Soliton-induced modification of the speed of sound in quasi-one-dimensional molecular crystals

Jasmina Tekić, Zoran Ivić and Željko Pržulj

The 'Vinča' Institute of Nuclear Sciences, Theoretical Physics Department—020, 11001 Belgrade, Serbia, Yugoslavia

Abstract. The influence of the anharmonic vibron–phonon coupling, arising on account of a 'dressing' effect, on the characteristics of the lattice subsystem in quasi-one-dimensional molecular crystals was examined within the 'pseudo-harmonic' phonon approximation. It was found that solitons could induce specific modifications of the speed of sound which shows a temperature dependence quite different to that in the case of the linear excitations. The possibility of an indirect experimental verification of the existence of solitons in molecular chains is suggested on the basis of these predictions.

Investigations of the properties of solitons in molecular crystals, especially those aimed at achieving an understanding of their role in the charge and energy transfer over large distances, have attracted considerable interest for more than twenty years [1–6]. The majority of the studies on the subject are concerned with the soliton formation occurring as a result of a single exciton (a vibrational one (a *vibron*) or an electronic one (a *Frenkel exciton*)) or electron being trapped by the induced local distortion of the host lattice. The possibility of the creation of such excitations was examined within the general theory of self-trapping (ST) phenomena [7, 8] and it was found [9–13] that Davydov's original proposal, i.e. soliton formation due to the single-exciton ST, cannot explain intramolecular vibrational energy transfer in α-helix and acetanilide (ACN). That is, according to the available data [3, 4], the width of the exciton band of these substances (7.9×10^{-23} to 1.55×10^{-22} J) is too small as compared with the maximal phonon frequency ($(18$–$21) \times 10^{-22}$ J) in the nonadiabatic limit, so one should expect the formation of the vibron analogue of Holstein's small polaron [14] rather than a soliton.

Nevertheless, the possibility of soliton creation in such substances cannot be excluded totally. In fact, recent analysis [15], carried out within the framework of the mean-field approximation based upon the variational extension of the Lang–Firsov unitary transform (LFUT) method [16], points to the possibility of soliton formation even in systems characterized by values of physical parameters for which Davydov's original proposal does not apply, i.e. even in the nonadiabatic limit. This, however, demands higher excitation concentrations in the system, where direct or indirect (phonon-mediated) exciton–exciton interaction significantly changes the conditions for soliton existence [15–20]. In this way, a solitonic mechanism for the intramolecular energy transfer in molecular crystals remains a possibility, but the idea should be based on different grounds. That is, as pointed out above, the width of the vibron band is about ten to thirty times smaller than that of the phonon

one, which excludes the possibility of ST as a mechanism of soliton formation. In that case an effective, phonon-induced, vibron–vibron interaction plays the dominant role in soliton creation, where the soliton now represents the bound state of the large number of vibron quanta [15]. The high degree of occupation of the vibron modes, necessary for the creation of such entities, may be achieved due to the excitation of the large number of so-called 'amid-I' quanta. In the case of the application of the soliton model in the explanation of energy transfer in biological systems (α-helix for example), it is usually assumed [1–6] that vibrons are excited on account of the resonant absorption of chemical energy released in the hydrolysis of adenosine triphosphate. Note also that the macroscopic occupation of the vibron modes indicates the applicability of the semiclassical approximation and justifies the selection of the coherent state *ansatz* as the method for making the choice of the trial state of the multi-vibron system (see [15] and references therein).

In our previous paper [15] we did not take into account: (i) possible changes of the phonon spectrum due to the induced phonon–phonon correlations which are the consequence of the anharmonic (in terms of phonon operators) interaction of 'dressed' quasiparticles and 'new' phonons; or (ii) the remaining interaction of the soliton with 'new' phonons. In the present paper we shall focus on the examination of the first of the above-mentioned issues, while the second one, which is interesting in its own right, will be examined separately. Our attention will be mainly concentrated on the soliton-induced modification of the speed of sound. According to the results of the previous analysis [15] these effects should be important in the nonadiabatic limit where the 'dressing' is maximal and where the effective vibron–vibron interaction plays the main role in the soliton formation.

