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## Radiation emission by a polaron in a molecular chain

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**Abstract.** We study the stability of the soliton-like polaron states in a molecular chain by means of a perturbation approach. We demonstrate that, under the influence of thermal fluctuations in the host lattice, the soliton gradually decays into delocalized ('excitonic') states. The soliton lifetime depends strongly on temperature and the coupling strength.

The state of the excess (quasi-) particle (electron, exciton, ...) in deformable media may be highly affected by a strong interaction with the underlying crystal lattice. So, for example, electrons in insulators or semiconductors may polarize and deform the host lattice and lead to the occurrence of a complex entity—the polaron, consisting of an electron and associated lattice distortion [1–4]. In quasi-one-dimensional systems with short-ranged electron (exciton)–phonon interaction in the adiabatic limit, polarons form large-radius, stable and mobile soliton-like states [4–7]. Therefore, the energy losses of the quasiparticle through dispersion and dissipation due to coupling with the environment may be prevented by formation of the soliton. For this reason the soliton concept has been proposed for understanding of the mechanisms of charge and energy transport in quasi-one-dimensional conductors [7] and molecular chains like  $\alpha$ -helix macromolecules and acetanilide [8]. In the latter case an idealized Davydov model (DM) [5, 6, 8], representing an extra quasiparticle (electron, exciton, ...) interacting with low-frequency acoustic modes of the underlying 1D lattice, has been proposed as a theoretical framework for the description of transport in molecular chains.

In applications to realistic physical systems, a crucial problem is examination of the soliton's dynamics, and, in particular, its stability under the influence of various perturbations that can arise during its motion. That is why various aspects of the DM theory concerning its relevance for the understanding of the fundamental transport mechanisms, especially in biological structures, have been critically re-examined over the last decade [9–11]. Special attention was paid to examination of the soliton's stability at biologically relevant temperatures and this problem still remains open [12]. We can safely accept, however, the applicability of the Davydov *ansatz* (DA) in the highly adiabatic and strong-coupling limit where the semiclassical treatment of phonons is justified.

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In the present paper we shall analyse some aspects of the soliton stability arising due to the non-integrability of the Davydov set of equations:

$$i\hbar\dot{\phi}(x, t) = (\Delta - 2J)\phi(x, t) - JR_0^2\phi_{xx} + \frac{1}{\sqrt{N}} \sum_q F_q e^{iqx} (\beta_q + \beta_{-q}^*)\phi(x, t) \quad (1a)$$

$$i\hbar\dot{\beta}_q(t) = \hbar\omega_q\beta(t) + F_q^* \frac{1}{\sqrt{N}} \int_{-\infty}^{\infty} \frac{dx}{R_0} e^{-iqx} |\phi(x, t)|^2. \quad (1b)$$

Here  $\phi(x, t)$  and  $\beta_q(t)$  denote the electron (exciton) wave function (normalized to unity) and the coherent phonon amplitude respectively;  $\Delta$  is the on-site excitation energy in the molecular chain,  $J$  is the intersite transfer matrix element, while  $R_0$  is the lattice constant.  $F_q = 2\chi i(\hbar/2M\omega_q)^{1/2} q R_0$  is the Fourier component of the electron (exciton)-phonon interaction where  $\chi$  is the coupling constant,  $M$  is the mass of the units in the host lattice, and for the phonon frequency  $\omega_q$  we adopt the acoustic linear dispersion law, i.e.,  $\omega_q = c_0|q|$  with  $c_0$  the speed of sound in the molecular chain.

