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Kinetic properties of multiquanta Davydov-like solitons in molecular chains

Jasmina Tekić, Zoran Ivić, Slobodan Zeković, and Željko Pržulj
Theoretical Physics Department 020, The ''Vinča'' Institute of Nuclear Sciences, 11001 Belgrade, Serbia, Yugoslavia

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The Fokker-Planck equation for multivibron solitons interacting with lattice vibrations in a molecular chain has been derived by means of the nonequilibrium statistical operator method. It was shown that a soliton undergoes diffusive motion characterized by two substantially different diffusion coefficients. The first one corresponds to the ordinary (Einsteinian or dissipative) diffusion and characterizes the soliton Brownian motion, while the second one corresponds to the anomalous diffusion connected with frictionless displacement of the soliton center of mass coordinate due to the interaction with phonons. Both processes are the consequence of the Cherenkov-like radiation of phonon quanta arising when soliton velocity approaches the phase speed of sound. [S1063-651X(99)01707-9]

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Examination of the possible role of the solitonic mechanism in charge and energy transfer over large distances in one-dimensional exciton (electron)-phonon systems has received considerable interest in the last twenty-five years [1–9]. A majority of these studies deal with the so-called Davydov model, which assumes soliton formation on account of single ''exciton'' (vibron, electron, Frenkel exciton, ...) trapping by the induced local distortion of the host lattice [self-trapping (ST) mechanism]. In order to avoid any confusion we note that in the present context, we use the term exciton to denote the quantum of the intramolecular vibrational excitation of the molecular chain or vibron. Investigations carried out within the general theory of the ST phenomena [5–7] indicate that the original Davydov proposal, i.e., soliton formation on account of the single exciton ST, cannot explain intramolecular energy (amide-*I* quanta) transfer in biopolymers such as the α helix and acetanilide (ACN). Namely, according to the available data [3–9], the width of the exciton band of these substances is too small compared to the maximal phonon frequency-nonadibatic limit, so that one should expect the formation of the small-polaron band states [5–10] rather than a soliton.

Nevertheless, recent analysis [11] points to the possibility of soliton formation in such systems but only for higher excitation concentrations, where, the so-called ''dressing'' effect which results in an additional (phonon mediated) exciton-exciton interaction, plays the dominant role in soliton formation, which now represents the bound state of several excitations. However, the results of that analysis, obtained within the framework of the mean-field method, are of limited validity. In particular, the starting point of these examinations was an effective, mean-field Hamiltonian describing the system of interacting ''dressed'' quasiparticles (polarons) completely disregarding the coupling of such excitations with the remaining phonons. As a result of such a coupling, energy exchange between the constituent subsystems takes place, which, in turn, may have a certain impact on soliton dynamics and stability and, in the final instance, would induce its decay.

The subject of the present paper is the examination of the kinetic properties of such solitons arising as a consequence of their coupling to the phonons which act as a thermal bath. Under these circumstances soliton dynamics can be described by the Fokker-Planck equation (FPE) for the soliton distribution function which will be derived below. For that purpose we shall use the method introduced in Ref. [12] for the examination of the related problem: kink dynamics under the influence of lattice vibrations. It is based upon the method of a nonequilibrium statistical operator as developed by Zubarev [13].

The starting point of our analysis is the well-known Frohlich-like Hamiltonian of the molecular chain specified as

$$H=\Delta\sum_{n} A_n^+A_n-J\sum_{n} A_n^+(A_{n+1}+A_{n-1}) +\frac{1}{\sqrt{N}}\sum_{q,n} F_q e^{iqnR_0}A_n^+A_n(b_q+b_{-q}^+)+\sum_{q} \hbar\omega_q b_q^+ b_q, \tag{1}$$

