

## Vanishing thermal damping of Davydov's solitons

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We consider Davydov's biophysical model in the context of nonequilibrium statistical thermodynamics. We show that excitations of the Davydov-soliton type that can propagate in the system, which are strongly damped in near-equilibrium conditions, become near dissipation-free in the Fröhlich-Bose-Einstein-like condensate and that this occurs after a certain threshold of pumped metabolic energy is reached. This implies the propagation of excitations at long distances in such biosystems.

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In the 1970s Davydov showed that, due to particular nonlinear interactions in biophysical systems, e.g., the  $\alpha$ -helix protein, a novel mechanism for the localization and transport of vibrational energy is expected to arise in the form of a solitary wave [1]. The subject was taken up by a number of contributors, and a long list of results published up to the first half of 1992 are discussed in the excellent review by Scott [2], who has also provided extensive research on the subject [3]. As pointed out in that review, one important open question concerning Davydov's soliton is that of its stability at normal physiological conditions, or in other words, the possibility of the excitation to transport energy (and so information) at long distances in the living organism, in spite of the relaxation mechanisms that are expected to damp it out at very short (micrometer) distances. We address this question here. First we note that there is equivalence between Davydov's model and the one used by Fröhlich [4,5], as shown by Tuszynski *et al.* [6]. In Fröhlich's work it is shown that, as a consequence of the nonlinear interactions to which we have already referred, under appropriate conditions a phenomenon akin to a Bose-Einstein condensation may occur in the system, provided there is a supply of metabolic energy exceeding a critical value. We proceed to analyze both phenomena in the Fröhlich-Davydov model under arbitrary nonequilibrium conditions. For that purpose we resort to an informational statistical thermodynamics based on the nonequilibrium statistical operator method (NSOM) [7]. The NSOM, which provides microscopic foundations for phenomenological irreversible thermodynamics [8], also allows for the construction of a nonlinear generalized quantum transport theory [9], which describes the evolution of the system at the macroscopic level in arbitrary nonequilibrium situations, a formalism to be used in our analysis below.

The model consists of a biosystem that can sustain longitudinal polar vibrations in interaction with a thermal bath of acousticlike vibrations. This interaction involves all possible three-particle collisions. An external source of metabolic energy is coupled to the polar vibrations, and the bath is assumed to be constantly kept at a fixed temperature  $T_0$  by an efficient homeostatic mechanism. Next, as the first step in the NSOM, it is necessary to

choose the basic variables deemed appropriate for the description of the macroscopic state of the system. We take the energy of the thermal bath,

$$E_b(t) = \text{Tr} \left[ \sum_{\mathbf{q}} \hbar \Omega_{\mathbf{q}} (b_{\mathbf{q}}^\dagger b_{\mathbf{q}} + \frac{1}{2}) \bar{\rho}(t, 0) \right], \quad (1a)$$

the population of the polar vibrations,

$$\nu_{\mathbf{q}}(t) = \text{Tr} \{ a_{\mathbf{q}}^\dagger a_{\mathbf{q}} \bar{\rho}(t, 0) \}, \quad (1b)$$

and the amplitudes of oscillation,

$$\begin{aligned} \langle a_{\mathbf{q}} | t \rangle &= \text{Tr} \{ a_{\mathbf{q}} \bar{\rho}(t, 0) \}, \\ \langle a_{\mathbf{q}} | t \rangle^* &= \text{Tr} \{ a_{\mathbf{q}}^\dagger \bar{\rho}(t, 0) \}, \end{aligned} \quad (1c)$$

where  $a$  and  $b$  ( $a^\dagger$  and  $b^\dagger$ ) are annihilation (creation) operators in the corresponding vibrational states of wave vector  $\mathbf{q}$ ,  $\Omega_{\mathbf{q}}$  is the frequency-dispersion relation of the modes of the bath, and, finally,

$$\begin{aligned} \bar{\rho}(t, 0) &= \exp \left[ -\phi(t) - \beta_0 H_b - \sum_{\mathbf{q}} F_{\mathbf{q}}(t) a_{\mathbf{q}}^\dagger a_{\mathbf{q}} \right. \\ &\quad \left. - \sum_{\mathbf{q}} [f_{\mathbf{q}}(t) a_{\mathbf{q}} + f_{\mathbf{q}}^*(t) a_{\mathbf{q}}^\dagger] \right] \end{aligned} \quad (2)$$