The system described by equations (1a) and (1b) is non-integrable (see also [13]). Therefore the interaction of the solitary excitation with phonons is expected to be inelastic, and the soliton should gradually decay into delocalized band states. This possibility is a consequence of the fact that the full spectrum of the electron (exciton) trapped by the lattice distortion contains one bound state (soliton) and a continuum of delocalized (band) states. In the context of the DM these delocalized states are usually called 'excitons' or exciton-like ones [14]. Thus, in the presence of perturbations there is a possibility of energy exchange between solitons and 'excitons' so that the soliton might decay into band states. In what follows below, we assume the applicability of the semiclassical approximation which provides the validity of the Davydov set of equations (1). It implies that we are dealing with systems for which the adiabatic and continuum approximations are meaningful. The first condition provides justification for the semiclassical time-dependent variational treatment (the so-called Davydov *ansatz*) and assumes large values of the adiabatic parameter,  $B \gg 1$ , where  $B \equiv 2JR_0/\hbar c_0$ . It represents the ratio of the exciton band width to the maximal phonon energy. The second condition imposes the restriction on the maximal value of the coupling constant, which is limited to small values [14, 15]. The relevant parameter is the ratio of the small polaron binding energy ( $E_b = \sum_q |F_q|^2/\hbar\omega_q$ ) to the maximum phonon energy, i.e.  $S = 2E_b R_0/\hbar c_0$ .

Under these conditions, the system (1) admits the well known soliton solution assuming that  $|\phi(x, t)|^2 = |\phi(x - vt)|^2$ , where  $v$  is the soliton velocity. This implies a particular form for the phonon amplitudes,  $\beta_q^s(t)$ , which can be immediately obtained from equation (1b):

$$\beta_q^s(t) = \frac{e^{-iqvt}}{\sqrt{N}} \frac{F_q^*}{\hbar(\omega_q - qv)} \int_{-\infty}^{\infty} \frac{dy}{R_0} e^{-iqy} |\phi(y)|^2 \quad (2)$$

(the integration variable is  $y \equiv x - vt$ ). Equation (2) represents, however, only a particular solution to the inhomogeneous equation (1b), while its general solution should also contain a solution to the corresponding homogeneous equation. The latter one is of the form  $\beta_q^h(t) = \beta_q(0)e^{-i\omega_q t}$ , and in the present context it represents the influence of the thermostat. Therefore the general solution to equation (1b) is

$$\beta_q(t) = \beta_q(0)e^{-i\omega_q t} + \beta_q^s(t). \quad (3)$$

For a system at  $T = 0$ , the incoherent part of  $\beta_q(t)$  is absent, while at a finite temperature it is this linear part that acts on the soliton as a perturbation representing random fluctuations

of the medium. The importance of this term for the soliton's stability has been pointed out [16, 17], but hitherto no quantitative examination of its influence has been carried out.

Substituting into equation (1a) the phonon amplitudes as per equation (3), we obtain a perturbed nonlinear Schrödinger (NLS) equation for the wave function  $\phi(x, t)$ :

$$i\hbar\dot{\phi}(x, t) - (\Delta - 2J)\phi(x, t) - JR_0^2\phi_{xx} + \frac{2E_b}{1 - v^2/c_0^2}|\phi(x, t)|^2\phi(x, t) = f(x, t)\phi(x, t) \quad (4)$$

with the effective fluctuation force  $f(x, t)$

$$f(x, t) = \frac{1}{\sqrt{N}} \sum_q F_q e^{iqx} (\beta_q(0)e^{-i\omega_q t} + \beta_{-q}^*(0)e^{i\omega_q t}). \quad (5)$$

For the initial conditions which correspond to a lattice in thermal equilibrium, one can find that the correlation function of the force (5) is

$$\langle f(x, t)f(x', t') \rangle = E_b k_B T R_0 \sum_{j=\pm 1} \delta[x - x' + c_{0j}(t - t')]. \quad (6)$$

Here  $T$  is the temperature, while the small polaron binding energy is given explicitly as  $E_b = 2\chi^2 R_0^2 / Mc_0^2$  and  $c_{0j} \equiv jc_0$  (recall  $j \equiv \pm 1$ ). Notice that a more general correlator of the effective random force in equation (4) was considered in [18], in terms of the interaction of a soliton with a random acoustic field (this was a model of the interaction between the Langmuir and ion-acoustic waves in a plasma, based on the famous Zakharov equations [19]). In [18], it was assumed that the random acoustic field was determined by independent random distributions of the acoustic field,  $n(x, t)$ , and of its time derivative  $n_t(x, t)$  at the initial moment  $t = 0$ . In the adiabatic approximation (the group velocities of the Langmuir waves were assumed much smaller than the speed of sound), this gave rise to the same equation (4); however, the correlator (6) is a special particular case of that considered in [18], whose analysis will be closely followed below.

