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Polaron-like features of the domain wall in a classical Ising chain with transverse field

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Abstract. The possibility of the creation of the bound state of a domain wall and surrounding lattice distortion was investigated in the framework of the one-dimensional Ising model with transverse field. It was found that the existence of such an entity is very sensitive to the mutual ratio of the basic physical parameters of the system. We obtain that, in the weak-coupling regime, such a 'dressed' excitation can arise in the so-called unadiabatic limit when the maximal phonon energy greatly exceeds the nearest-neighbour exchange energy. In that case, the 'dressing' effect can significantly modify domain-wall properties, causing the increase of its effective mass and lowering of the ground-state energy, while the domain-wall velocity cannot exceed the speed of sound.

1. Introduction

In a recent paper [1], hereafter called I, we have studied the dynamics of kink-like domain-wall (DW) excitations in the one-dimensional (1D) Ising chain (model) with transverse field (IMTF) within a vibrating three-dimensional (3D) crystal lattice. It was found that the dynamics of a DW has the character of Brownian motion arising as a consequence of the emission and absorption of acoustic phonons. These processes appear when the DW velocity (v) exceeds the phase speed of sound, i.e. when $v \geq \omega_q/q$, thus revealing typical Cherenkov character. These predictions could be relevant for the whole class of real substances where 1D magnetic, ferroelectric or other highly anharmonic (structurally unstable) subsystems exist within 3D crystal lattices. As an example, let us mention ferromagnetic $\text{CoCl}_2 \cdot 2\text{NC}_5\text{H}_5$, which consists of widely separated $-\text{CoCl}_2-$ chains embedded into a monoclinic crystal lattice, where each magnetic atom (Co) is surrounded by four Cl and two N atoms [2]. In such non-magnetic surroundings, the ratio of interchain (J') to intrachain (J) magnetic interaction is very small, being of the order of 10^{-2} [2, 3]. Therefore, although the real structure is 3D (monoclinic), considering the magnetic properties only, the system behaves as a collection of weakly coupled, practically non-interacting, ferromagnetic chains. Furthermore, this system shows pronounced Ising behaviour, as confirmed by the measurements of magnetic specific heat and magnetic susceptibility, which agree with exact solutions of the ferromagnetic Ising chain [2]. When exposed to a magnetic field orthogonal to the magnetization direction, the system can serve as an example of an IMTF. The whole family of 1D ferromagnets that belong to the series of isomorphous transition halides $\text{AMB}_3 \cdot 2\text{aq}$ ($\text{A}=\text{Cs, Rb}$; $\text{M}=\text{Mn, Co, Fe}$; $\text{B}=\text{Cl, Br}$; and $\text{aq}=\text{H}_2\text{O}$ or D_2O) [3], and uniaxial ferroelectric materials (CsH_2PO_4 and $\text{Pb}_5\text{Ge}_3\text{O}_{11}$, for example) [4, 5] also belong to the class of realistic systems in which 1D Ising-like subsystems exist within a 3D crystal lattice.

We have based our previous analysis [1] on the assumption of the weakness of the spin(pseudospin)–phonon interaction. Such an assumption enables one to utilize the collective coordinate method, which consists of treating kink momentum and position as a pair of canonically conjugated variables [1]. In such a way we have derived an effective Lagrangian and Hamiltonian of the kink–phonon system where the kink subsystem is represented in terms of its canonical variables: position $\xi(t)$ and momentum $p_{DW}(t)$. The resulting effective Hamiltonian of the system greatly resembles the polaron one provided that in this case our ‘polaron’ variables $\xi(t)$ and $p_{DW}(t)$ are purely classical. This correspondence with the polaron problem is not merely formal, since, in principle, a soliton in a deformable medium can cause a local distortion of the surrounding lattice which can follow its motion instantaneously. As a consequence of such an essentially polaronic effect, one could expect possibly significant modification of DW parameters, especially its effective mass and ground-state (GS) energy. The degree of these changes depends on the values of basic physical parameters of the system. The weakness of spin(pseudospin)–phonon coupling allowed us to neglect such possibilities in our previous paper [1]. However, it is not always justified; thence in the present paper we wish to investigate the influence of the phonon dressing (polaronic effect) on DW properties. In particular, special attention is paid to the analysis of the degree of modification of DW effective mass and energy due to kink–phonon coupling. As a starting point of our analysis we shall use the ‘non-relativistic’ limit of the effective kink–phonon Hamiltonian introduced in I (see equation (17) therein):

$$H_{\text{eff}} = \Delta E + \frac{1}{\sqrt{N}} \sum_q G_q \exp(iq \cdot \xi) (b_q + b_{-q}^\dagger) + \sum_q \hbar \omega_q b_q^\dagger b_q. \quad (1.1)$$

Here we have avoided the detailed derivation procedure of the above Hamiltonian, which is presented in I. Thus we quote only a few basic remarks concerning the parameters of the model. First, we recall that in the so-called critical regime (or ‘displacive’ regime, as it is customarily named in dynamics of highly anharmonic structurally unstable crystals) when $\lambda = J/2\Omega \geq \lambda_c$ ($\lambda_c = 1/2$), the DW excitation is represented by the kink-like profile [6]

$$S_z(x, t) = \frac{1}{2} S_z^0 \tanh[(\gamma/R_0)(x - x_0 - vt)/2] \quad (1.2)$$

where its amplitude and inverse width are, respectively, defined by

$$S_z^0 \simeq 2(\lambda - \lambda_c)^{1/2} \quad \gamma/R_0 \simeq (2\sqrt{2}/R_0)[(\lambda - \lambda_c)/(1 - \beta^2)]^{1/2}. \quad (1.3)$$