where $A_n^+(A_n)$ describes the presence (absence) of the excitation with the energy Δ on the nth molecular group, $b_q^+(b_q)$ creates (annihilates) phonon quanta with frequency ω_q, while F_q denotes the exciton-phonon coupling parameter. It is given by $F_q=2i\chi(\hbar/2M\omega_q)^{1/2}\sin qR_0$ in the case of coupling with acoustic phonons with frequency $\omega_q=\omega_B\sin|qR_0/2|$, $\omega_B=2(\kappa/M)^{1/2}$ denotes the maximal phonon frequency, κ is the spring constant, M denotes the mass of the molecular group, R_0 denotes the lattice constant, and finally J and χ represent intersite dipole-dipole transfer integral and coupling strength, respectively. In the case of coupling with dispersionless optical modes we have $\omega_q=\omega_0\equiv\text{const}$ and $F=\chi(\hbar/2M\omega_0)^{1/2}$, the meaning of symbols is as before. Obviously this corresponds to the known Holstein's molecular crystal model (MCM) [10]. Here we are primarily interested in the examination of the soliton dynamics in the context of their possible relevance for the intramolecular vibrational energy transfer in the systems such as the α helix and ACN, where the width of the exciton band is small compared to the width of the phonon band. Under these conditions the properties of the exciton-phonon system are dominated by the so-called ''dressing'' effect, and soliton formation arises on account of the effective exciton-exciton

1063-651X/99/60(1)/821(5)/$15.00

interaction [11]. As shown in Ref. [11], exciton dressing can be explicitly accounted for, with the help of the Lang-Firsov unitary transformation [14], by rewriting the Hamiltonian (1) in terms of the dressed exciton and new phonon operators. In such a way the model Hamiltonian of the system can be represented as a sum of two terms: $H=H_{\mathrm{eff}}+H_{\mathrm{int}}$ [11]. Here H_{eff} denotes the effective Hamiltonian of dressed excitations while the second term represents the interaction Hamiltonian with the remaining phonons. They are explicitly given as

$$\begin{aligned}H_{\mathrm{eff}}=[\Delta-E_B]\sum_n B_n^+B_n-J_{\mathrm{eff}}\sum_{n,l=\pm1}B_n^+B_{n+l}\\+\sum_q\hbar\omega_q a_q^+a_q-E_B\Bigg[\sum_n B_n^{+2}B_n^2\\+\frac{1}{2}\sum_{n,l=\pm1}B_n^+B_{n+l}^+B_{n+l}B_n\Bigg]\end{aligned}\tag{2}$$

and

$$H_{\mathrm{int}}=J\sum_n\{B_n^+B_{n+1}[\langle\Theta_n^+\Theta_{n+1}\rangle-\Theta_n^+\Theta_{n+1}]+\mathrm{H.c.}\}.\tag{3}$$

Here

$$\Theta_n=\exp\left\{\frac{1}{\sqrt{N}}\sum_q\frac{F_q}{\hbar\omega_q}e^{-iqnR_0}(a_q-a_{-q}^+)\right\}.$$

In the above expressions we use the same notation as in Ref. [11] so that $J_{\mathrm{eff}}=Je^{-S(T)}$ denotes the effective transfer integral with

$$S(T)=\frac{2}{N}\sum_q\frac{|F_q|^2}{(\hbar\omega_q)^2}\sin^2\frac{qR_0}{2}(2\overline{\nu}_q+1),$$

($\overline{\nu}_q$ is the equilibrium phonon distribution) denoting the temperature-dependent coupling constant introduced in Ref. [5–7].

$$E_B=\frac{1}{N}\sum_q\frac{|F_q|^2}{\hbar\omega_q}$$

denotes the small-polaron binding energy. Finally, the operators $B_n^+=U^+A_nU$ (B_n) describe the presence (absence) of a dressed excitation on the nth site of the molecular chain, while $a_q^+=U^+b_q^+U$ and $a_q=U^+b_qU$ are the creation and annihilation operators of the ‘‘new’’ phonons in the chain with the shifted equlibrium positions of the molecular groups. U is the Lang-Firsov unitary operator [12]

$$U=\exp\left\{\frac{1}{\sqrt{N}}\sum_{n,q}\frac{F_q}{\hbar\omega_q}e^{-iqnR_0}A_n^+A_n(b_{-q}-b_q^+)\right\}.$$

