \hbar^2 \Xi(\Theta)}$$

is its effective mass.

6. EXCITATION OF SOLITONS IN A ONE-DIMENSIONAL MOLECULAR SYSTEM⁴⁹

a) Method of the inverse scattering problem

The nonlinear Schroedinger equation (NSE) (2.29), describing stationary solutions moving with constant velocity V , in dimensionless units

$$\tau = \tilde{J}t/\hbar, \quad x = \zeta/a, \quad g = G/2\tilde{J}, \quad \tilde{J} = \hbar^2/2m_{\text{ex}}a^2 \quad (6.1)$$

can be transformed into the standard form

$$\left(i \frac{\partial}{\partial \tau} + \frac{\partial^2}{\partial x^2} + 2g|\Psi|^2 \right) \Psi(x, \tau) = 0, \quad \int |\Psi|^2 dx = 1. \quad (6.2)$$

This equation for arbitrary positive, nonzero value of g has a particular solution of the form

$$\Psi(x, \tau) = \frac{\sqrt{g} \exp[i(2kx - \omega\tau)]}{2 \operatorname{ch} \left[\frac{1}{2} g(x - 4k\tau) \right]} \quad (6.3)$$

for values

$$\omega = 4k^2 - g^2/4, \quad 2k = m_{\text{ex}}aV/\hbar. \quad (6.4)$$

It is interesting to study the change with time brought about by Eq. (6.2) in the excitation described initially by an arbitrary function $\Psi(x, 0)$. This is conveniently done by the method of the inverse scattering problem, which was first developed by Zakharov and Shabat⁹ for the NSE.

They showed that the NSE with the initial state corresponding to a function $\Psi(x, 0)$ decreasing arbitrarily rapidly at infinity can be compared to the linear problem of scattering for the characteristic vectors

$$v = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}, \quad (6.5)$$

satisfying the system of equations

$$\begin{aligned} v_1' - i\zeta v_1 &= q(x)v_2, & q(x) &= i\sqrt{g}\Psi(x, 0), \\ v_2' - i\zeta v_2 &= -q^*(x)v_1 \end{aligned} \quad (6.6)$$

with characteristic values $\zeta = \xi + i\eta$. Here and in what follows the prime in the functions indicates differentiation with respect to x . The system of equations (6.6) can also be written in the form

$$v_1'' - q'v_1/g + v_1(\zeta^2 + |q|^2 - i\zeta q'/q) = 0. \quad (6.7)$$

$$v_2 = (v_1' + i\zeta v_1)/q. \quad (6.7a)$$

According to the method of the inverse scattering problem, as a first step, it is necessary to find the solutions of the system (6.6) which have the following asymptotic behavior for a fixed function $q(x)$ and real $\zeta = \xi$:

$$\lim v(\xi, x) = \begin{cases} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \exp(-i\xi x), & \text{if } x \rightarrow -\infty, \\ a(\xi) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \exp(-i\xi x) + b(\xi) \begin{pmatrix} 0 \\ 1 \end{pmatrix} \exp(i\xi x), & x \rightarrow \infty. \end{cases} \quad (6.8)$$

The complex coefficients $a(\xi)$ and $b(\xi)$ satisfy the inequality

$$|a(\xi)|^2 + |b(\xi)|^2 = 1. \quad (6.9)$$

The quantity, inverse to $a|\xi|$, determines the transmission coefficient of a plane wave incident on the potential $q(x)$ out of the region $x \sim \infty$, while the ratio

$$R(\xi) = b(\xi)/a(\xi) \quad (6.10)$$

determines its coefficient of reflection.