Here $\beta = v/v_0$, $v_0 = \Omega R_0/\hbar\sqrt{2}$ is the limiting DW velocity, R_0 is the lattice constant of the Ising chain; the transverse (actual magnetic or effective tunnelling-like) field Ω is smaller than the value of the longitudinal (nearest-neighbour) intrachain coupling J , so the ordering (spontaneous polarization in S_z) can occur only if $\Omega \leq J$ ($\lambda \geq \lambda_c$) [7]. The corresponding energy of the single DW relative to the GS in (1.1) is defined by the expression [6]

$$\Delta E = (J/6\sqrt{2})(S_z^0)^3/(1 - \beta^2)^{1/2}. \quad (1.4)$$

Here, with respect to [1] and [6], a wrong numerical factor inessential for further analysis has been corrected. Namely the DW energy (1.4), which was obtained after direct substitution of kink solution (1.2) into the definition of the energy of a DW (equation (2.14) in [1]), is three times lower than the corresponding expression in [1] and [6] (i.e. equations (10) and (2.24) in [6] and [1], respectively). The numerical discrepancy is probably the consequence

of the qualitative character of the limiting value used in [6]. The interaction term in (1.1) is characterized by an effective kink-phonon coupling parameter $G_q = [f_1(\mathbf{q}) + f_2(\mathbf{q})]F_q$ with $f_1(\mathbf{q})$ and $f_2(\mathbf{q})$ being DW form factors defined in I:

$$f_1(\mathbf{q}) = \frac{(S_z^0)^2}{\gamma^2} \frac{\pi(\mathbf{q} \cdot \mathbf{R}_0)}{\sinh[\pi(\mathbf{q} \cdot \mathbf{R}_0)/\gamma]} \quad (1.5)$$

$$f_2(\mathbf{q}) = \frac{(S_z^0)^2 \gamma^2}{12} \frac{\pi(\mathbf{q} \cdot \mathbf{R}_0)[1 + \pi(\mathbf{q} \cdot \mathbf{R}_0)/\gamma]\{4 + [\pi(\mathbf{q} \cdot \mathbf{R}_0)/\gamma]^2\}}{\gamma^2 \sinh[\pi(\mathbf{q} \cdot \mathbf{R}_0)/\gamma]}$$

$$F_q = \alpha \left(\frac{\hbar}{2M\omega_q^2} \right)^{1/2} [\exp(i\mathbf{q} \cdot \mathbf{R}_0) - 1] \frac{\mathbf{e}_q \cdot \mathbf{R}_0}{|\mathbf{e}_q||\mathbf{R}_0|} \quad (1.6)$$

denotes the Fourier component of the original spin(pseudospin)-phonon interaction induced by the coupling strength $\alpha = (\partial J/\partial x)_{x=x_0}$, M is the mass of each magnetic (or ferroelectrically active) ion and \mathbf{e}_q is the polarization vector of longitudinal acoustic phonons with frequency ω_q ($\mathbf{e}_q = \mathbf{q}/|q|$). The last term in (1.1) is the pure phonon Hamiltonian in standard form. The effective Hamiltonian (1.1) was derived under the assumption that weak spin-phonon interaction does not change the character of soliton solution (1.2), causing only a slight modification of its parameters. Therefore our analysis of the influence of phonon dressing on DW properties will be restricted to the so-called intermediate- and weak-coupling limit. For that purpose we shall utilize the method of Lee, Low and Pines (LLP) [8]. Our approach to the spin-phonon coupling is quite different from that of Uchiyama *et al* [9], Tsang *et al* [10] and Zvezdin and Popkov [11]. They considered the coexistence and simultaneous propagation of magnetic and lattice solitons in order to explain anomalies in DW velocity (v) versus applied magnetic field (H) dependence, arising when DW velocity approaches the speed of sound. In the above-mentioned papers these anomalies, which were experimentally observed in orthoferrite-type ferromagnets YFeO_3 and TmFe_2O_3 [12-14], have been attributed to the enormous growth of the magnitude of lattice distortion (i.e. lattice soliton amplitude) occurring when the DW velocity tends to that of sound—longitudinal (c_{\parallel}) or transverse (c_{\perp}). On the other hand, in the series of papers by Bar'yakhtar and Ivanov with co-workers [15-17] the same effect was ascribed to the DW damping due to Cherenkov-like radiation of acoustic waves arising when the DW velocity in the rigid lattice exceeds the phase speed of sound (i.e. $v \geq \omega_q/q$). Their theory lies upon the assumption of weak spin-phonon coupling, which allows a perturbative treatment, thus disregarding the relevance of DW 'dressing' for the understanding of magnetoelastic anomalies. So we encounter the situation where the same experimentally observed effect has been assigned to two different, mutually opposite, types of phonon-field behaviour. The first concept [9-11] assumes the classical nature of phonons, predicting common propagation of lattice and spin (magnetic) solitons. On the other hand, the second concept presumes the purely quantum nature of the phonon field and propagation of the DW in a *rigid* lattice. The reason why we point out this controversy here is not to criticize any of these approaches but rather to illustrate, by this particular example, the necessity of determining the circumstances when 'dressing' (polaronic effect) should prevail with respect to the case when it can be neglected.

In the present paper we shall analyse the possibility of the creation of a 'dressed' kink (i.e. a kink surrounded by a cloud of virtual phonons) in the IMTF within a vibrating 3D lattice. Although confined to this particular model, we expect that our analysis, in principle, could also be relevant for a much wider class of materials including the above-mentioned examples of orthoferrite-type ferromagnets. Namely, in most materials with domain structure possessing weak magnetoelastic coupling, it is possible to obtain an

effective kink-phonon Hamiltonian similar to (1.1) with slightly modified parameters. Thus one can make the assertion that an analogous procedure can be carried out in those cases too.

2. Modification of domain-wall parameters due to polaronic effect

In order to examine the influence of phonon dressing on DW characteristics, we shall start with a 'non-relativistic' ($v \ll v_0$) version of the effective kink-phonon Hamiltonian

$$H_{\text{eff}} = E_0 + \frac{p_{\text{DW}}^2}{2m} + \frac{1}{\sqrt{N}} \sum_q G_q \exp(iq \cdot \xi) (b_q + b_{-q}^+) + \sum_q \hbar \omega_q b_q^+ b_q \quad (2.1)$$

where $E_0 = J(S_z^0)^3/6\sqrt{2}$ is the DW rest energy while N is the total number of lattice sites.

In accordance with such an approximation and henceforth adopting the continuum limit ($q \cdot R_0 \rightarrow 0$), for the convenience of further calculations we simply substitute the reduced parameters, $\gamma_0/R_0 \simeq 2\sqrt{2}(\lambda - \lambda_c)/R_0$, $f_1 \simeq (S_z^0)^2/\gamma_0$ and $f_2 \simeq (S_z^0)^2\gamma_0/3$, corresponding to an immobile soliton (DW) of mass $m = 2\hbar(S_z^0)^3/6JR_0^2$ [1, 6]. The index '0' herein indicates the limit $\beta \rightarrow 0$.