is the auxiliary (or coarse-grained) nonequilibrium operator in the NSOM, the whole (fine-grained) NSO being a functional of it [7]. In Eq. (2),  $\beta_0 = 1/kT_0$ ,  $\phi(t)$  ensures the normalization of  $\bar{\rho}$ , and  $F$  and  $f$  are the other Lagrange multipliers that the variational approach to the NSOM introduces [7];  $H_b$  is the Hamiltonian of the bath. Further, we note that, introducing the canonical transformation (reminiscent of Glauber's transformation to coherent states in laser theory [10]),

$$\bar{a}_{\mathbf{q}} = a_{\mathbf{q}} - \langle a_{\mathbf{q}} | t \rangle, \quad (3)$$

one finds that

$$\langle a_{\mathbf{q}} | t \rangle = -f_{\mathbf{q}}^*(t) / F_{\mathbf{q}}(t), \quad (4a)$$

$$\nu_{\mathbf{q}}(t) = \bar{\nu}_{\mathbf{q}}(t) + |\langle a_{\mathbf{q}} | t \rangle|^2, \quad (4b)$$

where

$$\bar{v}_q(t) = [e^{F_q(t)} - 1]^{-1} \quad (4c)$$

is the polar-mode population in the absence of the excitation of amplitude  $\langle a_q | t \rangle$ .

Applying the NSOM transport theory in the so-called second-order approximation in relation theory (SOART) [9] and using Zubarev's approach [11] to the NSOM, we find the equations of evolution

$$\tau_q^{-1} = \frac{2\pi}{\hbar^2} \frac{1}{v_q^0} \sum_{q'} |V_{qq'}^{(1)}|^2 [\eta_{q'} \eta_{q+q'} e^{\beta \hbar \Omega_{q'}} \delta(\Omega_{q+q'} - \Omega_{q'} - \omega_q) + \eta_{q'} \eta_{q'-q} \delta(\Omega_{q-q'} + \Omega_{q'} - \omega_q)] , \quad (6a)$$

$$\begin{aligned} \mathcal{F}_q(t) = & \frac{2\pi}{\hbar^2} \sum_{q'} |V_{qq'}^{(2)}|^2 \eta_{q+q'} \{ [1 + \bar{v}_{q'}(t)] [1 + \bar{v}_q(t)] - \bar{v}_{q'}(t) \bar{v}_q(t) e^{\beta \hbar \Delta_{qq'}^{(+)}} \} \delta(\Omega_{q+q'} - \omega_{q'} - \omega_q) \\ & + \frac{2\pi}{\hbar^2} \sum_{q'} |V_{qq'}^{(2)}|^2 \eta_{q-q'} \{ \bar{v}_{q'}(t) [1 + \bar{v}_q(t)] - [1 + \bar{v}_{q'}(t)] \bar{v}_q(t) e^{\beta \hbar \Delta_{qq'}^{(-)}} \} \delta(\Omega_{q-q'} + \omega_{q'} - \omega_q) \\ & + \frac{2\pi}{\hbar^2} \sum_{q'} |V_{qq'}^{(2)}|^2 \eta_{q'-q} \{ \bar{v}_{q'}(t) [1 + \bar{v}_q(t)] e^{-\beta \hbar \Delta_{qq'}^{(-)}} - [1 + \bar{v}_{q'}(t)] \bar{v}_q(t) \} \delta(\Omega_{q+q'} - \omega_{q'} + \omega_q) , \end{aligned} \quad (6b)$$

where

$$\Delta_{qq'}^{(+)} = \omega_q + \omega_{q'} , \quad (6c)$$

$$\Delta_{qq'}^{(-)} = \omega_q - \omega_{q'} , \quad (6d)$$

$V^{(1)}$  and  $V^{(2)}$  are the matrix elements of the interaction involving, respectively, collision of one polar phonon with two acoustic phonons and collision of two polar phonons with one acoustic phonon,  $\eta_q$  is the equilibrium Planckian distribution of acoustic phonons at temperature  $T_0$ , and  $\omega_q$  is the polar-mode frequency-dispersion relation.