The functions (6.8) can be analytically continued into the upper half-plane ($\eta > 0$) of the complex variable ζ . In the method of the inverse scattering problem (see Refs. 9-13) it is proved that from $a(\xi)$ and $b(\xi)$, found for time $\tau = 0$, it is possible to obtain their values at $\tau \neq 0$ using the equalities

$$a(\zeta, \tau) = a(\zeta), \quad b(\zeta, \tau) = b(\zeta) \exp(4i\zeta^2\tau). \quad (6.11)$$

If the coefficients $a(\xi_j)$ vanish in the upper half-plane of the complex ζ plane, then for these values of ξ_j the asymptotic behavior of the functions $v(\xi_j, x)$ is determined by the expressions

$$v(\xi_j, x) = \begin{cases} \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{\eta_j x} \exp(-i\xi_j x), & x \rightarrow -\infty, \quad j=1, \dots, N, \\ b(\xi_j) \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{-\eta_j x} \exp(i\xi_j x), & x \rightarrow \infty. \end{cases} \quad (6.12)$$

Therefore, the function (6.12) for $\eta_j \neq 0$ decrease asymptotically for $|x| \rightarrow \infty$ and describes bound states corresponding to complex characteristic values ξ_j of Eqs. (6.6).

The set of values

$$\begin{aligned} \xi_j, C_j(\tau) &= b(\xi_j, x) \left[\frac{\partial a(\zeta)}{\partial \zeta} \right]_{\zeta=\xi_j}^{-1}, \quad j=1, 2, \dots, N, \\ R(\xi, \tau) &= b(\xi, \tau)/a(\xi) \end{aligned} \quad (6.13)$$

forms the set of so-called "scattering data." With the help of these data we can determine the auxiliary function

$$F(x, \tau) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\xi R(\xi, \tau) e^{i\xi x} + \sum_{j=1}^N C_j(\tau) \exp(i\xi_j x), \quad (6.14)$$

which enters into the Gel'fand-Levitan-Marchenko integral equation

$$K(x, y) = F^*(x+y, \tau) - \int_{-\infty}^{\infty} ds \int_x^{\infty} dz F^*(s+y, \tau) F(s+z, \tau) K(x, z). \quad (6.15)$$

The function being sought $q(x, \tau)$ and the wave function

$$q(x, \tau) = -2K(x, x) \quad (6.16)$$

satisfying (6.2) with initial value $\Psi(x, 0)$ can be expressed in terms of the solution of Eq. (6.15) with the help of the equality

$$\Psi(x, \tau) = -iq(x, \tau)/\sqrt{g}. \quad (6.17)$$

As an illustration of the use of the inverse scattering problem method, in what follows, following the work of Brizhik and Davydov,⁴⁹ we examine special cases of initial conditions.

b) Initial pulse in the form of a hyperbolic secant

We shall assume that at $\tau = 0$ the initial momentum is given in the form

$$\Psi(x, 0) = \frac{1}{2} \sqrt{g} e^{2ihx} \operatorname{sech}(gx/2), \quad 2k = m_{\text{ex}}aV/\hbar. \quad (6.18)$$

In order to calculate the scattering data it is sufficient

to find the asymptotic solutions of Eq. (6.7) with values

$$q(x, 0) = i\sqrt{g}\Psi(x, 0) = \frac{ig}{2} e^{2ikx} \operatorname{sech}(gx/2). \quad (6.19)$$

If $|x| \rightarrow \infty$, then Eq. (6.7) goes over into the equation

$$v_1'' - (2ik \pm g/2)v_1' + \zeta(\zeta - k \mp ig/2)v_1 = 0. \quad (6.20)$$

The upper sign in (6.20) corresponds to $x \rightarrow -\infty$ and the lower sign corresponds to $x \rightarrow \infty$. This equation has the solution

$$v_1 \rightarrow \begin{cases} \exp\{[i(k+m_1) + g/4]x\}, & x \rightarrow -\infty, \\ \exp\{[i(k-m_2) - g/4]x\}, & x \rightarrow \infty, \end{cases} \quad (6.21)$$

where

$$m_1 = \zeta + k - ig/4, \quad m_2 = \zeta + k + ig/4. \quad (6.22)$$

For $g \neq 0$ the functions (6.21) coincide with the asymptotic functions (6.8) with the values

$$\zeta_1 = \xi_1 + i\eta_1, \quad \xi_1 = -k, \quad \eta_1 = g/4. \quad (6.23)$$