There are three basic physical parameters determining the energy spectrum of the kink-phonon system and consequently they also determine the degree of 'dressing' of the DW by the cloud of virtual phonons. The parameters are: nearest-neighbour exchange energy J , maximal phonon frequency (width of phonon band) ω_D and finally the so-called lattice relaxation energy $E_D = (1/N) \sum_q |G_q|^2/\hbar\omega_q$ representing the lowering of the GS energy of the system in the transportless limit ($J \rightarrow 0$ or $m \rightarrow \infty$) [18], when Hamiltonian (2.1) can be exactly diagonalized by appropriate unitary transformation [19]. E_D can be calculated easily using the well known rule for calculating the sums over the phonon quasimomenta

$$\frac{1}{N} \sum_q \dots = \begin{cases} \frac{3}{2q_D^3} \int_0^{q_D} q^2 dq \int_0^\pi \sin \theta d\theta & \text{for isotropic phonon spectrum:} \\ \omega_q = c_0|q| & \\ \frac{1}{q_{\parallel}^D (q_{\perp}^D)^2} \int_{-q_{\parallel}^D}^{q_{\parallel}^D} dq_{\parallel} \int_0^{q_{\perp}^D} q_{\perp} dq_{\perp} & \text{for anisotropic phonon spectrum:} \\ \omega_q = (c_{\parallel}^2 q_{\parallel}^2 + c_{\perp}^2 q_{\perp}^2)^{1/2}. & \end{cases} \quad (2.2)$$

Here c_0 , c_{\parallel} and c_{\perp} are average, longitudinal and transverse speeds of sound, respectively, while index D is associated with Debye's momentum. The limiting wavenumbers q_{\parallel}^D and q_{\perp}^D can be approximated by π/R_0 and π/R_{\perp} respectively, where R_{\perp} is the interchain distance. Explicit calculation gives the following results:

$$E_D = \frac{1}{3} E_D^{(0)} \quad (2.3a)$$

for the isotropic phonon spectrum and

$$E_D = \frac{E_D^{(0)}}{(1 - c_{\parallel}^2/c_{\perp}^2)(q_{\perp}^D)^2 q_{\parallel}^D} \left\{ \frac{(q_{\parallel}^D)^3}{3} \ln \left(\frac{1 + (q_{\perp}^D/q_{\parallel}^D)^2}{1 + (c_{\perp} q_{\perp}^D/c_{\parallel} q_{\parallel}^D)^2} \right) + \frac{2}{3} (q_{\perp}^D)^2 q_{\parallel}^D \left(1 - \frac{c_{\perp}^2}{c_{\parallel}^2} \right) \right. \\ \left. - \frac{2}{3} (q_{\perp}^D)^3 \left[\tan^{-1} \left(\frac{q_{\parallel}^D}{q_{\perp}^D} \right) - \frac{c_{\perp}^3}{c_{\parallel}^3} \tan^{-1} \left(\frac{c_{\parallel} q_{\parallel}^D}{c_{\perp} q_{\perp}^D} \right) \right] \right\} \quad (2.3b)$$

for the anisotropic phonon spectrum.

In the high-anisotropy limit, $q_{\parallel}^D \gg q_{\perp}^D$, and $c_{\parallel} \gg c_{\perp}$, one finds

$$E_D \simeq E_D^{(0)} \left[1 - \pi \frac{q_{\perp}^D}{q_{\parallel}^D} \frac{1 - c_{\perp}^3/c_{\parallel}^3}{1 - c_{\perp}^2/c_{\parallel}^2} + \left(\frac{q_{\perp}^D}{q_{\parallel}^D} \right) \left(\frac{1}{2} + \frac{c_{\perp}}{c_{\parallel}} \right) \right] \quad (2.4)$$

where terms proportional to the powers of $q_{\perp}^D/q_{\parallel}^D$ represent the corrections to the pure 1D result. Here $E_D^{(0)} = \alpha^2 R_0^2 (f_1 + f_2)^2 / 2M c_0^2$ ($c_0 \rightarrow c_{\parallel}$ for anisotropic phonons) defines the lattice deformation energy for the fully 3D or 1D system.

To evaluate the impact of 'dressing' on DW parameters, we use the LLP method. We first exploit the fact that the total momentum of the system

$$P = p_{DW} + \sum_q \hbar q b_q^+ b_q \quad (2.5)$$

is the constant of motion. So we perform the canonical transformation

$$\xi' = \xi \quad p_{DW} = P - \sum_q \hbar q b_q^+ b_q \quad (2.6)$$

and then following the LLP method we eliminate the kink position $\xi(t)$ by the unitary transformation

$$U_1 = \exp \left(i \sum_q \xi \cdot q b_q^+ b_q \right) \quad (2.7)$$

so we obtain transformed Hamiltonian

$$\bar{H} = U_1^+ H U_1 = E_0 + \frac{(P - \hbar \sum_q q b_q^+ b_q)^2}{2m} + \frac{1}{\sqrt{N}} \sum_q G_q (b_q + b_{-q}^+) + \sum_q \hbar \omega_q b_q^+ b_q \quad (2.8)$$