To achieve the above-proposed goal we shall utilize the pseudo-harmonic phonon approximation [21–24]. As presented in this article, such an approach represents a slightly modified version of the previous mean-field method [15]. It consists in a transition from the original Hamiltonian to an equivalent one with renormalized system parameters which should be determined self-consistently using the Bogolyubov theorem [24]. The starting point of our analysis represents the Hamiltonian of a 1-d molecular chain, rewritten, with the help of the LFUT method, in terms of 'dressed' vibrons (polarons) and new phonon operators [15]:

$$H = [\Delta - E_B] \sum_n B_n^+ B_n - J \sum_n (B_n^+ B_{n+1} \Theta_n^+ \Theta_{n+1} + \text{HC})$$
$$- E_B \sum_n [B_n^{+2} B_n^2 + \frac{1}{2}(B_n^+ B_{n+1}^+ B_{n+1} B_n + \text{HC})]$$
$$+ \frac{1}{2} \sum_q \left[\frac{p_q p_{-q}}{M} + M\omega_q^2 u_q u_{-q} \right] \tag{1}$$

where

$$\Theta_n = \exp \left\{ \frac{1}{\sqrt{N}} \sum_q \frac{F_q^*}{\hbar\omega_q} e^{-iqR_0}(a_q - a_{-q}^+) \right\}.$$

The operators B_n^+ (B_n) describe the 'dressed' vibron, Δ is the excitation energy of the nth molecular group and

$$p_q = i\sqrt{\frac{\hbar\omega_q M}{2}}(a_q^+ - a_{-q}) \qquad \text{and} \qquad u_q = \sqrt{\frac{\hbar}{2M\omega_q}}(a_q + a_{-q}^+)$$

represent the Fourier components of the momentum and displacement operators of the molecular groups of the molecular chain (a_q^+ and a_q are the phonon creation and annihilation

operators). The meaning of the remaining parameters is the same as in [15]: J is the intersite dipole–dipole transfer integral, $\omega_q = \omega_B \sin|q R_0/2|$ is the phonon frequency ($\omega_B = 2\sqrt{\kappa/M}$ is the phonon bandwidth while κ and M denote the spring constant and mass of the molecular group respectively),

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

represents the small-polaron binding energy,

$$F_q = 2i\chi \sqrt{\frac{\hbar}{2M\omega_q}} \sin q R_0$$

denotes the exciton–phonon coupling parameter, χ is the vibron–phonon coupling strength, R_0 denotes the lattice spacing and finally $N \gg 1$ is the number of molecular groups in the chain. Here we have corrected the misprints present in the equations (3) and (4) of reference [15] where the vibron–vibron interaction term is half the size that it should be. Please note that this does not affect the results of the previous analysis qualitatively. To be precise, all of the conclusions of the previous paper are valid after the simple substitution of $2\mathcal{N}$ for $\mathcal{N}$ in formulae (17) to (20) ($\mathcal{N}$ represents the total number of vibrons engaged in the soliton formation). The pure phonon part of the above expression is written in terms of p_q and u_q for further mathematical convenience. Since the present analysis concerns the strict nonadiabatic limit where, as mentioned above, phonon–phonon correlations are the most significant, the choice of the maximal value of the dressing fraction $\delta = 1$ in (1) is justified.

The next step of our mean-field approach is the choice of the so-called effective (harmonic in terms of phonon operators) Hamiltonian:

$$
\begin{aligned}
H_{eff} = {}& [\Delta - E_B] \sum_n B_n^+ B_n - J_{eff} \sum_n B_n^+ (B_{n+1} + B_{n-1}) \\
& - E_B \sum_n \left[B_n^{+2} B_n^2 + \frac{1}{2}(B_n^+ B_{n+1}^+ B_{n+1} B_n + \text{HC}) \right] \\
& + \frac{1}{2} \sum_q \left[\frac{p_q p_{-q}}{M} + M\tilde{\omega}_q^2 u_q u_{-q} \right]
\end{aligned}
\tag{2}
$$

where J_{eff} and $\tilde{\omega}_q$ are variational parameters representing the effective dipole–dipole transfer integral of the dressed excitations and the frequency of the so-called pseudo-harmonic phonons, respectively. In accordance with the standard procedure [21–24] they will be determined by minimizing the trial free energy of the system:

$$\mathcal{F}_1 = \mathcal{F}_0 + \langle H - H_{eff} \rangle_0 \tag{3}$$

where $\mathcal{F}_0 = \mathcal{F}_{sol} + \mathcal{F}_{ph}$ represents the free energy of the fully decoupled vibron (soliton)–phonon model, while $\langle \cdots \rangle_0$ denotes averaging over the assembly of the noninteracting vibrons (solitons) and phonons. Therefore we may write

$$
\begin{aligned}
\langle H - H_{eff} \rangle_0 = {}& -\sum_n \left[(J \langle \Theta_n^+ \Theta_{n+1} \rangle_0 - J_{eff}) \langle B_n^+ B_{n+1} \rangle_0 + \text{HC} \right] \\
& + \frac{1}{2} \sum_q M(\omega_q^2 - \tilde{\omega}_q^2) \langle u_q u_{-q} \rangle_0.
\end{aligned}
\tag{4}
$$