From (6.8) it follows that for $x \rightarrow \infty$, $v_2(\xi) = b(\xi)e^{i\tau\xi}$. On the other hand, for values (6.21) it follows from Eq. (6.7a) that the function $v_2(\infty) = 0$. Thus, for the potential (6.19), the factor $b(\xi)$ and the coefficient of reflection $R(\xi)$ are equal to zero. Such potentials are called nonreflective potentials and they cannot be observed by scattering of plane waves arriving from infinity.

Thus, in our problem the spectral data (6.13) have the values

$$R(\xi, \tau) = 0, \quad \zeta_1 = -k + ig/4, \quad (6.24)$$

$$C_1(\tau) = C_0 \exp(4i\zeta_1^* \tau), \quad C_0 = ig/2.$$

For this reason, the function (6.14) has the simple form

$$F(x, \tau) = C_1(\tau) \exp(i\zeta_1 x). \quad (6.25)$$

Substituting this expression into Eq. (6.15) and assuming that

$$K(x, y) = f(x) \exp(-ik_1^* y),$$

we find

$$f(x) = C_1^*(\tau) e^{-ik_1^* x} \left[1 + \frac{4|C_1(\tau)|^2}{g^2} \exp(-gx) \right]^{-1}.$$

Thus the square of the modulus of the wave function, in accordance with the exact solution (6.3) up to time τ , including (6.16) and (6.17), will be determined by the expression

$$|\Psi(x, \tau)|^2 = \frac{1}{g} |q(x, \tau)|^2 = \frac{g/4}{\operatorname{ch}^2[g(x-x_0-4k\tau)/2]}, \quad (6.26)$$

where

$$x_0 = \frac{2}{g} \ln(2|C_0|/g) = 0.$$

Thus the initial pulse (6.18) propagates with time with velocity V in the form of a single soliton with arbitrary nonzero value of g .

c) Initial pulse in the form of a rectangular step

Let us assume that at time $\tau = 0$ the pulse is given in the form

$$\Psi_{(x,0)} = \begin{cases} \frac{1}{\sqrt{l}} \exp(2ikx), & \text{if } 0 \leq x \leq l, \\ 0, & \text{if } x < 0 \text{ and } x > l. \end{cases} \quad (6.27)$$

In this case the solution of the system of equations (6.6) can be sought in the form

$$v = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \exp(-i\zeta x) \text{ for } x < 0, \\ v = a(\zeta) \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-i\zeta x} + b(\zeta) \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{i\zeta x} \text{ for } x > l,$$

while in the region $0 \leq x \leq l$

$$v_1 = \{A_1 \sin mx + A_2 \cos mx\} e^{i\tau x}, \\ v_2 = \frac{1}{Q_0} \{[(\zeta + k)A_1 + imA_2] \sin mx + [(\zeta - k)A_2 - imA_1] \sin mx\} e^{-i\tau x},$$

where

$$Q_0 = \sqrt{g^2 l}, \quad m^2 = Q_0^2 - (\zeta - k)^2. \quad (6.28)$$

From the condition of continuity of the solutions it follows that

$$A_1(\zeta) = -i(k + \zeta)/m, \quad A_2 = 1, \quad (6.29)$$

$$a(\zeta) = m^{-1} S(\zeta, k) e^{i(k+\zeta)l}, \quad b(\zeta) = im^{-1} Q_0 e^{-i(k+\zeta)l},$$

where

$$S(\zeta, k) = m \cos ml - i(k + \zeta) \sin ml. \quad (6.30)$$

Using (6.29) we find the coefficient of reflection at time $\tau = 0$

$$R(\xi) = iQ_0 S^{-1}(\xi, k) \exp[-2i(k + \xi)l].$$

At time τ , according to (6.11), it assumes the value

$$R(\xi, \tau) = R(\xi) \exp(4i\xi^* \tau). \quad (6.31)$$

The parameters of the bound states are determined from the condition

$$S(\zeta, k) = 0.$$

This equation has the solution

$$\zeta_0 = -k + i\eta_0, \quad (6.32)$$

in which η_0 is determined by the transcendental equation

$$l\eta_0 = -\sqrt{gl - l^2\eta_0^2} \operatorname{ctg} \sqrt{gl - \eta_0^2} l. \quad (6.33)$$