In what follows, we shall consider very slow solitons ( $v/c_0 \ll 1$ ), and equations (5) and (6) will be written in the dimensionless form using the definitions  $z \equiv x/R_0$ ,  $\tau \equiv 2Jt/\hbar$ , and  $G \equiv E_b/J$ , so that they transform into

$$i\psi_\tau + \frac{1}{2}\psi_{zz} + |\psi(z, \tau)|^2\psi(z, \tau) = g(z, \tau)\psi(z, \tau) \quad (4')$$

$$\langle g(z, \tau)g(z', \tau') \rangle = \epsilon^2(T) \sum_{j=\pm 1} \delta[z - z' + jc(\tau - \tau')]. \quad (6')$$

The nonlinearity parameter  $G$  was absorbed into the scaled amplitude  $\tilde{\psi}(z, \tau) \equiv \sqrt{G}\phi(x, t)$ , while the constant multiplier  $\Delta - 2J$  is removed by the simple transformation  $\tilde{\psi}(x, t) \equiv e^{i(\Delta - 2J)t}\psi(x, t)$ . In equation (6'),  $\epsilon(T) \equiv \sqrt{E_b k_B T / 2J^2}$ , while  $c = \hbar c_0 / 2JR_0$  ( $\equiv B^{-1}$ ) plays the role of the speed of sound in dimensionless units. Clearly, the applicability of the adiabatic (semiclassical) condition restricts our analysis to the small- $c$  limit, which is still assumed to be larger than the soliton's velocity and the group velocity of the 'radiation'.

The unperturbed NLS equation has a soliton solution and a continuum set of delocalized (band) states. In the context of the underlying single-polaron problem we are interested only in the long-time behaviour of the soliton solution. In the absence of perturbations equation (4') is an exactly solvable one, possessing an infinite set of integrals of motion. Here we will only need the first one involving the norm or particle number:

$$N \equiv \int_{-\infty}^{+\infty} dz |\psi(z, \tau)|^2 = 2\eta + \int_{-\infty}^{+\infty} \mathcal{N}(\lambda) d\lambda \quad (7)$$

where  $\eta$  comes from the normalization of the soliton solution,

$$\psi_{\text{sol}}(z, \tau) = i\eta \operatorname{sech}[\eta(z - v\tau)]e^{i[vz - \frac{1}{2}(v^2 - \eta^2)\tau]} \quad (8)$$

and  $\mathcal{N}(\lambda) = \pi^{-1} \ln |a(\lambda)|^2$  comes from the continuum component and represents the spectral particle number density of the 'radiation field' at the wave number  $2\lambda$ .  $a(\lambda)$  is the transmission coefficient known in the inverse scattering transform (IST) [20]. For the single-polaron problem  $N = 1$ . The perturbation in equation (4') is a norm-conserving one ( $\partial N/\partial \tau = 0$ ), so that the possible decay of the soliton amplitude is the result of the increase of the number of 'quanta' (particles) in the radiation field. According to the general perturbation theory based upon IST [20, 21], the decay of the soliton's amplitude is connected with the averaged emission rate spectral density [18, 20]:

$$\frac{d\eta}{d\tau} = -\frac{1}{\pi} \int_{-\infty}^{\infty} d\lambda \left\langle \frac{d}{d\tau} \mathcal{N}(\lambda) \right\rangle. \quad (9)$$