The values averaged over the phonon ensemble in (4) are given as $\langle \Theta_n^+ \Theta_{n\pm1} \rangle_0 = e^{-S(T)}$ where

$$S(T) = \frac{2}{N} \sum_q \frac{|F_q|^2}{(\hbar\omega_q)^2} \sin^2 \frac{qR_0}{2} (2\bar{\nu}_q + 1) \equiv \frac{4}{N} \sum_q \frac{|F_q|^2}{(\hbar\omega_q)^2} \sin^2 \frac{qR_0}{2} \frac{M\tilde{\omega}_q}{\hbar} \langle u_q u_{-q} \rangle_0$$

represents the temperature-dependent coupling constant defined in analogy with [9–11,15], while $\bar{\nu}_q = \{e^{\hbar\tilde{\omega}_q/kT} - 1\}^{-1}$ is the 'pseudo-harmonic' phonon average number.

As was shown in [21–24], minimization of the trial free energy over J_{eff} and $\tilde{\omega}_q$ is fully equivalent to its minimization over the correlation functions $\langle B_n^+ B_{n\pm1} \rangle_0$ and $\langle u_q u_{-q} \rangle$, respectively. Thus from $\partial \mathcal{F}_1 / \partial \langle B_n^+ B_{n\pm1} \rangle_0 = 0$ we found $J_{eff} = J e^{-S(T)}$ while $\partial \mathcal{F}_1 / \partial \langle u_q u_{-q} \rangle_0 = 0$ leads to

$$\tilde{\omega}_q^2 = \omega_q^2 - 8J_{eff} \frac{\tilde{\omega}_q}{\hbar} \frac{|F_q|^2}{(\hbar\omega_q)^2} \sin^2 \frac{qR_0}{2} \left[\frac{1}{N} \sum_n \langle B_n^+ (B_{n+1} + B_{n-1}) \rangle_0 \right]. \tag{5}$$

The effective transfer integral, due to its dependence on $\bar{\nu}_q$, is a complicated function of the frequency of the 'pseudo-harmonic' phonons, so the last expression represents a rather complicated self-consistent equation for $\tilde{\omega}_q$ which cannot be found in a closed form. We may find, however, an approximate result obtained after the replacement of all of the $\tilde{\omega}_q$ on the right-hand side of the above equation with the ω_q. This is justified due to the fact that the second term on the right-hand side of the above equation is proportional to the product of the adiabaticity parameter and the coupling constant which is small in the region where we expect solitons to exist. In this way, substituting F_q and ω_q into (5) and using the explicit form of the temperature-independent coupling constant, namely

$$S(0) = \frac{8}{3\pi} \frac{E_B}{\hbar\omega_B}$$

and the adiabaticity parameter, namely

$$B(0) = \frac{8}{3\pi} \frac{2J}{\hbar\omega_B}$$

as defined in [9–11, 15], we found straightforwardly

$$\tilde{\omega}_q^2 = \omega_B^2 \left[1 - 11.1 e^{-S(T)} S(0) B(0) \frac{1}{N} \sum_n \langle B_n (B_{n+1} + B_{n-1}) \rangle_0 \cos^2 \frac{qR_0}{2} \right] \sin^2 \frac{qR_0}{2}. \tag{6}$$

From the above equation we can find the speed of sound as modified by the soliton (vibron)–phonon interaction $c = \lim_{q \to 0} \tilde{\omega}_q / q$:

$$c = c_0 \sqrt{1 - 11.1 e^{-S(T)} S(0) B(0) \frac{1}{N} \sum_n \langle B_n (B_{n+1} + B_{n-1}) \rangle_0} \tag{7}$$

where $c_0 = \omega_B R_0$ denotes the speed of sound in the absence of soliton (exciton)–phonon coupling.

So far we have not specified the type of the excitation of the vibron subsystem, so the above formulae are quite general and could be applied for the examination of both soliton- and vibron-induced changes of the phonon spectrum. The contribution from the particular type of excitation is defined through the explicit form of the static correlation function in equations (6) and (7).

