

Polarons in quantum chains with XY exchange and Dzyaloshinsky-Moriya interaction

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Abstract. Excitations of the polaron types are investigated in the spin-1/2 quantum chain with XY exchange and Dzyaloshinsky-Moriya interaction, both coupled to acoustic vibrations of the substrate lattice. The study is carried out via Jordan-Wigner transformation with the help of which the spin chain is mapped onto a chain of spinless fermions. From the resulting effective fermion-lattice Hamiltonian, the discrete equations of motion are derived. These equations are solved in the continuum limit for self-trapped states near the bottom of the fermion spectrum interacting with long-wavelength acoustic lattice modes. The associate polaron solution, which has a pulse shape, is shown to propagate bound to the induced lattice kink distortion by translation along the chain at a constant velocity v . The pair can also experience an additional acceleration ϑ_0 when the free fermion charge is excited above its groundstate. The polaron binding energy is strongly reduced, depending quadratically on the ratio D/J of the Dzyaloshinsky-Moriya interaction strength D to the isotropic XY exchange interaction J . It is also found that polaron parameters depend only on the XY spin-lattice coupling but not on the Dzyaloshinsky-Moriya contribution.

PACS. 63.20.Ry Anharmonic lattice modes – 71.38.-k Polarons and electron-phonon interactions – 75.10.Pq Spin chain models

1 Introduction

Neutron-scattering experiments [1] have reported the presence of field-dependent incommensurate low-energy modes in copper benzoate. While the incommensurability was found to be consistent with Bethe's exact solution of the Heisenberg model in a magnetic field, the system also exhibited an unexpected excitation gap induced by the applied field. This excitation gap is as surprising as the coexistence of a gap and a finite magnetization is inconsistent with the rotational symmetry around the direction of magnetization [2] in the Heisenberg spin chain. The origin of the excitation gap has been the subject of great interest, namely it was suggested [1,3–5] that the gap could be due to a staggered magnetic field generated by the alternating g tensor in Cu benzoate under the applied field. However, Affleck and Oshikawa [6] established unambiguously the consistency between the proposed mechanism of gap formation involving the generation of a staggered field perpendicular to the direction of the applied magnetic field, and the Dzyaloshinsky-Moriya interaction [7–9] present in Cu benzoate [6]. From this they showed that all the experiments reported on Cu benzoate could well be understood in the unified framework of a model of spin-1/2 quantum

chain with an antisymmetric Dzyaloshinsky-Moriya interaction, of a Dzyaloshinsky-Moriya vector orthogonal to the b axis.

From the theoretical standpoint, Cu benzoate is believed to possess attribute of an $S = 1/2$ antiferromagnetic quantum spin chain [1–6]. The Heisenberg spin-1/2 quantum chain has long served as a paradigm for strongly correlated quantum many body systems, for instance its quantum critical behaviour can be tuned by a magnetic field. In the absence of Dzyaloshinsky-Moriya interaction, the excitation spectrum of the model is dominated by a gapless spinon continuum but a soft mode can be created at the incommensurate wave vector by the application of high fields [10]. However, at relatively moderate fields the system can also accommodate a singlet-triplet gap and a low-temperature non-magnetic groundstate resulting from a structural transition due to the coupling with the molecular substrate. This structural instability, best known as spin-Peierls instability [11,12], is the magnetic counterpart of the Peierls transition [13]. Thus, within the framework of Jordan-Wigner transformation [12] that maps spins onto spinless fermions, the spin-Peierls transition can be shown to occur as the result of a gap developing at the Fermi level k_F of the fermion spectrum due to the coupling of the spinless fermions to the $2k_F$ lattice distortion.

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In recent years, the microscopic basis of the spin-Peierls instability provided by Jordan-Wigner transformation has motivated a great number of theoretical attempts on various aspects of the instability, in a close analogy with theories developed for the Peierls transition. For instance the similarity between the fermion-lattice model derived from the deformable XY model and the tight-binding model [14] without the electronic spins, is a natural source of motivation for considering possible polaronic features in the groundstate of the pseudo fermion spectrum [15].

The tight-binding version of the quantum spin-1/2 chain with Dzyaloshinsky-Moriya interaction has been introduced by Moriya [9], and formally identified [6,16] as Anderson's superechange model [17] equivalent to the Heisenberg chain including the Dzyaloshinsky-Moriya interaction term. Very recently it was used as basis of the microscopic fermion-phonon model [18–21] for an hypothetical structural instability of the spin-Peierls type, which otherwise is fully justified in Cu benzoate given the quasi-one-dimensional anisotropy of the fermion spectrum corresponding to the associate quantum spin model.