Equation (5) is then of the type proposed by Fröhlich, where the nonlinear terms in  $\mathcal{F}$  account for the transfer of energy (through mediation of the acoustic phonons) from the high-frequency to the low-frequency modes, leading to Fröhlich-Bose condensation. Let us show this in numerical calculations. Taking into account the mentioned type of energy transfer, we introduced a quite simplified model, that is, we take a mode as representative of all high-frequency modes (index 0 below), and another for the low-frequency modes (index 1 below). We are then left with a coupled set of equations, namely,

$$\begin{aligned} \frac{\partial}{\partial t} \bar{v}_0(t) = & I_0 - \tau_0^{-1} [\bar{v}_0(t) - v_0^0] - g_1 \eta e^{\beta \hbar \Delta} \bar{v}_0(t) \\ & + g_1 \eta \bar{v}_1(t) - g_2 \bar{v}_1(t) \bar{v}_0(t) , \end{aligned} \quad (7a)$$

$$\begin{aligned} \frac{\partial}{\partial t} \bar{v}_1(t) = & I_1 - \tau_1^{-1} [\bar{v}_1(t) - v_1^0] - g_0 \eta \bar{v}_1(t) \\ & + g_0 \eta e^{\beta \hbar \Delta} \bar{v}_0(t) + g_0 \bar{v}_0(t) \bar{v}_1(t) , \end{aligned} \quad (7b)$$

where  $g_0$  and  $g_1$  are coupling constants,  $\Delta = \omega_0 - \omega_1$ , and

$$\eta = [\exp(\beta \hbar \Delta) - 1]^{-1} . \quad (8)$$

After a certain transient has elapsed (estimated to be of the order of picoseconds (12), a steady state is attained, i.e.,  $\partial \bar{v} / \partial t = 0$  in Eqs. (7). For a numerical solution we

$$\frac{\partial}{\partial t} v_q(t) = I_q - \tau_q^{-1} [\bar{v}_q(t) - v_q^0] - \mathcal{F}_q(t) , \quad (5)$$

where  $I_q$  is the pumping intensity rate,  $\tau$  is a relaxation time associated with the decay of a polar vibration in two acoustic vibrations in the bath,  $v^0$  is the equilibrium value, and  $\mathcal{F}$  is a lengthy collision operator associated with the collisions of two polar phonons with one acoustic-like phonon. They are given by

choose  $\tau_0 \approx \tau_1 (= \bar{\tau})$ ,  $g_0 \bar{\tau} = g_1 \bar{\tau} \approx 10^{-5}$ ,  $\omega_0 = 10^{13} \text{ sec}^{-1}$ , and  $\Delta = 2 \times 10^{12} \text{ sec}^{-1}$ .  $\Omega_q = sq$  with  $s = 10^5 \text{ cm/sec}$  and we write  $S = I_0 \bar{\tau} = I_1 \bar{\tau}$  for the pumping intensities. The result is shown in Fig. 1: One may clearly see the onset of

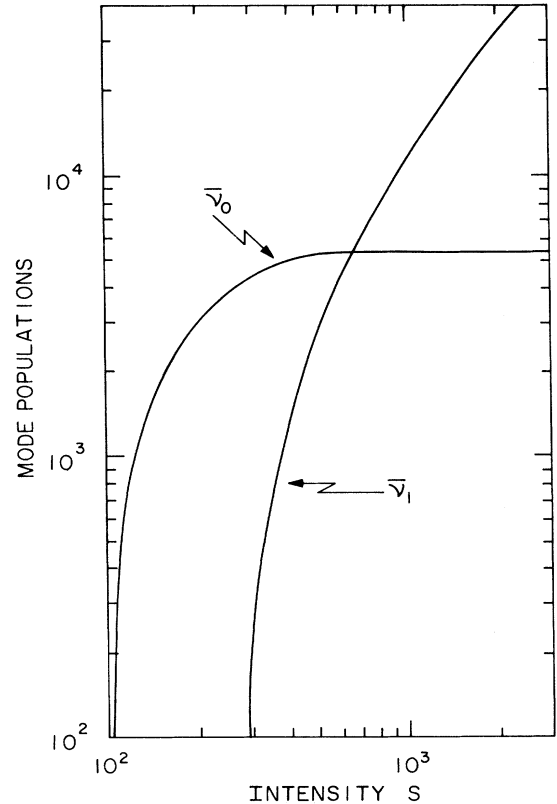


FIG. 1. Population of the representative modes of high frequency,  $\bar{v}_0$ , and that of the representative modes of low frequency,  $\bar{v}_1$ , as a function of the source power.

the *Fröhlich effect*, that is, a large increase of population in the low-frequency modes, which follows at an intensity threshold (roughly given by the value of  $S$  where  $\nu_1$  steeply increases) of 500. Figure 2 shows, for the case of an  $\alpha$ -helix protein, the domain in frequency space in which the Fröhlich condensate occurs [12].