In the spirit of the semiclassical analysis of reference [15], calculation of the soliton input in the above correlation function demands the following procedure. We first simply

replace the vibron operators by their coherent amplitudes β_n. Then we apply the continuum approximation which leads to

$$\sum_n \langle B_n^+(B_{n+1} + B_{n-1})\rangle_0 \rightarrow 2\mathcal{N} - R_0^2 \int_{-\infty}^{\infty} \frac{dx}{R_0} \left\langle \left| \frac{\partial \beta(x)}{\partial x} \right|^2 \right\rangle_0$$

$$= 2\mathcal{N} - \frac{\mathcal{N}^3 E_B^2}{3 J_{eff}^2} - R_0^2 \mathcal{N} \langle k^2 \rangle_0. \tag{8}$$

Here

$$\beta(x, t) = e^{i(kx - \omega t)} \mathcal{N} \left(\frac{\mu}{2} \right)^{1/2} \operatorname{sech} \frac{\mu \mathcal{N}}{R_0}(x - x_0 - vt)$$

represents the soliton solution of the effective Hamiltonian (2). It is normalized as follows:

$$\mathcal{N} = \frac{1}{R_0} \int dx \, |\beta(x, t)|^2.$$

The soliton parameters are defined as follows:

$$k = \frac{m^* v}{\hbar} \qquad \mu = \frac{E_B}{J_{eff}} \qquad \hbar\omega = \Delta - E_B - 2J_{eff} + \frac{m^* v^2}{2} - \frac{\mathcal{N}^2 E_B^2}{J_{eff}}$$

and finally

$$m_s = \mathcal{N} m^* \left[1 + \frac{16 E_B^2 \mathcal{N}^2 R_0^2}{3 c^2 \hbar^2} \right]$$

represents the effective mass of the soliton with

$$m^* = \frac{\hbar^2}{2 J_{eff} R_0^2}$$

being a dressed-vibron effective band mass.

The statistical averages in the above expression will be calculated within the phenomenological approach assuming that solitons behave as an ideal gas of classical particles. This is justified since the soliton in a molecular crystal behaves as a classical particle [15–19] carrying the energy and momentum

$$E_s = \varepsilon_0 + \frac{m_s v^2}{2} \qquad P_s = m_s v \tag{9}$$

where v denotes the soliton velocity while

$$\varepsilon_0 = \mathcal{N}[\Delta - E_B - 2J_{eff}] - \frac{E_B^2 \mathcal{N}^3}{3 J_{eff}}.$$

This concept has been successfully applied in the analysis of the thermodynamics of soliton-bearing systems, in which the appearance of the central peak in the energy spectrum of slow neutrons scattered by some uniaxial ferroelectrics or by quasi 1-d ferromagnets and antiferromagnets [25–30] was quite well explained on the basis of the soliton concept. The further procedure is straightforward and consists of two steps [25–27, 30]: we first assume that only one soliton is excited in the system and then we generalize that result to the case of a system with a finite soliton density. In the presence of the single soliton, the statistical averaging in (8) simply represents an integration over the soliton phase space, i.e. over its position and momentum, with the canonical distribution function

$$\langle \cdots \rangle_{01} = \frac{1}{Z_1} e^{-\varepsilon_0/kT} \int_{-L/2}^{L/2} \int_{-\infty}^{\infty} \frac{dx_0 \, dP_s}{h} \, (\cdots) \exp\left(-\frac{P_s^2}{2 m_s kT} \right) \tag{10}$$

where

$$Z_1 = e^{-\varepsilon_0/kT} \int_{-L/2}^{L/2} \int_{-\infty}^{\infty} \frac{dx_0\, dP_s}{h} \exp\left(-\frac{P_s^2}{2m_s kT}\right) = \frac{L}{h} e^{-\varepsilon_0/kT} \sqrt{2\pi m_s kT}$$

is the canonical ensemble partition function, and $L = N R_0$ and h represent the length of the system and Planck's constant, respectively.

The total contribution arising from many solitons is simply the product of the so-obtained result and the soliton average number

$$\langle N_S \rangle = kT \frac{\partial}{\partial \mu_S} \ln Z.$$

Here Z denotes the grand canonical partition function of the soliton ideal gas: $Z = \exp(Z_1 e^{\mu_s/kT})$ and μ_S denotes the soliton chemical potential.