The right-hand side of equation (5) can be evaluated using the results of the perturbation theory based on the IST

$$\left\langle \frac{d}{d\tau} \mathcal{N}(\lambda) \right\rangle = \frac{2}{\pi} \operatorname{Re} \left\langle B^*(\lambda) \frac{dB(\lambda)}{d\tau} \right\rangle \quad (10)$$

where the quantity  $B(\lambda, \tau) \equiv b(\lambda, \tau)e^{-4i\lambda^2\tau}$  ( $b(\lambda, \tau)$  is the IST reflection coefficient) may be calculated as

$$\frac{dB}{d\tau} = -4e^{-i\lambda^2\tau} a(\lambda) \int_{-\infty}^{\infty} dz \{ [\psi^{(1)*}(z, \lambda)]^2 P^*(z) + [\psi^{(2)*}(z, \tau)]^2 P(z) \}. \quad (11)$$

Here  $\psi^{(1,2)}(z, \lambda)$  stands for the two-component one-soliton Jost function for the NSE equation which can be found in [20], while  $P(z)$  stands for the right-hand side of equation (4').

In order to justify the application of the perturbation theory, let us estimate the values of the relevant physical parameters of the system. At first we can easily relate the unperturbed soliton's amplitude to the energy parameters of the underlying polaron system by evaluating the norm of  $\psi_s(z, \tau)$ . We assume that initially radiation is absent and, using the soliton solution for  $\psi(z, \tau)$  (or  $\phi(z, \tau)$ ), we find  $2\eta = G$ . Since  $G$  is equal to the inverse soliton's width, applicability of the continuum approximation demands that  $\eta \ll 1$ . On the other hand, the perturbation theory demands the smallness of the parameter  $\epsilon^2(T)$  in equation (6') as compared with  $\eta^3$ , i.e.  $\epsilon^2(T) \ll \eta^3$  [18, 21]. Using the explicit form of  $\epsilon(T)$ , this condition becomes  $(k_B T/J) \ll \eta^2$ . Since the soliton's width is expected to be typically of the order of ten to twenty lattice constants, the adiabatic condition can be satisfied in a large class of materials of interest. We note that  $J$  is estimated to be of the order of 1 eV [22, 23], which provides the applicability of the perturbative treatment even at high temperatures (we actually need  $\eta^2 \gg 10^{-4} \text{ K}^{-1} \text{ T}$ ). In addition, we have assumed that the group velocity of the delocalized states is small as compared to the speed of sound. This condition imposes a restriction on the maximum value of the wave number of the 'radiation field':  $|\lambda| \ll c/4$  [18].

It is more convenient to express the fluctuation force in equation (4') in the form [16]

$$g(z, \tau) = \sum_{j=\pm 1} \int_{-\infty}^{\infty} dq A_j(q) e^{-ijc|q|\tau} e^{-iqz} \quad (12)$$

where the corresponding coefficients are

$$A_1(q) = \frac{1}{4\pi J} F_q^* \beta_{-q} \quad A_{-1}(q) = \frac{1}{4\pi J} F_q^* \beta_q^* \quad (13)$$

The only non-vanishing correlators of these are given by

$$\langle A_1(q)A_1^*(q') \rangle = \langle A_{-1}(q)A_{-1}^*(q') \rangle = \frac{E_b k_B T}{16\pi^2 J^2} \delta(q - q'). \quad (14)$$

Using equation (11), after substitution of the single-soliton Jost functions (see, e.g., appendix A in [20]) we have

$$\frac{dB(\lambda)}{d\tau} = \frac{i\pi}{4} \frac{1}{\lambda^2 + \eta^2/4} \int_{-\infty}^{\infty} dq q^2 \sum_{j=\pm 1} \frac{A_j e^{i[Uc|q|-4(\lambda^2 + \eta^2/4)]\tau}}{\cosh((\pi/2\eta)(q + 2\lambda))}. \quad (15)$$