The aim of this work is to take advantage of the existing microscopic model for the quantum spin-1/2 chain with Dzyaloshinsky-Moriya interaction, to investigate the influence of this interaction on the shape and dynamics of nonlinear excitations of the polaron type in the groundstate of the pseudo-fermion spectrum [15,22–25]. This study has direct connection with previous studies of polaron modes in the tight-binding model coupled to acoustic lattice vibrations [15,22–24] and therefore provides a natural extension of these previous works to one-dimensional quantum systems dominated by competing antiferromagnetic correlations. More concretely, the point of focus of our attention is on the self-trapped states resulting from the coupling of fermion states near the bottom of the fermion spectrum to long-wavelength lattice distortions. Indeed, while the interaction of fermion states near the Fermi level with the $2k_F$ lattice distortion triggers the structural instability, thermal transport properties of the system much more involve long-wavelength lattice displacements. Consequently, the mechanism of heat transport in the spin-lattice system can strongly deviate from the classic mechanism known for the free monoatomic lattice. As we will see, the formed long-wavelength polaron induces a kink soliton distortion in the lattice such that the lattice dynamics and thermodynamics are governed by kinks. Thus, through our study we wish to provide insights onto an understanding of both qualitative and quantitative effects of the Dzyaloshinsky-Moriya interaction on thermal transport properties of systems concerned with the model, including copper benzoate [6] and copper metaborate [26].

In Section 2, we introduce the spin-lattice model and carry out necessary transformations to obtain the effective single-particle Hamiltonian consisting of spinless fermions coupled to quantum lattice vibrations. This Hamiltonian is next used to derive the discrete equations of motion for both the wavefunctions of fermion occupation proba-

bilities and the lattice displacement fields. In Section 3, the shape of the fermionic polaron, as well as its excitation spectrum and binding energy, are explicitly derived exactly in the continuum limit. In Section 4 a brief conclusion of the study is given.

2 The effective fermion-lattice Hamiltonian and equations of motion

Consider an antiferromagnetic system consisting of a spin-1/2 quantum chain with an isotropic XY exchange J coexisting with an antisymmetric exchange $\mathbf{D} = D\mathbf{z}$ of the Dzyaloshinsky-Moriya type. We assume in addition that the spins interact with acoustic vibrations of the molecular substrate lattice. The total Hamiltonian of the magneto-elastic system is then:

$$H = H_{ph} + H_{mag}. \quad (1)$$

The first term

$$H_{ph} = \sum_n \left[\frac{1}{2M} P_n^2 + \frac{1}{2} K (u_{n+1} - u_n)^2 \right], \quad (2)$$

represents the contribution of the lattice where u_n and P_n are position and conjugate momentum of an atom M at site n of the one-dimensional lattice, and K is the spring constant of Hooke's springs that couple nearest-neighbour atoms along the monoatomic chain. The second term of H , i.e.

$$H_{mag} = \sum_n J_n (S_n^x S_{n+1}^x + S_n^y S_{n+1}^y) + \sum_n D_n (S_n^x S_{n+1}^y - S_n^y S_{n+1}^x) \quad (3)$$

is the magnetic energy where

$$J_n = J [1 + \lambda (u_n - u_{n+1})], \\ D_n = D [1 + \lambda \beta (u_n - u_{n+1})]. \quad (4)$$

In this second part S_n^ℓ denotes the $\ell (\equiv x, y, z)$ component of the spin-1/2 operator \mathbf{S}_n at site n , J_n and D_n are the isotropic XY and antisymmetric or Dzyaloshinsky-Moriya antiferromagnetic exchange integrals respectively. According to (4), they are assumed to have a homogeneous part J and D while depending linearly on the relative displacement of atoms M at sites $n+1$ and n with spin-phonon couplings λ and $\lambda\beta$ respectively.

The Hamiltonian (2)–(4) is apparently quite rich compared to the usual spin-lattice model for the spin-Peierls transition based on the XY chain coupled to the lattice. Thus, from the standpoint of fundamental physics, it stands as a good generic model for studying structural instabilities in a great number of quantum spin chains characterized by the coexistence of different exchange anisotropies including the symmetric and antisymmetric exchanges of the Dzyaloshinsky-Moriya type. In

particular the Hamiltonian (2)–(4) should provide relevant and rich insights onto the spin-Peierls transition in Cu benzoate. Regarding this last remark this Hamiltonian has recently been used [19–21] to investigate the influence of the Dzyaloshinsky-Moriya interaction on the zero-temperature phase diagram of XY -based spin-Peierls compounds. These recent studies, based on variational numerical approaches, predicted surprising phenomena indicating a net deviation of the mechanism of the spin-Peierls transition from the standard mechanism known through the XY model [12]. It has thus been shown [20] that when the Dzyaloshinsky-Moriya interaction is uniform and only the XY part couples to the lattice, a strong Dzyaloshinsky-Moriya interaction will always act against a dimerized groundstate. Moreover, a reentrance transition from the gapless phase to the gapped phase was observed with an increase of the Dzyaloshinsky-Moriya dimerization rate β and when the Dzyaloshinsky-Moriya interaction was in direct competition against the isotropic XY exchange J . Interesting enough, these numerical predictions are confirmed [27] by analytical results within the mean-field theory, in particular the mean-field theory confirms unambiguously the crossover character of the reentrance transition [20] which is manifest in the dependence of the spin-Peierls transition temperature on the Dzyaloshinsky-Moriya interaction parameters D and β .