The thermodynamics of the vibron system should be similar to the thermodynamics of phonons. This means that there is no external constraint on their number, which implies that the vibron chemical potential is equal to zero. Consequently the chemical potential of the multi-vibron soliton ideal gas should also be set equal to zero, and for the soliton mean number we found

$$\langle N_S \rangle = kT \left[\frac{\partial}{\partial \mu_S} \ln Z \right]_{\mu_S=0} \equiv \frac{L}{h} \sqrt{2m_S \pi kT}\, e^{-\varepsilon_0/kT}. \tag{11}$$

In accordance with the above-proposed procedure, the further calculations are straightforward and give

$$c = c_0 \sqrt{1 - 11.1 e^{-S(T)} S(0) B(0) \left(\frac{2N}{N} - \frac{N^3 E_B^2}{3N J_{eff}^2} - \frac{R_0 m^* N kT}{m_s J_{eff}} n_s \right)} \tag{12}$$

where $n_S = \langle N_S \rangle / L$ denotes the soliton density. Let us recall that the present analysis concerns the nonadiabatic regime $(B < 1)$ and that soliton existence demands $S(T) < B(T)/N$ [15]. This implies that the validity of our results is restricted to the weak-coupling limit. Under these circumstances the second term in the brackets in (12) is of the order of

$$\frac{N^3 S^2}{3 B^2} \approx \frac{\alpha^2 N}{3}$$

(α is a numerical factor less than unity due to the above-mentioned condition for soliton existence) and can therefore be disregarded as compared with the first term. The third term may be approximated as

$$\frac{1}{1 + 16 S^2 N^2 / 3} \frac{kT}{J} n_S \approx \frac{kT}{J} n_S$$

and could play a significant role for higher temperatures $(kT/J \sim 27$ for α-helix at 300 K [3–5, 9–13]). This, however, depends on the value of the soliton density, which is determined by the value of the parameter ε_0 playing the role of the soliton creation (excitation) energy. In the region where one should expect soliton existence, it may be approximated as $\varepsilon_0 \approx N[\Delta - 2J - E_B - N E_B/3]$. The dominant terms in this expression are the first and the last ones, whose balance determines the magnitude of the soliton density and consequently determines the character of the temperature dependence of the above-predicted modifications of the speed of sound. For the particular values of the physical parameters, characterizing α-helix and ACN, Δ greatly exceeds the other energy parameters of the system (see reference [9], for example), so the soliton density is negligible and changes of the speed of sound are temperature independent. To estimate the possible degree of these changes we may use, for

these substances, the following approximate result: $c = c_0\sqrt{1 - 22.2\alpha B^2/N}$. Specifying $\alpha = 0.5$, $B = 0.65$ and choosing $N = 25$ to 200 sites, which are the values typically used in numerical calculations [3–5], we obtain that c may be reduced by up to 10%. In the systems where the soliton excitation energy is not so high, the presence of the solitons in molecular chains may induce specific modifications of the speed of sound. At low temperatures ($J \ll kT$) they reduce it with respect to that in the absence of the coupling with the vibron subsystem (c_0). With the rise of temperature it should tend to c_0, and above some critical temperature, which can be estimated roughly as $T \sim (2\mathcal{N}J/k)n_s$, it exceeds c_0.

The above-predicted behaviour of the speed of sound as influenced by solitons is quite different from that arising from the 'dressed' vibrons exclusively. That is, expanding the operators B_n in Fourier series we easily obtain

$$\frac{1}{N}\sum_n \langle B_n^+(B_{n+1} + B_{n-1})\rangle_0 = \frac{2}{N}\sum_K \langle n_K\rangle \cos K R_0$$

where $\langle n_K\rangle = \{e^{\varepsilon_K/kT} - 1\}^{-1}$ is the vibron average number and $\varepsilon_K = \Delta - 2J_{eff}\cos K R_0$ is its energy. From this expression it follows that, like solitons, linear modes may also cause a reduction of the speed of sound while, unlike in the previous case, increasing of the temperature leads to an additional reduction of the speed of sound.

These results are analogous to those of reference [31], where we predicted characteristic behaviour of the speed of sound in quasi-one-dimensional ferromagnets depending on the type of the excitation of the magnetic subsystem: solitons or magnons. Thus, like in that case, here there arises the interesting possibility of an indirect experimental examination of solitons in molecular crystals based upon the above-predicted temperature dependence of the speed of the sound, which should show quite different behaviour for different types of the excitation of the vibron subsystem. Relevant experiments should be Brillouin scattering, ultrasonic propagation and Young modulus measurements, analogous to those used in the investigation of the large elastic softening induced by spin–phonon interaction [32–34].

Acknowledgments

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