After the second unitary transformation

$$U_2 = \exp \left(\sum_q \beta_q b_q^+ - \beta_q^* b_q \right) \quad (2.9)$$

we find the new transformed Hamiltonian consisting of two parts

$$H_{\text{new}} = H_0 + H_1 \quad (2.10)$$

where H_0 and H_1 are defined as follows:

$$\begin{aligned} H_0 = E_0 &+ \frac{(P - \hbar \sum_q q b_q^+ b_q)^2}{2m} + \frac{1}{\sqrt{N}} \sum_q G_q (\beta_q + \beta_{-q}^*) + \sum_q \hbar \omega_q b_q^+ b_q \\ &+ \frac{\hbar^2}{2m} \left(\sum_q q |\beta_q|^2 \right)^2 + \frac{\hbar^2}{2m} \sum_{q, q'} q \cdot q' b_q^+ b_q |\beta_{q'}|^2 \\ &+ \sum_q |\beta_q|^2 \left(\hbar \omega_q - \frac{\hbar q \cdot P}{m} + \frac{\hbar^2 q^2}{2m} \right) \\ &+ \sum_q \left\{ b_q^+ \left[\frac{G_q^*}{\sqrt{N}} + \beta_q \left(\hbar \omega_q - \frac{\hbar q \cdot P}{m} + \frac{\hbar^2 q^2}{2m} \right) \right. \right. \\ &\left. \left. + \frac{\hbar^2}{2m} \sum_{q'} q \cdot q' |\beta_{q'}|^2 \right] \right\} + \text{HC} \end{aligned} \quad (2.11)$$

and

$$H_1 = \frac{\hbar^2}{2m} \sum_{q,q'} \mathbf{q} \cdot \mathbf{q}' [\beta_q^* \beta_{q'}^* b_q b_{q'} + \text{HC} + 2\beta_q \beta_{q'}^* b_q^+ b_{q'}] + \frac{\hbar^2}{m} \sum_{q,q'} \mathbf{q} \cdot \mathbf{q}' (b_q^+ b_q b_{q'} \beta_{q'}^* + \text{HC}). \quad (2.12)$$

Here β_q is a variational parameter determined by the minimization of GS energy, $E_{\text{GS}} = \langle 0 |_{\text{ph}} H_{\text{new}} | 0 \rangle_{\text{ph}}$:

$$\beta_q = -\frac{1}{\sqrt{N}} G_q^* / \left(\hbar\omega_q - \frac{\hbar\mathbf{q} \cdot \mathbf{P}}{m} + \frac{\hbar^2 q^2}{2m} + \frac{\hbar^2}{2m} \sum_q \mathbf{q} \cdot \mathbf{q}' |\beta_{q'}|^2 \right). \quad (2.13)$$

The total momentum \mathbf{P} of the system, being the constant of motion, should be considered as a classical variable. It defines the only preferred direction in the problem, therefore $\hbar \sum_q \mathbf{q} |\beta_q|^2$ can only differ from \mathbf{P} by a scalar factor. Thus we can write:

$$\hbar \sum_q \mathbf{q} |\beta_q|^2 = \eta \mathbf{P}. \quad (2.14)$$

The scalar parameter η can be determined self-consistently from the relation

$$\eta \mathbf{P} = \frac{1}{N} \sum_q \frac{\hbar \mathbf{q} |G_q|^2}{[\hbar\omega_q + \hbar^2 q^2 / (2m) - \hbar \mathbf{q} \cdot \mathbf{P} (1 - \eta) / m]^2} \quad (2.15)$$

which follows from (2.13) and (2.14). We can now substitute β_q into E_{GS} to obtain the energy of the 'dressed' DW:

$$E(\mathbf{P}) = E_0 + \frac{P^2}{2m} (1 - \eta^2) - \frac{1}{N} \sum_q \frac{|G_q|^2}{\hbar\omega_q + \hbar^2 q^2 / (2m) - \hbar \mathbf{q} \cdot \mathbf{P} (1 - \eta) / m}. \quad (2.16)$$

According to this relation the kink velocity reads

$$\begin{aligned} \mathbf{v} &= (1/m) \nabla_{\mathbf{P}} E(\mathbf{P}) \equiv (\mathbf{P}/m) (1 - \eta) \\ \nabla_{\mathbf{P}} &= \mathbf{e}_x \frac{\partial}{\partial P_x} + \mathbf{e}_y \frac{\partial}{\partial P_y} + \mathbf{e}_z \frac{\partial}{\partial P_z}. \end{aligned} \quad (2.17)$$

Writing the kink momentum as $\mathbf{P} = m^* \mathbf{v}$ we see that the effective mass of a 'dressed' kink takes the form

$$m^* = m / (1 - \eta). \quad (2.18)$$

Further evaluation of both kink effective mass and energy becomes a rather technical problem since it is reduced to the calculation of sums over the phonon quasimomenta in (2.15) and (2.11). Transforming the summation to an integration in accordance with the above-adopted rule (2.2) we have

$$E(\mathbf{P}) = E_0 + (P^2/2m)(1 - \eta^2) - E_{\text{D}}^{(0)} J(\mathbf{v}) \quad (2.19)$$

and

$$\eta|P| = E_0^{(0)} \frac{\partial}{\partial v} J(v) \quad (2.20)$$

where $v = |v|$, while the integral

$$J(v) = \frac{3}{2q_D^3} \int_0^{q_D} q^2 dq \int_{-1}^1 \frac{\mu^4 d\mu}{1 + b(q/q_D) - (v/c)\mu} \quad (\mu = \cos\theta) \quad (2.21)$$

stands for the case of the isotropic phonon spectrum. Parameter $b = \hbar q_D / 2mc_0$ plays the role of the so-called 'adiabatic parameter' known from the polaron theories [20]. For anisotropic phonons $J(v)$ is given by

$$J(v) = \frac{1}{q_{\parallel}^D (q_{\perp}^D)^2} \int_0^{q_{\perp}^D} q_{\perp} dq_{\perp} \int_{-q_{\parallel}^D}^{q_{\parallel}^D} \frac{c_{\parallel}^2 q_{\parallel}^4 dq_{\parallel}}{(q_{\parallel}^2 + q_{\perp}^2)[\omega_q - q_{\parallel}v + (\hbar^2/2m)(q_{\parallel}^2 + q_{\perp}^2)]\omega_q} \quad (2.22)$$

For isotropic phonons, the calculation is straightforward, and after a long and rather tedious procedure one obtains

$$\begin{aligned} J(v) = & \frac{3}{10} \left(\frac{1}{b} - \frac{2}{b^2} \right) + \frac{3}{b^3} \left[\left(\frac{c_0}{v} \right)^5 \sum_{k=0}^4 \sum_{l=0}^2 b^l (1+b)^k \binom{2}{l} \binom{4}{l} \right. \\ & \times \left(\frac{(1+v/c_0+b)^{7-l-k} \ln(1+v/c_0+b) - (1-v/c_0+b)^{7-l-k} \ln(1-v/c_0+b)}{7-l-k} \right. \\ & \left. - \frac{(1+v/c_0+b)^{7-l-k} - (1-v/c_0+b)^{7-l-k}}{(7-l-k)^2} \right) - 4 \left(\frac{c_0}{v} \right)^5 \ln \left(\frac{1+v/c_0}{1-v/c_0} \right) \\ & - 2 \left(\frac{c_0}{v} \right)^4 \frac{1}{1-v^2/c_0^2} + \left(\frac{c_0}{v} \right)^4 \\ & \left. \times \sum_{k=2}^4 (-1)^k \binom{4}{l} \frac{(1+v/c_0)^{k-1} - (1-v/c_0)^{k-1}}{k+1} \right]. \quad (2.23) \end{aligned}$$