To find  $B(\lambda)$ , we first multiply equation (15) by  $e^{\alpha\tau}$ , keeping in mind that at some later stage we will take the limit  $\alpha \rightarrow 0$  [18]. This trick corresponds to adiabatically turning on the perturbation which was absent at  $\tau = -\infty$ . Then after the integration over  $\tau$  we have

$$B^*(\lambda) = \frac{\pi}{4} \frac{1}{\lambda^2 + \eta^2/4} \int_{-\infty}^{\infty} dq q^2 \times \sum_{j=\pm 1} \frac{A_j(q)}{\cosh((\pi/2\eta)(q + 2\lambda))} \frac{e^{\tau[\alpha - i(Uc|q| - 4(\lambda^2 + \eta^2/4))]}{\alpha + jc|q| - 4(\lambda^2 + \eta^2/4)}. \quad (16)$$

Combining the last two equations and averaging their product over the initial (equilibrium) lattice degrees of freedom, we finally obtain

$$\left\langle \frac{d}{d\tau} \mathcal{N}(\lambda) \right\rangle = \frac{2}{\pi} \frac{E_b k_B T}{c^5 J^2} \left( \lambda^2 + \frac{\eta^2}{4} \right)^2 \sum_{j=\pm 1} \operatorname{sech}^2 \left( \frac{\pi}{\eta} \left[ \lambda + \frac{2j}{c} \left( \lambda^2 + \frac{\eta^2}{4} \right) \right] \right). \quad (17)$$

In deriving this equation, we used the identity  $(x + i\alpha)^{-1} = P(1/x) + i\pi\delta(x)$ ,  $P$  being the symbol of the principal value.

Combining the last equation with equation (9) we may find the averaged soliton decay rate. For that purpose we have to calculate the total mean power of the emission (averaged emission rate), which demands evaluation of  $\int_{-\infty}^{+\infty} d\lambda \langle (d/d\tau) \mathcal{N}(\lambda) \rangle$ . The evaluation of this integral is quite difficult and in the general case its explicit expression cannot be found in a closed form analytically. However, it can be satisfactorily estimated by means of the approximations proposed in [18, 20–21] if one of the following conditions is satisfied: (i)  $\eta \ll c$  or (ii)  $\eta \gg c$ .

The first condition ( $\eta \ll c$ ) is valid at a sufficiently late stage of the soliton's decay or in the case when the soliton is initially spread over a large number of lattice sites and the adiabaticity parameter is not too high. Using the expression for the soliton amplitude and rescaled speed of sound this condition can be written as  $S \ll 1$ . On the other hand the second condition holds in the strong-coupling ( $S \gg 1$ ) limit, which, in this particular case, is equivalent to the high-adiabatic limit: namely, if the adiabatic parameter is very large (in [21, 22] it was found that  $B \sim 10^2$ ), then condition (ii), which demands large values for the coupling constant, is satisfied if the continuum approximation ( $\eta \sim 10^{-1}$ ) holds.

Let us note that smallness of the coupling constant is one of the most important conditions for the generation and existence of solitons in molecular chains [17]. However, soliton existence is not restricted to the weak-coupling case only. In particular, in recent studies [14] of the self-trapping phenomena in the one-dimensional electron (exciton)-phonon systems it was found that solitons could be formed even in the strong-coupling case if the adiabaticity parameter is large enough. Therefore analysis of the soliton decay demands the estimation of the total averaged emission rate in both cases mentioned above. More details concerning the influence of the values of the physical parameters on soliton existence can be found in [14]. It is straightforward to see that, under this condition, the spectral

density in equation (17) has two pronounced maxima at the points  $\lambda_{\pm} \equiv \lambda \approx \mp \eta^2/2c$ , at which the argument of the function  $\cosh$  in equation (17) vanishes (it vanishes also at the points  $\lambda \approx \mp \frac{1}{2}c$ , which, however, lie beyond the framework of applicability of the above adiabatic approximation,  $|\lambda| \ll c/4$ ). Widths of these maxima are  $\Delta\lambda \sim \eta$ , so that they are well separated under the adopted assumption  $\eta^2 \ll c^2$ . Consequently, the main contribution to the integral in equation (9) comes from the vicinities of the points  $\lambda_{\pm}$ . Calculating the integral in this approximation, we obtain from equation (9) the following evolution equation for the soliton's amplitude:

$$\frac{d\eta}{d\tau} = -\frac{1}{2\pi^2} \frac{E_b k_B T}{c^5 J^2} \eta^5. \quad (18)$$