For values \sqrt{gl} less than $\pi/2$, this equation does not have nonzero solutions. In this case the starting pulse (6.27) does not give rise to solitons, but, oscillating, spreads out along the chain with probability density decreasing with time according to the law $1/\sqrt{\tau}$.

If the inequality

$$\pi/2 < \sqrt{gl} \leq 3\pi/2, \quad (6.34)$$

is satisfied, then Eq. (6.33) is satisfied by a single positive value $\eta_0 \leq Q_0$. When the inequality $3\pi/2 < \sqrt{gl} \leq \sigma\pi/2$ is satisfied, Eq. (6.33) has two roots. Figure 12 indicates the dependence of the ratio η_0/Q_0 on the quantity \sqrt{gl} .

For $\eta_0 \neq 0$, according to (6.11), (6.13), and (6.28)

$$C_0(\tau) = \alpha \exp(4i\zeta_0^* \tau), \quad (6.35)$$

$$\alpha = \frac{m_1^2 \exp(2l\eta_0)}{Q_0(m_1 l \cos m_1 l - \sin m_1 l)}, \quad m_1^2 = Q_0^2 - \eta_0^2. \quad (6.36)$$

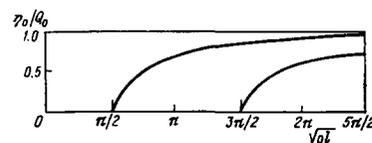


FIG. 12. Dependence of the ratio η_0/Q_0 on the quantity \sqrt{gl} .

Thus the function (6.14) assumes the value

$$F(x, \tau) = C_0(\tau) e^{i\epsilon_0 \tau} - \frac{1}{2\pi} \int_{-\infty}^{\infty} R(\xi, \tau) e^{i\xi x} dx, \quad (6.37)$$

where $C_0(\tau)$ and $R(\xi, \tau)$ are determined by expressions (6.35) and (6.31), respectively.

The first term in (6.37) determines the soliton solutions, while the second term determines the "tail" accompanying the soliton.

For long times τ the value of the integral can be approximated by the expression

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} R(\xi, \tau) e^{i\xi x} d\xi \approx \frac{i V^{-1} g \exp \left\{ -i \left[\frac{(x-2l)^2}{46\tau} + 2 \left(kl - \frac{\pi}{8} \right) \right] \right\}}{4 \sqrt{\tau} S(0, k)}. \quad (6.38)$$

Thus, for long times, the amplitude of the "tail" decreases with time according to the law $1/\sqrt{\tau}$.

Retaining for long times in (6.37) only the first term and solving Eq. (6.15), we determine the value of $K(x, y)$ and the wave function

$$\Psi_s(x, \tau) = \frac{2i\eta_0 \exp \{ 2i [kx - 2(k^2 - \eta_0^2)\tau] \}}{\sqrt{g} \operatorname{ch} z}, \quad (6.39)$$

where

$$z = 2\eta_0(x - x_0 - 4k\tau), \quad x_0 = \frac{1}{2\eta_0} \ln \frac{|\alpha|}{2\eta_0}. \quad (6.40)$$

Thus, with the initial excitation in the form of the pulse (6.27), soliton solutions appear with a nonlinearity parameter g exceeding the critical value

$$g_{cr} = \pi^2/4l. \quad (6.41)$$

The amplitude of the soliton increases and its width decreases with increasing g . For $g = \pi^2/4l$, the soliton makes the main contribution to normalization of the wave function, since

$$\int |\Psi_s(x, \tau)|^2 dx \approx 0.85.$$

The role of the "tail" in this case is negligibly small.