The last term in Eq. (2) represents the effective exciton-exciton interaction responsible for multiquanta soliton formation. Their properties have been examined in detail in Ref. [11] where the criteria for their existence were formulated in terms of temperature, coupling constant $[S(T)]$, and the so-called adiabaticity parameter $B(T)=(8/3\pi)(2J/\hbar\omega_B)S(T)$. It was found that the whole parameter space of the system (S-B plane) is divided into two regions in which two different types of nonlinear excitations, soliton and so-called intrinsic self-localized mode, exist. These regions are separated by the continuum boundary $S(T)=B(T)/\mathcal{N}$, where $\mathcal{N}$ denotes the number of quanta engaged in the soliton creation. Soliton solutions correspond to those points of the system parameter space for which the condition for the applicability of the continuum approximation is satisfied and the soliton sector lies below that line [11]. In the systems we are primarily interested in the adiabaticity parameter lies in nonadiabatic region ($B\ll1$) so that the soliton sector corresponds to the weak-coupling limit. Consequently, the exponential term in H_{int} containing the ‘‘small parameter’’ proportional to the square root of the coupling constant, may be expanded in power series where we may safely keep the first two terms only. Under these conditions our interaction Hamiltonian becomes

$$\begin{aligned}H_{\mathrm{int}}=\frac{1}{\sqrt{N}}J_{\mathrm{eff}}\sum_{n,q}\frac{F_q}{\hbar\omega_q}(1-e^{iqR_0})e^{iqnR_0}B_n^+B_{n+1}(a_q^+-a_{-q})\\+\mathrm{H.c.}\end{aligned}\tag{4}$$

The next step is the derivation of an effective Lagrangian of the soliton-phonon system in which the soliton subsystem is described by the collective variables: its momentum and center of mass.

In order to introduce a collective variable Hamiltonian (Lagrangian) let us recall that the equations of motion for the soliton amplitudes (soliton wave function) follow from the time-dependent variational principle—i.e., demanding the stationarity of the action $\mathcal{A}=\int_{t_1}^{t_2}d\tau\mathcal{L}[\psi^*(\tau),\psi(\tau)]$ ($\delta\mathcal{A}=0$). Here $\mathcal{L}=(i\hbar/2)[\langle\Psi|\dot{\Psi}\rangle-\langle\dot{\Psi}|\Psi\rangle]-\mathcal{H}(\Psi^*,\Psi)$ denotes the Lagrangian of the system with $\mathcal{H}(\Psi^*,\Psi)=\langle\Psi|H|\Psi\rangle$ and where $|\Psi\rangle$ denotes an appropriate trial state. In the present context it is chosen as a product of the polaron operator coherent states $|\Psi(t)\rangle=|\beta(t)\rangle,|\beta(t)\rangle=\Pi_n|\beta_n(t)\rangle$. Derivation of the collective variable Hamiltionian assumes the following steps: (i) substututing the proposed form of the trial state into the explicit expression for the Lagrangian, (ii) going over to a continuum approximation $\beta_n(t)\rightarrow\beta(x,t)$, (iii) substitution of the explicit soliton solution in the form $\beta(x,t)=\beta[x-\xi(t)]$ [$\xi(t)$ denotes soliton center of mass] into the so obtained Lagrangian, and finally (iv) integration over the spatial coordinate x. The first two steps give us

$$\mathcal{L}=\frac{i\hbar}{2}\int_{-\infty}^{\infty}\frac{dx}{R_0}(\dot{\beta}\beta^*-\beta\dot{\beta}^*)-\mathcal{H}_s-\mathcal{H}_{\mathrm{int}}+\mathcal{L}_{\mathrm{ph}}.\tag{5}$$