From this expression it is readily seen that kink velocity cannot exceed the speed of sound, since, in accordance with (2.19), the DW energy becomes singular when v approaches c_0 . For a slow DW one can expand the above expression (2.23) in powers of small v/c_0 to put it in the form

$$J(v) \simeq \frac{3}{10} \left(\frac{1}{b} - \frac{2}{b^2} + \frac{2}{b^3} \ln(1+b) \right) + \frac{3v^2}{7c_0^2 b^3} \left(\ln(1+b) - \frac{3b^2 + 2b}{2(1+b)^2} \right). \quad (2.24)$$

For anisotropic phonons $J(v)$ can be calculated only approximately. After some simple manipulations we can rewrite (2.22) in a form that is more appropriate for practical calculation:

$$\begin{aligned} J(v) = & \frac{2c_{\parallel}^2}{q_{\parallel}^D (q_{\perp}^D)^2} \int_0^{q_{\perp}^D} q_{\perp} dq_{\perp} \int_0^{q_{\parallel}^D} q_{\parallel}^4 dq_{\parallel} \left(\frac{1}{q_{\parallel}^2 + q_{\perp}^2} - \frac{\hbar/m}{\omega_q + (\hbar/2m)(q_{\parallel}^2 + q_{\perp}^2)} \right) \frac{1}{\omega_q^2 - q_{\parallel}^2 v^2} \\ & + \frac{c_{\parallel}^2}{(q_{\perp}^D)^2 q_{\parallel}^D} \int_0^{q_{\perp}^D} q_{\perp} dq_{\perp} \\ & \times \int_0^{q_{\parallel}^D} \frac{\hbar}{2m} \frac{q_{\parallel}^4 dq_{\parallel}}{[\omega_q + (\hbar/2m)(q_{\parallel}^2 + q_{\perp}^2)][\omega_q - q_{\parallel}v + (\hbar/2m)(q_{\parallel}^2 + q_{\perp}^2)]}. \quad (2.25) \end{aligned}$$

These integrals can be calculated in the high-anisotropy limit:

$$J(v) \simeq \frac{1}{b} \ln(1+b) \left(\frac{1}{1 - (v^2 + c_{\perp}^2)/c_{\parallel}^2} - \frac{v^2/c_{\parallel}^2}{1 - v^2/c_{\parallel}^2} \right) + \frac{v^2/c_{\parallel}^2}{1 - v^2/c_{\parallel}^2} \frac{1}{2b} \left(1 - \frac{1}{(1+b)^2} \right) - \frac{1}{1 - (v^2 + c_{\perp}^2)/c_{\parallel}^2} \times \left[\frac{\pi}{3} \frac{q_{\perp}^D}{q_{\parallel}^D} \left(1 - \frac{c_{\perp}^3}{c_{\parallel}^3(1 - v^2/c_{\parallel}^2)^{3/2}} \right) + \left(\frac{q_{\perp}^D}{q_{\parallel}^D} \right) \left(1 - \frac{c_{\perp}^4/c_{\parallel}^4}{1 - v^2/c_{\parallel}^2} \right) \right] \quad (2.26)$$

where now $b = \hbar q_{\parallel}^D / 2mc_{\parallel}$.

With the help of these results we can find the energy of the slowly moving dressed DW

$$E(P) = E_0 - \delta E + P^2/2m^* \quad (2.27)$$

which is valid for both types of phonon spectrum we have analysed here. δE denotes the lowering of the kink energy caused by the polaronic effect. It is given by the following expressions:

(i) Isotropic phonons

$$\delta E = \hbar\omega_D S \frac{3}{10} \left(\frac{1}{b} - \frac{2}{b^2} + \frac{2}{b^3} \ln(1+b) \right) \quad (2.28)$$

$$\eta = \frac{A}{1+A} \quad A = \frac{6E_D^{(0)}}{7mc_{\parallel}^2 b^3} \left(\ln(1+b) - \frac{3b^2 + 2b}{(1+b)^2} \right)$$

where $S = E_D/\hbar\omega_D$ is the kink-phonon coupling constant as usually defined in the context of the polaron problem [20].

(ii) Anisotropic phonons

$$\delta E = \hbar\omega_D S \left[\frac{1}{b} \ln(1+b) - \frac{\pi}{3} \frac{q_{\perp}^D}{q_{\parallel}^D} \left(1 - \frac{c_{\perp}^3}{c_{\parallel}^3} \right) - \left(\frac{q_{\perp}^D}{q_{\parallel}^D} \right)^2 \left(1 - \frac{c_{\perp}^4}{c_{\parallel}^4} \right) \right]$$

$$\eta = \frac{A'}{1+A'}$$

$$A' = \frac{2E_D^{(0)}}{mc_{\parallel}^2} \left[\frac{1}{b} \ln(1+b) \left(1 - \frac{1}{(1+b)^2} \right) + \frac{c_{\perp}^2}{c_{\parallel}^2} \frac{1}{b} \ln(1+b) - \frac{\pi}{3} \frac{q_{\perp}^D}{q_{\parallel}^D} \left(1 - \frac{c_{\perp}^3}{c_{\parallel}^3} \right) - \left(\frac{q_{\perp}^D}{q_{\parallel}^D} \right)^2 \left(1 - \frac{c_{\perp}^2}{c_{\parallel}^2} \right) \right]. \quad (2.29)$$