In the inertia-free approximation, i.e., when the nonlinearity parameter g does not depend on the soliton velocity V , the excitation described by Eq. (6.2) corresponds in units of $\hbar^2/2ma^2$ to the energy

$$E_0(v) = \int \left(\left| \frac{\partial \Psi}{\partial x} \right|^2 - g_0 |\Psi|^4 \right) dx.$$

If the nonlinearity parameter $g = g_0/(1 - s^2)$ depends on velocity, then the inertia of the displacements of peptide groups appears. In this case, the energy integral, including deformation of the chain is determined by the expression

$$E(v) = \int \left(\left| \frac{\partial \Psi}{\partial x} \right|^2 - g(1 - 2s^2) |\Psi|^4 \right) dx. \quad (6.42)$$

In the initial state this energy is determined by two terms:

$$E(v) = E(0) + E_k, \quad (6.43)$$

where

$$E(0) = -g_0/l, \quad (6.44)$$

$$E_k = 4k^2(1 + \beta g/l), \quad \beta \equiv \hbar^2/m^2 a^2 V^2.$$

For $k=0$ the energy (6.43) is less than the bottom of

the exciton band by an amount $E(0)$.

For $\tau > 0$ the part of the energy (6.43) is transported by the "tail," and the remaining part

$$E_s(v) = E_s(0) + E_{s,k}, \quad (6.45)$$

where

$$E_s(0) = -16\eta_0^3/3g_0, \quad E_{s,k} = 16\eta_0 k^2(1 + 20\eta_0^2\beta/3)g_0^{-1} \quad (6.46)$$

is carried by the soliton. The excitation loses part of its initial energy in establishing the asymptotic single-soliton form (6.39).

The calculations performed in this section show that the presence (or absence) of a threshold for excitation of solitons and the magnitude of the threshold depend on the nature of the spatial distribution of the initial pulse.

¹N. J. Zabusky and M. D. Kruskal, Phys. Rev. Lett. 15, 240 (1965).

²J. Scott-Russell, Proc. Roy. Soc. Edinburgh (1844), p. 319.

³D. J. Korteweg and G. de Vries, Phil. Mag. 39, 422 (1895).

⁴R. Z. Sagdeev, Voprosy teorii plazmy i problema upravlyayemykh termoya derykh reaktsii (Problems in plasma theory and the problem of controlled thermonuclear reactions). Publ. by Acad. Sci. USSR vol. 4, p. 384, 1958.

⁵R. Z. Sagdeev, In the book Voprosy teorii plazmy (Problems in plasma theory), Atomizdat, M., No. 4, p. 20, 1964.

⁶B. B. Kadomtsev and V. I. Karpman, Usp. Fiz. Nauk 109, 193 (1973) [sic].

⁷C. S. Gardner, J. M. Green, M. D. Kruskal, and R. M. Miura, Phys. Rev. 19, 1095 (1967).

⁸V. E. Zakharov and L. D. Faddeev, Funkts. analiz i ego prilozhenie (Functional analysis and its applications) 5, No. 4, 18 (1971).

⁹V. E. Zakharov and A. B. Shabat, ibid. 8, No. 3, 43 (1974).

¹⁰F. Cologero and A. Degasperis, Nuovo Cimento B 32, 201 (1976); ibid. B 39, 1 (1977).

¹¹B. A. Dubrovin, V. B. Matveev, and S. P. Novikov, Usp. Matem. Nauk 31(1), 55 (1976).

¹²V. A. Marchenko, Operatory Shturma-Liuvillya i ikh prilozheniya (Sturm-Liouville Operators and Their Application), Naukova Dumka, Kiev (1977).

¹³V. I. Zakharov, S. V. Manakov, S. P. Novikov, and L. P. Pitaevskii, Teoriya solitonov, Metod obratnoy zadachi (Theory of solitons. Method of the Inverse Problem), Nauka, Moscow (1980), p. 320.