Here $\mathcal{H}_s$ represents the Hamiltonian function of the solitonic subsystem which, in accordance with the above proposed procedure, may be approximated by the Hamiltonian of the nonlinear Schrödinger model (NSM)

$$\begin{aligned}\mathcal{H}_s=(\Delta-E_B-2J_{\mathrm{eff}})\int_{-\infty}^{\infty}\frac{dx}{R_0}|\beta|^2+J_{\mathrm{eff}}\,R_0^2\int_{-\infty}^{\infty}\frac{dx}{R_0}|\beta_x|^2\\-2E_B\int_{-\infty}^{\infty}\frac{dx}{R_0}|\beta|^4,\end{aligned}\tag{6}$$

while

$$\mathcal{H}_{\text{int}}=\frac{R_0 J_{\text{eff}}}{\sqrt{N}}\sum_q \int_{-\infty}^{\infty}\frac{dx}{R_0}\frac{F_q(1-e^{iqR_0})}{\hbar\omega_q}\times e^{iqx}(a_q^{+}-a_{-q})(\beta^{*}\beta_x-\text{c.c.}) \tag{7}$$

denotes the soliton-phonon interaction Hamiltonian. As usual dots and subscripts denote derivation with respect to t and x, respectively. Finally,

$$\mathcal{L}_{\text{ph}}=\frac{i\hbar}{2}\sum_q (\dot{a}_q^{+}a_q-\text{H.c.})-H_{\text{ph}} \tag{8}$$

denotes the phonon subsystem Lagrangian. Following the above proposed procedure we take the soliton amplitude as follows: $\beta(x,t)=\beta[x-\xi(t),t]\equiv\tilde{\beta}[x-\xi(t)]e^{i\{k_s[x-\xi(t)]-\omega t\}}$. Here $k_s=P_{\text{sol}}/\hbar\mathcal{N}$ denotes the soliton quasimomentum, $\tilde{\beta}[x-\xi(t)]$ is the soliton envelope given by $\tilde{\beta}(x,t)=\mathcal{N}(\mu/2)^{1/2}\operatorname{sech}(\mu\mathcal{N}/R_0)[x-\xi(t)]$, while ω represents a soliton phase whose explicit form is irrelevant in the present context. After straightforward calculation we obtain the following collective variable Lagrangian:

$$\mathcal{L}=\dot{\xi}P_{\text{sol}}-\frac{P_{\text{sol}}^2}{2m_s}-\frac{P_{\text{sol}}}{\sqrt{N}}\sum_q G_q e^{iq\xi}(a_q^{+}-a_{-q})+\mathcal{L}_{\text{ph}}, \tag{9}$$

where $m_s=\mathcal{N}\hbar^2/2J_{\text{eff}}R_0^2$ denotes the soliton effective mass [11]. In this expression we have neglected a constant term which does not contain soliton collective variables and which consequently does not influence its dynamics. The soliton-phonon coupling parameter is given explicitly as

$$G_q=\frac{2iR_0J_{\text{eff}}}{\hbar}\frac{F_q(1-e^{iqR_0})}{\hbar\omega_q}\frac{\pi qR_0/2\mu\mathcal{N}}{\sinh(\pi qR_0/2\mu\mathcal{N})}. \tag{10}$$

The model specified by the above Lagrangian describes the system consisting of the classical particle(s) (soliton) interacting with a quantum-mechanical thermal bath (phonons). It has precisely the same form as the one derived in Ref. [12] for the examination of the kinetic properties of kink solitons interacting with a three-dimensional phonon field and we may safely follow the procedure proposed there. Thus the next step is the derivation of the FPE for the soliton distribution function $[f(P_{\text{sol}},\xi)]$ which characterizes the macroscopic state of the system and which is defined as an average value of the soliton density $[n(P_{\text{sol}},\xi)=\Sigma_i\delta(P_{\text{sol}}-P_i)\delta(\xi-\xi_i)]$: $f(P_{\text{sol}},\xi)=\langle n(P_{\text{sol}},\xi)\rangle$, where $\langle\ \ldots\ \rangle$ denotes the averaging over the nonequlibrium statistical operator [13]. In such a way, strictly following Ref. [12], we obtain the FPE

$$\frac{\partial f}{\partial t}+\frac{P_{\text{sol}}}{m_{\text{sol}}}\frac{\partial f}{\partial\xi}=\frac{\partial}{\partial\xi}\left(L_{11}kT\frac{\partial f}{\partial\xi}\right)+\frac{\partial}{\partial P_{\text{sol}}}\left[L_{22}\left(\frac{P_{\text{sol}}}{m_s}f+kT\frac{\partial f}{\partial P_{\text{sol}}}\right)\right], \tag{11}$$