We consider now the dynamic aspects associated with the propagation of signals in Fröhlich condensate, that is, we look for quantities  $\langle a_q | t \rangle$  that, in SOART-NSOM, satisfy the equations of evolution

$$\frac{\partial}{\partial t} \langle a_q | t \rangle = -i\tilde{\omega}_q \langle a_q | t \rangle - \Gamma_q \langle a_q | t \rangle - iW_q \langle a_q | t \rangle^* + \Gamma_q \langle a_q | t \rangle^* + \sum_{q_1 q_2} [R_{q_1 q_2} \langle a_{q_1} | t \rangle \langle a_{q_2} | t \rangle \langle a_{q_1+q_2-q} | t \rangle^* + \text{c.c.}] \quad (9)$$

and the accompanying complex conjugated equation, where  $\tilde{\omega}_q = \omega_q + W_q$ ,

$$2\Gamma_q = \tau_q^{-1} + \frac{2\pi}{\hbar^2} \sum_{q'} |V_{qq'}^{(2)}|^2 \eta_{q+q'} [(e^{\beta\hbar\Delta_{qq'}^{(+)}} - 1) \bar{\nu}_q - 1] \delta(\omega_q + \omega_{q'} - \Omega_{q+q'}) \\ + \frac{2\pi}{\hbar^2} \sum_{q'} |V_{qq'}^{(2)}|^2 \eta_{q-q'} [(1 + \bar{\nu}_{q'}) e^{\beta\hbar\omega_q} - \bar{\nu}_q e^{\beta\hbar\omega_{q'}}] \{ e^{-\beta\hbar\omega_q} \delta(\omega_q - \omega_{q'} - \Omega_{q-q'}) + e^{-\beta\hbar\omega_{q'}} \delta(\omega_q - \omega_{q'} + \Omega_{q-q'}) \}, \quad (10)$$

with  $\tau_q$  of Eq. (6a) [we omit to write down the long expression for  $W$  (it is a term of renormalization of frequency of no relevance in what follows)], and

$$R_{q_1 q_2} = i \frac{2\pi}{\hbar^2} |V_{q_1 q_2}^{(2)}|^2 \{ (\omega_{q_1} + \omega_{q_2} - \Omega_{q_1+q_2} + i\epsilon)^{-1} + (\omega_{q_1} + \omega_{q_2} + \Omega_{q_1+q_2} + i\epsilon)^{-1} \\ + (\omega_{q_1} - \omega_{q_2} + \Omega_{q_1+q_2} + i\epsilon)^{-1} + (\omega_{q_1} - \omega_{q_2} - \Omega_{q_1+q_2} + i\epsilon)^{-1} \}, \quad (11)$$

where  $\epsilon$  is to be taken in the limit  $+0$ .

Equation (9) is of the Davydov-soliton type, but with the presence of the damping term with damping constant  $\Gamma$ . We mention that if we approximate the polarvibration frequency dispersion by  $\omega_q = \omega_0 - \alpha q^2$ , where  $\alpha$  is a constant (a good approximant in real cases), after neglecting the coupling terms with the conjugated equation, once we introduce the average field operator in the continuum (in one dimension)

$$\psi(x, t) = \sum_q \langle a_q | t \rangle e^{iqx}, \quad (12)$$

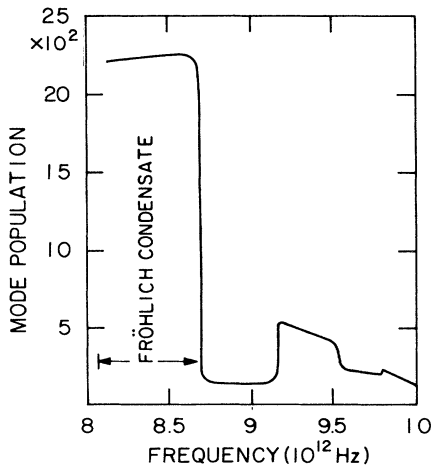


FIG. 2. Modes (in frequency space) in Fröhlich's condensate for a one-dimensional model for the  $\alpha$ -helix protein. After Ref. [12].