Straightforward integration of equation (18) yields the solution

$$\eta^4(\tau) = \frac{\eta_0^4}{1 + (4\pi^2) S^5 (k_B T/J) \tau} \quad (19)$$

where  $\eta_0 = E_b/2J$  is an initial value of the soliton's amplitude. In accordance with what was said above and restoring the physical time  $t \equiv \hbar\tau/2J$ , we obtain from equation (19)

$$\eta^4(t) = \frac{\eta_0^4}{1 + (8/\pi^2) S^5 (k_B T/\hbar) t} \quad (20)$$

from which one can easily estimate a soliton's lifetime

$$t_{1/2} = 1.42(T S^5)^{-1} \times 10^{-10} \text{ s}. \quad (21)$$

Notice that the decay of the soliton into 'radiation', described by equations (19) and (20), is very slow.

In the case when the condition (ii) holds ( $\eta \gg c$ ), the averaged spectral density is symmetric with respect to the point  $\lambda = 0$  and has two maxima for  $\lambda_j = \pm c/4$ , while for  $\lambda = 0$  it approaches its minimum. However, as follows from (17), the magnitude of the averaged emission rate spectral density in all three  $\lambda$  points is practically identical. Following [21], we may estimate the total averaged emission rate directly integrating equation (17) over  $\lambda$  by adopting the following approximation:

$$\left\langle \frac{d}{d\tau} \mathcal{N}(\lambda) \right\rangle \approx \frac{8}{\pi} \frac{E_b k_B T}{c^5 J^2} \left( \lambda^2 + \frac{\eta^2}{4} \right)^2 e^{-\pi\eta/c} e^{-4(\pi/\eta c)(\lambda + jc/4)^2} \quad (22)$$

to obtain

$$\int_{-\infty}^{\infty} d\lambda \left\langle \frac{d}{d\tau} \mathcal{N}(\lambda) \right\rangle \approx \frac{1}{2\pi} \frac{E_b k_B T}{J^2} \left( \frac{\eta}{c} \right)^{9/2} e^{-\pi\eta/c}. \quad (23)$$

This equation cannot be used for an explicit evaluation of the time dependence of the soliton amplitude, but contains enough information for a qualitative description of the soliton decay in the strong-coupling and high-adiabatic limit. In order to estimate the rate of the soliton amplitude decay, we plot in figure 1 the function  $P(z) = z^{9/2} e^{-\pi z}$  (where  $z = \eta/c$ ), which practically determines the dependence of the total averaged emission rate on  $\eta$ . The small- $z$  case is what we examined in condition (i). In the region where condition (ii) is well satisfied, i.e.  $z \gg 1$ ,  $d\eta/dt$  almost vanishes, which means that, in the strong-coupling and highly adiabatic limit, the soliton is extremely stable, having practically an infinite lifetime. Its stability breaks down if  $z$  is not too large ( $1.5 < z < 4.0$ ). In terms of the basic physical parameters ( $S, B$ ), this case corresponds to the intermediate region where, as shown in [14], quantum fluctuations of the lattice play an important role. Therefore, this intermediate case (when  $P(z) \neq 0$ ) lies beyond the validity of the classical equations (1)–(6'). Consequently

satisfactory analysis of the soliton decay under these circumstances requires taking into account the quantum nature of the phonon field which causes renormalization of the system parameters due to the so-called 'dressing' effect [14].