Here L_{11} and L_{22} are kinetic coefficients given as

$$L_{11}=\frac{1}{kT}\int_{-\infty}^{0}e^{\varepsilon t}dt\left\langle\frac{\partial\mathcal{H}_{\text{int}}}{\partial P_{\text{sol}}}\frac{\partial\mathcal{H}_{\text{int}}(t)}{\partial P_{\text{sol}}}\right\rangle_0, \tag{12}$$

$$L_{22}=\frac{1}{kT}\int_{-\infty}^{0}e^{\varepsilon t}dt\left\langle\frac{\partial\mathcal{H}_{\text{int}}}{\partial\xi}\frac{\partial\mathcal{H}_{\text{int}}(t)}{\partial\xi}\right\rangle_0, \tag{13}$$

where $\langle\cdots\rangle_0$ stands for the averaging over the thermal bath while $\mathcal{H}_{\text{int}}$ denotes the soliton-phonon interaction Hamiltonian expressed in terms of collective variables (ξ,P_{sol}). Its explicit form is given by the third term in the collective variable Lagrangian in Eq. (9). Here, in the final calculations, one must set $\varepsilon\rightarrow 0$. Explicit time dependence of $\mathcal{H}_{\text{int}}$ in the above expressions appears only through the time dependence of phonon operators and soliton momentum and center of mass coordinate and, in the first approximation, will be specified by the solutions of their equations of motion with respect to the unperturbed case. In particular, for the calculation of the above kinetic coefficients we shall adopt the following approximation: $a_q(t)=a_q e^{-i\omega_q t}$, $a_q^{+}(t)=a_q e^{i\omega_q t}$, and $\xi(t)=x_0+vt$ (v-soliton velocity). Thus we get

$$L_{11}=\frac{1}{kT}\frac{2\pi}{N}\sum_{q>0}|G_q|^2\left(\nu_q+\frac{1}{2}\right)\delta(\omega_q-qv), \tag{14}$$

$$L_{22}=\frac{1}{kT}\frac{2\pi P_{\text{sol}}^2}{N}\sum_{q>0}q^2|G_q|^2\left(\nu_q+\frac{1}{2}\right)\delta(\omega_q-qv). \tag{15}$$

It follows from the above derived FPE, that due to the interaction with phonons, the soliton undergoes diffusive motion as result of two different mechanisms. The first one determines the Brownian motion of the soliton and corresponds to the ordinary (Einsteinian or dissipative) diffusion characterized by the diffusion coefficient $D=kT/L_{22}$, where L_{22} has the meaning of the viscosity or friction coefficient. The second mechanism, on the contrary, is not connected with dissipation and arises as a result of the shift of the soliton center of mass coordinate due to the interaction with phonons. The quantity $D^{*}=kTL_{11}$ plays the role of the coefficient of this diffusion. Both mechanisms are the consequence of the Cherenkov-like radiation of phonon quanta arising when the soliton velocity (v) approaches the phase speed of sound ω_q/q. This is obvious from the presence of a δ function in the expressions for the kinetic coefficients which are different from zero only when the argument of the δ function vanishes, i.e., when $\omega_q=qv$. The appearance of a δ function in the above expressions enables one to calculate explicitly both diffusion coefficients. Furthermore, adopting the long wavelength limit ($qR_0\approx 0$) we may approximate the soliton form factor, the last factor in the expression for the soliton-phonon coupling parameter (10), by unity. This is justified since it is highly peaked for $qR_0\approx 0$ and rapidly diminishes as qR_0 increases. In such a way we obtain

$$L_{11}\approx 12\frac{B^2R_0^2\omega_B S}{kT\sqrt{1-v/c_0}}\left(\nu_{q_0}+\frac{1}{2}\right), \tag{16}$$