The degree of dressing is determined by the mean number of virtual phonons \bar{v} ($\bar{v} = \sum_q |\beta_q|^2$) involved in the formation of lattice distortion. Using a similar procedure as for calculation of δE and η for isotropic and anisotropic phonons we find respectively:

$$\bar{v} = \frac{3S}{4} \left(\frac{c_0}{v} \right)^5 \left[6 \frac{v}{c_0} + \frac{2v^3}{3c_0^3} - 4 \ln \left(\frac{1+v/c}{1-v/c} \right) + 2 \frac{v/c_0}{1-v^2/c_0^2} \right] - 2Sb \left(\frac{c_0}{v} \right)^5 \left[\frac{v/c_0}{(1-v^2/c_0^2)^2} - \frac{4v/c_0}{1-v^2/c_0^2} + 3 \ln \left(\frac{1+v/c_0}{1-v/c_0} \right) - 3 \frac{v}{c_0} \right] \quad (2.30)$$

and

$$\bar{v} = \frac{S}{2} \frac{1 + v^2/c_{\parallel}^2}{1 - v^2/c_{\parallel}^2} \left\{ 1 - \frac{1}{2} \left(\frac{q_{\perp}^D}{q_{\parallel}^D} \right)^2 \left(1 + \frac{c_{\perp}^2}{c_{\parallel}^2} \right) - \frac{Sb(1 + 2v^2/c_{\parallel}^2)}{1 - v^2/c_{\parallel}^2} \right. \\ \left. \times \left[1 - \frac{\pi}{3} \frac{q_{\perp}^D}{q^D} \left(1 + \frac{c_{\perp}}{c_{\parallel}} + \frac{c_{\perp}^2}{c_{\parallel}^2} \right) - \frac{1}{2} \left(\frac{q_{\perp}^D}{q_{\parallel}^D} \right)^2 \left(1 + \frac{v^2}{c_{\parallel}^2} \right) \right] \right\}. \quad (2.31)$$

The above results show that DW dressing in a weak-coupling limit is the most significant in the non-adiabatic regime ($b \ll 1$). In that case modifications of kink parameters as well as the number of virtual phonons approach their maximal values, while the ‘dressing’ effect vanishes in the adiabatic regime ($b \gg 1$).

However, it does not mean that phonon ‘dressing’ does not affect DW at all in that regime. Quite on the contrary it only reflects the inadequacy of the present ‘weak-coupling’ approach in the adiabatic limit when the phonon subsystem can be regarded as a classical one.

3. Range of validity

Having in mind the approximate character of the variational treatment discussed above, we need to try to estimate the range of validity of our results. It is of particular interest to compare the present results with those obtained in I. Namely, since in both cases we have assumed the weakness of the kink–phonon interaction, in the sense that it does not change the character of soliton solutions, it is necessary to determine whether the DW behaves as a ‘dressed’ entity rather than a bare one.

Writing the effective kink–phonon Hamiltonian (2.1) in the dimensionless form

$$\frac{H}{\hbar\omega_D} = \frac{E_0}{\hbar\omega_D} + b\tilde{P}^2 + \frac{\sqrt{S}}{\sqrt{N}} \sum_{\mathbf{Q}} i\sqrt{|\mathbf{Q}|} \frac{\mathbf{e}_{\mathbf{Q}} \cdot \mathbf{R}_0}{|\mathbf{e}_{\mathbf{Q}}||\mathbf{R}_0|} \frac{\mathbf{Q} \cdot \mathbf{R}_0}{|\mathbf{R}_0|} \exp(i\mathbf{Q} \cdot \tilde{\xi})(b_{\mathbf{Q}} + b_{-\mathbf{Q}}^+) + \sum_{\mathbf{Q}} |\mathbf{Q}| b_{\mathbf{Q}}^+ b_{\mathbf{Q}} \quad (3.1)$$

we see that all the main features of the DW within a vibrating lattice are determined by two parameters only: adiabatic parameter b and kink–phonon coupling constant S , which were defined in the previous section. Here $\tilde{P} = P_{DW}/\hbar^2 q_D^2$ and $\tilde{\xi} = \xi/q_D$ are the corresponding dimensionless DW momentum and position, respectively, while $\mathbf{Q} = \mathbf{q}/q_D$. From (2.8) it follows that the first LLP transformation exactly diagonalizes this Hamiltonian in the transportless limit ($b \rightarrow 0$ or $m \rightarrow \infty$). In the case of finite adiabaticity the value of the coupling constant S plays the essential role. So, for example, in the strict weak-coupling regime $S \ll 1$, the dressing effect does not influence DW properties significantly. Thus the problem of kink–phonon interaction can be treated perturbatively, as was done in I. In that case the DW propagates along the rigid lattice and its dynamics is determined by the interaction with real phonons excited when the DW velocity exceeds the phase speed of sound. Such an interpretation is satisfactory as long as the adiabatic parameter is high enough. However, if $b \ll 1$ the properties of the DW should be similar to those of small polarons and the continuum model used here is no longer applicable. For that reason the theoretical approach should be modified to incorporate the proper treatment of discreteness effects and the real quantum nature of the spin (pseudospin) system.

According to the results of the preceding section the DW 'dressing' becomes significant if $S > 1$ and for small but finite values of b . In that case the DW recoil kinetic energy introduces a correlation between the emission of successive virtual phonons, which will tend to limit the validity of the method employed here. Since the variational calculation that was performed is equivalent to the transformation $H \rightarrow H_0 + H_1$, we can estimate the validity of our calculation by determining the lowest-order correction to the DW energy resulting from that part of the Hamiltonian which was neglected so far. Since we have found β_q by minimizing the energy, H_0 is diagonal and the lowest phonon state is simply the vacuum one ($|0\rangle_{\text{ph}}$), while H_1 should be considered as small, so it is possible to estimate its contribution using standard perturbation theory. However, in what follows we shall deviate from that general rule and instead of a perturbation calculation we shall find the new normal modes of that part of the transformed Hamiltonian which is quadratic in phonon operators. For that purpose we rewrite the transformed Hamiltonian as

$$\mathcal{H} = \sum_{n=0}^4 \mathcal{H}^{(n)}$$

where

$$\mathcal{H}^{(0)} = E_0 + P^2/2m^* - \delta E$$

$$\mathcal{H}^{(1)} = 0$$

$$\mathcal{H}^{(2)} = \sum_q \hbar \tilde{\omega}_q b_q^\dagger b_q + \frac{\hbar^2}{2m} \sum_{q,q'} (\mathbf{q} \cdot \mathbf{q}') [2\beta_{q'}^* \beta_q b_q^\dagger b_{q'} + (\beta_q \beta_{q'} b_q^\dagger b_{q'}^\dagger + \text{HC})] \quad (3.2)$$