¹⁴A. C. Scott, F. Y. Chu, and D. W. McLaughlin, Proc. IEEE 61, 1443 (1973).

¹⁵E. I. Rashba, Opt. Spektrosk. 2, 75 (1957).

¹⁶E. I. Rashba, ibid., p. 88.

¹⁷Y. Toyazawa, Progr. Theor. Phys. 26, 29 (1961); Techn. Report ASSP (Japan) Ser. A, No. 648 (1974).

¹⁸V. K. Fedyanin and L. V. Yakushevich, Teor. Mat. Fiz. 30, 133 (1977).

¹⁹A. S. Davydov, Fiz. Tverd. Tela 9, 2230 (1967) [Sov. Phys. Solid State 9, 1749 (1968)].

²⁰A. S. Davydov, Phys. Stat. Sol. Ser. B 59, 465 (1973).

²¹N. N. Bogolyubov, Ukr. Mat. Zh. 2, 3 (1950).

²²S. V. Tyablikov, Zh. Eksp. Teor. Fiz. 21, 377 (1951).

²³G. E. Volovik and V. M. Edel'shtein Zh. Eksp. Teor. Fiz. 65, 1946 (1973) [Sov. Phys. JETP 38, 972 (1974)].

²⁴V. M. Mel'nikov, Zh. Eksp. Teor. Fiz. 72, 2345 (1977) [Sov. Phys. JETP 45, 1233 (1977)].

²⁵A. S. Davydov and N. I. Kislukha, Zh. Eksp. Teor. Fiz. 71, 1090 (1976) [Sov. Phys. JETP 44, 571 (1976)].

²⁶A. S. Davydov and A. A. Eremko, Ukr. Fiz. Zh. 22, 881 (1977).

²⁷A. S. Davydov, Phys. Scripta 20, 387 (1979).