$$L_{22}\approx 288\frac{\omega_B v^2 m_S^2 B^2 S}{kT}\sqrt{1-\frac{v}{c_0}}\left(\nu_{q_0}+\frac{1}{2}\right), \tag{17}$$

in the case of the soliton coupling with acoustical phonons. Here $B=(3\pi/8)(2J/\hbar\omega_B)$ and $S=(3\pi/8)(E_B/\hbar\omega_B)$ represent the adiabaticity parameter and the coupling constant, respectively, while $q_0=(4.9/R_0)\sqrt{1-v/c_0}$ denotes a nontrivial solution of the equation $\omega_q-qv=0$. It is necessary for one to evaluate integrals of the form $\int_0^{\pi/R_0}dq q^n|G_q|^2(\nu_q+\frac{1}{2})\delta(\omega_q-qv)$ appearing in the expressions for kinetic coefficients after the replacement of the summation over the phonon quasimomenta by an integration. For the explicit calculations we used $\omega_q\simeq c_0q(1-q^2R_0^2/12)$, where $c_0=R_0\sqrt{\kappa/M}$ denotes the speed of sound. From the demand that q_0 must lie in the interval $(0,\pi/R_0)$, otherwise these integrals vanish, the following condition for the Cherenkov-like radiation of acoustic phonons arises: $0.6c_0\leqslant v<c_0$.

In the case of interaction with optical phonons, an analogous procedure results in

$$L_{11}\approx\frac{B^2R_0^5\omega_0^4S}{kTv^3}\left(\nu_{q_0}+\frac{1}{2}\right), \tag{18}$$

$$L_{22}\approx\frac{\omega_0^6R_0^5m_S^2B^2S}{kTv^3}\left(\nu_{q_0}+\frac{1}{2}\right). \tag{19}$$

Here $q_0=\omega_0/v$ is the zero of the argument of a δ function, while the coupling constant and adiabaticity parameter take the forms $S=E_B/\hbar\omega_0$ and $B=2J/\hbar\omega_0$. Analogously as in the previous case we found the following condition for the Cherenkov-like radiation: $v\geqslant\omega_0R_0/\pi$.

Thus, irrespective of the type of the soliton-phonon coupling, the "anomalous" as well as the ordinary diffusion exhibits the same temperature dependence but quite different dependence on soliton velocity. Precisely, in the low-temperature limit ($kT\ll\hbar\omega_{q_0}$ for acoustic and $kT\ll\hbar\omega_0$ for optical phonons), the anomalous diffusion coefficient is temperature independent ($D^*\sim$const) while the ordinary one becomes $D\sim T^2$. However, in the high-temperature limit we have $D^*\sim T$ and $D\sim T$. Considering the dependence on the soliton velocity we have (i) in the case of acoustical phonons the coefficient of the anomalous diffusion increases with the increase of the soliton velocity, while the ordinary diffusion coefficient decreases in the range $0.6c_0\leqslant v\leqslant0.8c_0$ and increases for $0.8c_0\leqslant v<c_0$, (ii) for optical phonons, D^* decreases while D increases with the increase of soliton velocity.

In summary we note that the kinetics of the multivibron solitons in a molecular chain, induced by the soliton-phonon coupling, is characterized by the two substantially different diffusion processes. The first, an ordinary (dissipative) one, is connected to the soliton viscosity while the second, so to speak anomalous one, arises due to the phonon induced shift of the soliton position. This is the consequence of the fact that the soliton-phonon interaction depends on soliton position and momentum as well. A similar situation arises also in the case of the kink-soliton diffusion in some nearly integrable systems [15–17] (magnetic, ferroelectric, etc.). In contrast to these systems, where radiationless processes, soliton scattering by the linear excitations (magnons, for example) dominate their dynamics, and where both types of diffusion coefficients are independent of soliton velocity, here the soliton dynamics is the consequence of the Cherenkov-like radiation of phonon quanta which is the reason why diffusion coefficients in our case depend on soliton speed.