$$\mathcal{H}^{(3)} = \frac{\hbar^2}{m} \sum_{q,q'} (\mathbf{q} \cdot \mathbf{q}') (b_q^\dagger b_q b_{q'} \beta_{q'}^* + \text{HC})$$

$$\mathcal{H}^{(4)} = \frac{\hbar^2}{2m} \sum_{q,q'} (\mathbf{q} \cdot \mathbf{q}') b_q^\dagger b_{q'}^\dagger b_{q'} b_q \quad \tilde{\omega}_q = \omega_q - \mathbf{q} \cdot \mathbf{v} + \frac{\hbar q^2}{2m}$$

$\mathcal{H}^{(2)}$ can be exactly diagonalized using standard Bogoliubov–Tyablikov (BT) unitary transformation [21]. In order to simplify the practical calculations, we first perform the Fourier transform of phonon operators

$$b_q = \frac{1}{\sqrt{N}} \sum_n \exp(-i\mathbf{q} \cdot \mathbf{n}) b_n$$

to obtain $\mathcal{H}^{(2)}$ in a form that is very convenient for direct application of the BT method:

$$\mathcal{H}^{(2)} = \sum_{n,m} Z_{nm} b_n^\dagger b_m - \frac{1}{2} \sum_{n,m} A_{nm} b_n^\dagger b_m^\dagger + A_{nm}^* b_n b_m \quad (3.3)$$

where

$$Z_{nm} = \frac{1}{N} \sum_q \hbar \tilde{\omega}_q \exp[i\mathbf{q} \cdot (\mathbf{n} - \mathbf{m})] + \frac{1}{N} \sum_{q,q'} \frac{\hbar^2}{m} (\mathbf{q} \cdot \mathbf{q}') f_q f_{q'} \exp[i(\mathbf{q} \cdot \mathbf{n} - \mathbf{q}' \cdot \mathbf{m})] \quad (3.4)$$

$$A_{nm} = \frac{1}{N} \sum_{q,q'} \frac{\hbar^2}{m} (\mathbf{q} \cdot \mathbf{q}') f_q f_{q'} \exp[i(\mathbf{q} \cdot \mathbf{n} + \mathbf{q}' \cdot \mathbf{m})]$$

and

$$f_q = -i\beta_q.$$

Introducing the new Bose operators $\eta_k^{\pm}(\eta_k)$ in accordance with standard BT procedure

$$b_n = \sum_k u_{nk} \eta_k + v_{nk}^* \eta_k^{\dagger} \quad \eta_k = \sum_n u_{nk}^* b_n - v_{nk}^* b_n^{\dagger} \quad (3.5)$$

we can write Hamiltonian (3.3) in the diagonal form

$$\mathcal{H}^{(2)} = \Delta E + \sum_k E_k \eta_k^{\dagger} \eta_k. \quad (3.6)$$

Here functions u_{nk} and v_{nk} satisfy the orthogonality conditions

$$\begin{aligned} \sum_k u_{nk}^* u_{n'k} - v_{nk} v_{n'k}^* &= \delta_{nn'} & \sum_n u_{nk}^* u_{nk'} - v_{nk}^* v_{nk'} &= \delta_{kk'} \\ \sum_k u_{nk} v_{n'k}^* - v_{nk}^* u_{n'k} &= 0 & \sum_n u_{nk} v_{nk'} - v_{nk} u_{nk'} &= 0. \end{aligned} \quad (3.7)$$

$\Delta E = -\sum_{k,n} E_k |v_{nk}|^2$ represents the first correction to the DW energy. The spectrum of new phonons E_k can be determined from the following set of eigenequations:

$$\begin{aligned} E_k u_{nk} &= \sum_{\nu} Z_{\nu\nu} u_{\nu k} - \sum_{\nu} A_{\nu\nu} v_{\nu k} \\ - E_k v_{nk} &= \sum_{\nu} Z_{\nu\nu}^* v_{\nu k} - \sum_{\nu} A_{\nu\nu} u_{\nu k}. \end{aligned} \quad (3.8)$$

Choosing

$$u_{nk} = \frac{1}{\sqrt{N}} u_k e^{ik \cdot n} \quad \text{and} \quad v_{nk} = \frac{1}{\sqrt{N}} v_k e^{ik \cdot n}$$

and after summation over n , we obtain

$$\begin{aligned} E_k u_k &= Z_k u_k - A_k v_k \\ - E_k v_k &= Z_k v_k - A_k u_k. \end{aligned} \quad (3.9)$$

Here

$$A_k = \frac{1}{N} \sum_{n,\nu} A_{\nu\nu} \exp[i(\nu - n) \cdot k] \quad \text{and} \quad Z_k = \frac{1}{N} \sum_{n,\nu} Z_{\nu\nu} \exp[i(\nu - n) \cdot k].$$

From the condition that homogeneous system (3.9) has non-trivial solutions u_k and v_k we find the spectrum E_k in the form

$$E_k = (Z_k^2 - A_k^2)^{1/2} = [\hbar^2 \tilde{\omega}_k^2 + (2\hbar^3/m)k^2 \tilde{\omega}_k f_k^2]^{1/2}. \quad (3.10)$$

Finally, using equations (3.9) and the orthogonality condition for the functions (u, v) , which in this case reads

$$u_k^2 - v_k^2 = 1 \quad (3.11)$$

one can easily prove the following relations:

$$u_k^2 = \frac{Z_k + E_k}{2E_k}, \quad v_k^2 = \frac{Z_k - E_k}{2E_k}, \quad u_k v_k = \frac{A_k}{2E_k}. \quad (3.12)$$

With the help of these relations we can find the corresponding correction to the GS energy

$$\Delta E = -\frac{\hbar^2}{4m^2} \frac{1}{N} \sum_k \frac{k^4 f_k^4}{\hbar \tilde{\omega}_k} - \frac{\hbar^2}{2m} \frac{1}{N} \sum_k k^2 u_k^2 v_k^2. \quad (3.13)$$