we obtain

$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = \left[ \hbar\omega_0 + \hbar\alpha \frac{\partial^2}{\partial x^2} \right] \psi(x, t) \\ - i\hbar \int dx' \Gamma(x - x') \psi(x', t) \\ + \int dx' dx'' R(x', x'') \psi(x', t) \\ \times \psi(x'', t) \psi^*(x, t), \quad (13)$$

where

$$R(x', x'') = \sum_{q_1 q_2} R_{q_1 q_2} e^{iq_1 x' + iq_2 x''}, \quad (14a)$$

$$\Gamma(x - x') = \sum_q \Gamma_q e^{iq(x - x')}. \quad (14b)$$

Equation (13) is a nonlinear Schrödinger-type equation with damping [13]. In a local approximation, Eq. (13) becomes, except for the term in  $\Gamma$ , Davydov's equation for the soliton. Here the damping effect governed by the  $\Gamma$  of Eq. (10) is clear. Inspection of Eq. (10) tells us that the damping constant implies in the near-equilibrium condition a lifetime for the excitation of the order of  $\tau$ , i.e., in the picosecond range. However, the nonlinear contributions are responsible for the fact that with increasing population  $\bar{\nu}$  the lifetime decreases for the high-frequency modes, while it *increases* for the low-frequency modes. Let us again resort to the model of two representative sets of modes as already described. Numerical calculations lead to the results shown in Fig. 3.

Clearly the situation is substantially modified if the excitation propagates in the nonequilibrium background

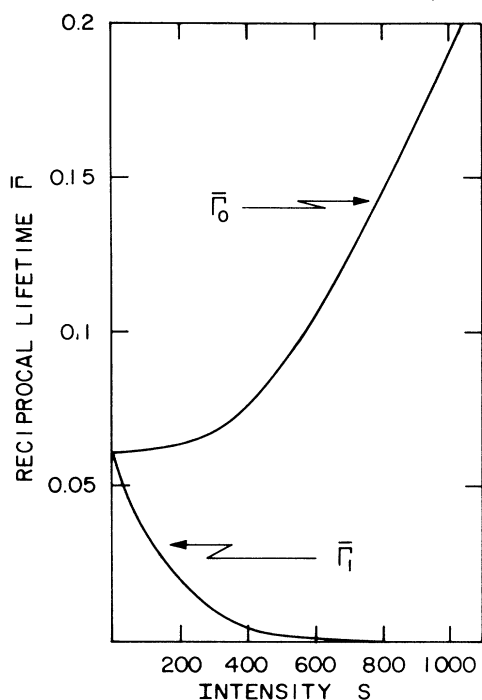


FIG. 3. Reciprocal lifetime ( $\bar{\Gamma} = \Gamma\tau$ ) of the representative high-frequency modes,  $\bar{\Gamma}_0$ , and that of the low-frequency modes,  $\bar{\Gamma}_1$ , as a function of the power source.

provided by Fröhlich's condensate. We reemphasize that this is the result of the fact that the damping constants depend on the actual state of the system, being affected by the nonlinear kinetic effects that are responsible, on the one hand, by Fröhlich effect, and, on the other, by

Davydov's mechanism for exciton propagation. Consequently, while there occurs a very rapid damping of amplitudes corresponding to the high-frequency modes, those at low frequencies become undamped. Hence, in the expression for the average field operator in the continuum, Eq. (12), following a very short time (sub picosecond range) after the exciting pulse initiating the propagation of the signal, only the contributions from the modes in the condensate survive (see Fig. 2). In terms of energy, we comment that if the metabolic energy is provided by hydrolysis of adenosine 5'-triphosphate (ATP) (7.3 kcal/mol), and if there is total absorption of this energy in the process, to sustain the Fröhlich condensate for a signal to propagate during, say,  $10^{-6}$  sec (group velocity is expected to be of the order of  $10^5$  cm/sec; then the travel length is 1 cm) would require roughly  $10^{-11}$  moles of ATP, a seemingly accessible value. (This value greatly decreases if one includes double excitation instead of the single excitation we considered.)

Summarizing, our results show that *propagation of a coherent Davydov-soliton-like excitation, composed of low-lying excited vibrational states, is possible. This propagation can travel long distances if metabolic energy is provided to produce a Fröhlich-Bose-Einstein-like condensation, in an open system under nonequilibrium thermodynamic conditions.* As final points we mention that Fröhlich's condensation and propagation of Davydov's soliton are *quantum effects*, which are nonexistent in classical theory, and that there exists a certain similitude of the phenomenon described here with laser action.

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