We note that the proposed ansatz of deriving of the collective variable Lagrangian, based upon the choice of soliton solution as proposed below Eq. (8), is not the most accurate one since it disregards dynamics of the soliton phase. A better choice would be $\beta(x,t)=\beta[x-\xi(t),t]\equiv\tilde{\beta}[x-\xi(t)]e^{i\{k_s[x-\xi(t)]-\Omega(t)\}}$. As a result the collective coordinate Lagrangian would be expressed in terms of the two pairs of conjugated variables: soliton momentum and its center of mass coordinate, characterizing soliton translational motion, and an additional pair, generalized "momentum" $\mathcal{N}$ and "coordinate" Ω, describing the evolution of the soliton phase. Kinetics of the soliton in that case would be described in terms of a bit more complicated FPE which can be derived in analogous way as Eq. (11). However, due to the fact that the interaction Hamiltonian (7) does not depend on the generalized "coordinate" Ω and weakly depends on its conjugated "momentum" ($\mathcal{N}$) only through the appearance of the soliton form factor in Eq. (10) which, in the soliton sector, tends to unity, dynamics of the soliton phase is practically unaffected by the coupling to phonons. Thus one can accept that the FPE (11) describes the dynamics of the multiexciton solitons fairly well.

The method presented does not take into account soliton decay, which may arise as the result of the soliton-phonon interaction. Accounting of this effect demands, however, taking into account the whole spectrum of the NSM describing the vibron subsystem which, besides the soliton mode contains also the band of linear excitations, "excitons." Therefore the phonon coupling with both "branches" of vibron spectra may induce "particles" exchange between them. This should result in the time dependence of the soliton amplitude and consequently its life time becomes finite. Examination of this problem will be presented separately.

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[1] A.S. Davydov and N.I. Kislukha, Phys. Status Solidi B **59**, 465 (1973).

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

[3] See, for example, *Davidov's Soliton Revisited*, edited by P.L. Christiansen and A.C. Scott (Plenum, New York, 1990).

[4] A.C. Scott, Phys. Rep. **217**, 1 (1992).

[5] D.W. Brown and Z. Ivić, Phys. Rev. **40**, 9876 (1989).

[6] D.W. Brown, K. Lindenberg, and X. Wang, in *Davidov's Soliton Revisited*, edited by P.L. Christiansen and A.C. Scott (Plenum, New York, 1990).

[7] Z. Ivić, D. Kapor, M. Škrinjar, and Z. Popović, Phys. Rev. B **48**, 3721 (1993).

[8] D.M. Alexander, Phys. Rev. Lett. **54**, 138 (1985).

[9] D.M. Alexander and J.A. Krumhansl, Phys. Rev. B **33**, 7172 (1986).

[10] T. Holstein, Ann. Phys. (N.Y.) **8**, 326 (1959); **8**, 343 (1959).

[11] Z. Ivić, D. Kostić, Ž. Pržulj, and D. Kapor, J. Phys.: Condens. Matter **9**, 413 (1997).

[12] J. Tekić, Z. Ivić, S. Stamenković, and R. Žakula, J. Phys.: Condens. Matter **4**, 231 (1992).

[13] D.N. Zubarev, *Nonequlibrum Statistical Thermodynamics* (Consultants Bureau, New York, 1974), Chap. 4.

[14] I.G. Lang and Yu.A. Firsov, Zh. Éksp. Teor. Fiz. **43**, 1832 (1962) [Sov. Phys. JETP **16**, 1293 (1962)].

[15] V.G. Bar'yakhtar, B.A. Ivanov, A.L. Sukstanskiĭ, and E.V. Tartakovskaya, Teor. Mat. Fiz. **74**, 46 (1988).

[16] B.A. Ivanov and A.K. Kolezhuk, Pis'ma Zh. Eksp. Teor. Fiz. **49**, 489 (1989) [JETP Lett. **49**, 561 (1989)]; Phys. Lett. A **146**, 190 (1990).

[17] B.A. Ivanov, A.K. Kolezhuk, and E.V. Tartakovskaya, J. Phys.: Condens. Matter **5**, 7737 (1993).