The second sum in this expression represents the contribution to the energy which arises from $\mathcal{H}^{(4)}$ after its proper ordering in terms of new operators η_k and η_k^\dagger . Transforming the summation in (3.13) to an integration, in accordance with previously adopted rules (2.2), we can finally express ΔE through the parameters S and b as follows:

$$\Delta E \simeq \begin{cases} -\hbar \omega_D \frac{S^2 b^2}{3} \left(\frac{1}{4} - \frac{4}{5} b + \frac{3}{2} b^2 \right) & \text{for isotropic phonons} \\ -\hbar \omega_D S^2 b^2 (1 - 3b + 7b^2) & \text{for anisotropic phonons.} \end{cases} \quad (3.14)$$

In performing the explicit calculation of ΔE we have assumed the smallness of adiabatic parameter ($b < 1$), which is precisely the limit where one can expect considerable influence of phonon 'dressing' on DW properties. Since, in principle, the first correction to the energy ΔE should not exceed the basic contribution δE , we expect that the present approach is satisfactory as long as $\Delta E \ll \delta E$. Adopting this criterion one can find the maximal value of the coupling constant S , for each b , which represents the upper bound of the applicability of the present method. Unfortunately this criterion does not offer any possibility for the precise determination of the numerical values of S and b for which the DW demonstrates polaron-like behaviour. So, for example, for $b = 0.5$ we found that $S < 7.8$, while for $b = 0.1$, $S \ll 102$. So the estimated value of the coupling constant is too high and we believe that the maximal realistic value of S should be significantly smaller. This follows from the fact that the spin-phonon interaction in the strong-coupling limit should modify the character of soliton solutions and therefore the effective Hamiltonian (2.1) is no longer a good basis for a description of a kink-phonon interaction. Consequently the method utilized here is no longer applicable and the theoretical description as well as the physical picture depend on the values of the 'bare' adiabatic parameter $b_0 \sim J/\hbar \omega_D$ and the strength of the original spin-phonon coupling $S_0 = (1/N) \sum_q |F_q|^2 / \hbar^2 \omega_q^2$, which we define in analogy with corresponding parameters known from the polaron problem and theories of self-trapping [18, 20].

If $b \gg 1$ the classical nature of phonons prevails and for that reason theoretical treatment of the spin(pseudospin)-phonon coupling should be analogous to the theories of large adiabatic polarons [18, 20, 22]. In that case the problem is practically reduced to the analysis of the system of coupled non-linear equations describing the simultaneous evolution of magnetic (or dipolar electric) and elastic degrees of freedom. Such a theory predicts coexistence and simultaneous propagation of the spin (pseudospin) and lattice solitons as was shown in a number of related papers [9-11, 23-26]. However, at present, owing to the differences in the dimensionality of spin and phonon subsystems, such an analysis is much more complicated. It particularly follows from the recent study of Brown and Ivić [27], where the existence and stability of large adiabatic polarons in linear molecular crystals within a 3D lattice was examined. For that reason this interesting aspect of spin-phonon coupling deserves separate examination.

In the strong-coupling *non-adiabatic* regime, $S_0 \gg 1$ and $b_0 \ll 1$, the real quantum nature of both subsystems plays the essential role, so we encounter a problem that cannot be successfully treated by any of the above-mentioned methods. In that case the spin-phonon Hamiltonian can be partially diagonalized by appropriate unitary transformation known from the theory of small polarons [19]. The subsequent diagonalization can be carried out in a form of perturbation expansion in terms of small parameter b_0 . However, this case, as well as the strong-coupling adiabatic limit, is beyond the scope of the present study. For that reason we are not in a position to determine precise numerical values of S and b or S_0 and b_0 which support any of the above-mentioned types of DW behaviour.

Therefore we can only roughly estimate that the predicted polaron-like behaviour of DWs should occur in the *non-adiabatic* ($b < 1$) *intermediate-coupling* ($S \geq 1$) *limit*. Choosing the values of S and b from this intermediate region of parameter space (approximately $0.1 < b < 0.5$ and $1 < S < 5$) we find a relative correction of the energy of approximately 1 to 15%.

4. Summary

Concluding this paper, we emphasize that the method employed here provides a reasonably good basis for the understanding of kink-phonon interaction in the intermediate-coupling limit. In that case we predicted polaron-like behaviour of DWs, which motion is that of a free particle with an effective mass $m^* = m/(1-\eta)$, which is higher than that of a bare DW, while its energy is lower than in the rigid lattice. Applicability of the method is satisfactory as long as DW velocity is sufficiently small so that no spontaneous Cherenkov-like emission of real phonons can occur (i.e. $v < c_0$ and $v < c_{\parallel}$ for isotropic and anisotropic phonon spectra, respectively).

The influence of the difference in dimensionality of two constituent subsystems is manifested through a significant lowering of the polaronic effect in such systems with respect to those where both subsystems are of the same dimensionality. It can be seen from the explicit expressions for the lattice relaxation energy E_D and the shift of GS energy δE , which are five times less than in the purely 1D or 3D systems (equations (2.3) and (2.28)) for isotropic phonons. For the anisotropic phonons this lowering of 'dressing' can be seen from equations (2.4) and (2.29) where all terms proportional to powers of small parameter $q_{\perp}^D/q_{\parallel}^D$ represent corrections to the pure 1D result. This lowering of the polaronic effect is the consequence of the angular dependence of the Fourier component of the spin-phonon interaction through the term $e_q \cdot e_x = \cos \theta \leq 1$. In purely 1D and 3D systems this term approaches unity.

We would finally like to point out that the spin-phonon interaction is not the only mechanism that can induce DW dressing. Namely a proper treatment of DW dynamics in realistic substances demands taking into account the interaction of DWs with the linear excitations of spin (pseudospin) system—magnons (pseudomagnons), which could also contribute to DW dressing. An analogous effect was discovered by Koehler *et al* [29] in the molecular dynamics simulation of a φ -four model (φ^4) where linear excitations around soliton solutions (i.e. 'phonons') played precisely the same role as magnons (pseudomagnons) in the framework of IMTF. Therefore the magnon dressing of DWs and its examination should also be an interesting problem.

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