- ²⁸A. A. Eremko and A. I. Sergienko, Preprint ITF AN USSR 80-90R, Kiev (1980).
- ²⁹J. R. Klauder and E. C. G. Sudarshan, *Fundamentals of Quantum Optics*, Benjamin, New York, 1968 [Russ. Transl. Mir, Moscow (1970), p. 428].
- ³⁰*Coherent States in Quantum Theory* [Russian translation], Mir, M. (1972), p. 232.
- ³¹D. E. Green, *Science* **181**, 583 (1973).
- ³²*Ann. N. Y. Acad. Sci.* **227**, General discussion, pp. 108-115 (1974).
- ³³A. S. Davydov, *J. Theor. Biol.* **66**, 379 (1977).
- ³⁴A. S. Davydov in: *Metodologicheskie i teoreticheskie problemy v biofizike* (Methodological and Theoretical Problems in Biophysics), Nauka, Moscow (1979), p. 243.
- ³⁵A. S. Davydov, *Intern. J. Quant. Chem.* **26**, 5 (1979).
- ³⁶M. V. Vol'kenshtein, *Molekulyarnaya biofizika* (Molecular Biophysics), Nauka, M. (1975), p. 616.
- ³⁷A. S. Davydov, *Biologiya i kvantovaya mekhanika* (Biology and Quantum Mechanics), Naukova Dumka, Kiev (1979).
- ³⁸L. Pauling, R. B. Corey, and R. Hayward, *Sci. American* **191**, 51 (1954).
- ³⁹N. A. Nevskaya and Yu. N. Chirgadze, *Biopolymers* **15**, 637 (1976).
- ⁴⁰A. A. Eremko and A. I. Sergeenko, Preprint ITF AN USSR N80-IP, Kiev (1980).
- ⁴¹A. S. Davydov, A. A. Eremko, and A. I. Sergeenko, *Ukr. Fiz. Zh.* **23**, 983 (1978).
- ⁴²A. S. Davydov, *Ukr. Fiz. Zh.* **19**, 44 (1974).
- ⁴³A. C. Scott, *Phys. Lett. A* **86**, 60 (1981).
- ⁴⁴A. C. Scott, *Dynamics of Davydov Solitons*; Los Alamos Scientific Lab. LA-UR 81-3268; *Phys. Rev. B* **26** (5), 2474 (1982).
- ⁴⁵A. C. Scott, "The vibrational structure of Davydov solitons," *Los Alamos Sci. Lab. LA-UR 81-3711*; *Phys. Scripta* (1982) (to appear).
- ⁴⁶S. J. Webb, *Phys. Rept.* **60**, 201 (1980).
- ⁴⁷J. M. Hyman, D. W. McLaughlin, and A. C. Scott, "On Davydov's alpha-helix solitons," *Los Alamos Sci. Lab.* (1979); *Physica D* **3**, 23 (1979).
- ⁴⁸J. C. Eilbeck, "Davydov solitons: A 16 mm mute film available from Swift Film Productions, 1 Wool Road, Wimbledon, London.
- ⁴⁹L. S. Brizhik and A. S. Davydov, "Excitation of solitons in one-dimensional molecular systems," Preprint ITF AN USSR 82-11, p. 1982.
- ⁵⁰A. S. Davydov, *Phys. Stat. Sol. Ser B* **102**, 275 (1980).
- ⁵¹E. Del Giudice, S. Doglia, and M. Milani, *Phys. Scripta* **23**, 307 (1981).
- ⁵²J. Hanson and H. E. Huxley, *Nature* **173**, 973 (1954).
- ⁵³A. F. Huxley and R. Nidergerke, *ibid.*, p. 971.
- ⁵⁴J. M. Murray and A. Weber, *Sci. American* **230**, 59 (1974).
- ⁵⁵A. S. Davydov, *J. Theor. Biol.* **38**, 559 (1973).
- ⁵⁶A. S. Davydov, *Biofizika* **19**, 670 (1974).
- ⁵⁷A. S. Davydov, *Ukr. Fiz. Zh.* **20**, 179 (1975).
- ⁵⁸A. S. Davydov in: *Biofizika i biokhimiya myshechnogo sokrashcheniya* (Biophysics and Biochemistry of Muscle Contraction), Nauka, Moscow (1976), p. 254.
- ⁵⁹A. S. Davydov, *Studia Biophys.* **47**, 221 (1974).
- ⁶⁰K. M. Ragulskis, R. J. Bansevichyus, R. B. Didzgalvis, and V. I. Ragulskiene, *Theory of Machines and Mechanisms*, Nauka, M. (1976).
- ⁶¹K. M. Ragulskis, *The Shock and Vibration Information Center, Naval Research Lab., Washington, Vol. 12, No. 2*, p. 27 (1980).
- ⁶²V. I. Karpman and E. M. Maslov, *Zh. Eksp. Teor. Fiz.* **73**, 537 (1977) [*Sov. Phys. JETP* **46**, 281 (1977)].
- ⁶³M. B. Fogel, S. E. Trullinger, A. R. Bishop, and J. A. Krumhansl, *Phys. Rev. Lett.* **36**, 1411 (1976).
- ⁶⁴J. P. Keener and D. W. McLaughlin, *Phys. Rev. A* **16**, 777 (1977).
- ⁶⁵A. S. Davydov and A. A. Eremko, *Teor. Mat. Fiz.* **43**, 367 (1980).
- ⁶⁶N. N. Bogolyubov and Yu. A. Mitropol'skiĭ, *Asimptoticheskie metody v teorii nelineĭnykh kolebaniĭ* (Asymptotic Methods in the Theory of Nonlinear Oscillations), Nauka, M. (1974), p. 296.
- ⁶⁷Y. H. Ichikawa, *Phys. Scripta* **20**, 296 (1979).
- ⁶⁸V. I. Karpman, *Phys. Scripta* **20**, 462 (1979).
- ⁶⁹A. S. Davydov, *Zh. Eksp. Teor. Fiz.* **78**, 789 (1980) [*Sov. Phys. JETP* **51**, 397 (1980)].

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