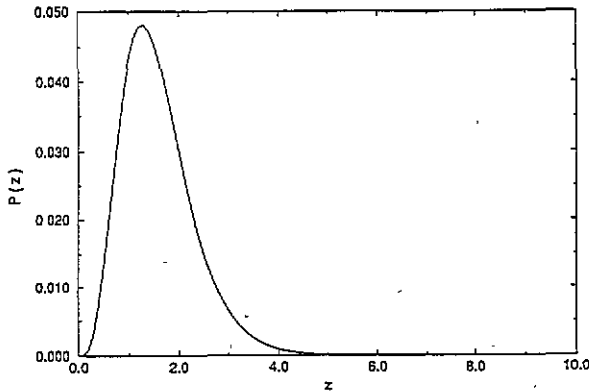


Figure 1. Plot of the function  $P(z)$  where  $z \equiv \eta/c$ .

On the basis of the present analysis we conclude that soliton evolution may display quite different behaviour depending on the values of the basic physical parameters. Thus, in the weak-coupling case thermal fluctuations of the host lattice act perturbatively on the soliton, tending to destroy it by causing leakage of the 'radiation' from it. Unlike the  $T = 0$  case, when the soliton's lifetime is infinite, at finite temperatures its amplitude gradually decays while its width increases. This is a consequence of the flow of energy from the soliton to the band states. The rate of this process is strongly influenced by the value of the coupling constant whose growth enhances soliton decay. Since our analysis concerns the weak-coupling limit, the rate of this process, as described by equations (19)–(21), is very small. Note that although this part of our analysis is focused on the weak-coupling case,  $S$  cannot be extremely small since soliton formation demands that it should be bigger than some small but finite threshold value [14, 17]. Thus the coupling constant plays a twofold role: while, on one hand, formation of the soliton (polaron) demands finite coupling, on the other hand it also determines (at  $T = 0$ ) the strength of the influence of the thermal fluctuations which have an opposite effect on the soliton stability. Thus, the stability of the soliton at finite temperatures is determined by a balance between these two effects.

In [18], analysis of the radiative decay of the soliton with the above-mentioned correlators for the random force in equation (4), more general than those given by equation (6), has demonstrated that in the general case the decay is exponential, i.e., it is essentially faster than as per equations (19) and (20). Only in a special particular case does the model considered in [18] lead to the same slow law of the soliton's decay as in the present work. Nevertheless, it is clear that an estimate for the characteristic soliton lifetime in physical units, following from equation (20), will be the same whatever the particular assumption about the correlators.

If, however, the system parameters fall in the strong-coupling and adiabatic limit, solitons become extremely stable. In the case of intermediate coupling and not too high adiabaticity the present method should be modified in order to take into account quantum effects.

In conclusion, in this work we have demonstrated that thermal fluctuations of the host lattice act perturbatively on the soliton, tending to destroy it, causing leakage of the 'radiation'. Unlike the  $T = 0$  case, when the soliton's lifetime is infinite, at finite  $T$  its amplitude gradually decays while its width increases. This is a consequence of the flow of



energy from the soliton to the band states. The rate of this process is strongly influenced by the value of the coupling constant and even at very low temperatures in the strong-coupling limit the soliton may decay rapidly enough. Thus the strength of the coupling constant plays a twofold role: while, on one hand, the formation of the polaron (soliton) demands a strong coupling, on the other hand it also defines (at  $T \neq 0$ ) the strength of the influence of thermal excitations, which has the opposite effect on the soliton's stability. Obviously, stability of the soliton at finite temperatures demands a trade-off between these two tendencies; therefore the ratio  $S$  of the polaron binding energy to the maximum phonon energy should not be very large. This conclusion is supported by some recent results [14] where it was shown that the combined effects of the quantum nature of phonons and adiabaticity leads to a reduction of the admitted values of the coupling constant.

Finally, let us note that the present analysis is carried out in a classical manner and is thus a counterpart of the quantum procedure of Schweitzer [15], who considered the decay of the soliton into exciton states by treating the linearized lattice modes as an interaction which generated such a process. In the region of the parameter space where we expect the applicability of semiclassical methods, we feel that the present analysis is more relevant.

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