In this work, we take advantage of the possible representation of the spin-phonon Hamiltonian (2)–(4) in terms of fermion degrees of freedom to investigate low-lying excitations in the groundstate of the quantum spin-1/2 chain coupled to dynamic phonons. More explicitly, we are interested with the dynamics of Bloch-type excitations localized about the groundstate of the fermion spectrum in the presence of the XY exchange, Dzyaloshinsky-Moriya interaction and their simultaneous coupling to non adiabatic lattice distortions. As a prior step we perform Jordan-Wigner transformation [12] which allows us map the spin degrees of freedom in (3) onto spinless fermions, leading to the effective single-fermion Hamiltonian:

$$H_{eff} = \frac{1}{2} \sum_n \left[G_n c_n^\dagger c_{n+1} + G_n^* c_{n+1}^\dagger c_n \right], \quad (5)$$

where c_n^\dagger and c_n creates and destroys single-fermion states respectively at site n of the one-dimensional chain, and where we defined:

$$G_n = J_n + i D_n, \quad G_n^* = J_n - i D_n. \quad (6)$$

It will also be useful for our next developments to recast G_n and G_n^* in simple forms [6]. Using the explicit expressions (4) we rewrite G_n as:

$$\begin{aligned} G_n &= G_o + G_1 (u_n - u_{n+1}), \\ G_o &= J + i D, \quad G_1 = \lambda (J + i \beta D). \end{aligned} \quad (7)$$

Next, introducing the phase parameters

$$\alpha = \arctg \left(\frac{D}{J} \right), \quad \alpha_1 = \arctg \left(\frac{\beta D}{J} \right), \quad (8)$$

as well as the effective couplings

$$\epsilon = \frac{1}{2} J \sqrt{1 + \left(\frac{D}{J} \right)^2}, \quad \lambda_1 = \frac{1}{2} \lambda J \sqrt{1 + \left(\frac{\beta D}{J} \right)^2}, \quad (9)$$

the single-particle Hamiltonian (5) becomes:

$$\begin{aligned} H_{eff} &= \sum_n \left[\epsilon e^{i\alpha} + \lambda_1 e^{i\alpha_1} (u_n - u_{n+1}) \right] c_n^\dagger c_{n+1} \\ &+ \sum_n \left[\epsilon e^{-i\alpha} - \lambda_1 e^{-i\alpha_1} (u_{n+1} - u_n) \right] c_{n+1}^\dagger c_n. \end{aligned} \quad (10)$$

Remarkably this last formula describes the one-particle Hamiltonian of a chain of spinless fermions coupled to acoustic vibrations in which the free-fermion spectrum experiences a phase shift α , which is reflected on the coupling of fermions to the lattice distortion through a phase factor α_1 . In addition, we see from the definitions of α and α_1 in (8) that finite values of the phase shifts in the quantum spin system are intrinsic manifestations of nonzero values of the Dzyaloshinsky-Moriya interaction D .

An inspection of the electronic structure of the effective Hamiltonian (10) in momentum space indicates that the phase factor α gives rise to a shift of the Fermi level by α , such that the new Fermi wave vector $k_F^\alpha = \pi/2 - \alpha$. However, from symmetry considerations this shift does not affect the size of the Fermi sea since all the states are uniformly shifted by the same amount α . It follows that the filling condition of the system is not affected by the Dzyaloshinsky-Moriya interaction, i.e. the renormalized fermion spectrum is still half filled with respect to the Fermi level k_F^α . But the dependence of the effective coupling ϵ defined in (9) on the Dzyaloshinsky-Moriya interaction D , suggests a possible influence of this last parameter on the Fermi velocity v_F^α . Owing to this last effect, the quantum dynamics of electronic states should experience drastic changes as we vary D with direct incidence on polaronic excitations as the Dzyaloshinsky-Moriya interaction is varied. To see these changes with more details, we solve the equations governing the dynamics of atoms and the Bloch states. These equations are derived from (2) and (10) by applying Hamilton and Heisenberg formalisms which lead to the two coupled discrete equations:

$$\begin{aligned} M\ddot{u}_n &= K (u_{n+1} - 2u_n + u_{n-1}) \\ &- \lambda_1 e^{i\alpha_1} \left(c_n^\dagger c_{n+1} - c_{n-1}^\dagger c_n \right) \\ &+ \lambda_1 e^{-i\alpha_1} \left(c_{n+1}^\dagger c_n - c_n^\dagger c_{n-1} \right), \end{aligned} \quad (11)$$

$$\begin{aligned} i\hbar\dot{c}_n &= - \left[\epsilon e^{i\alpha} + \lambda_1 e^{i\alpha_1} (u_n - u_{n+1}) \right] c_{n+1} \\ &- \left[\epsilon e^{-i\alpha} + \lambda_1 e^{-i\alpha_1} (u_{n-1} - u_n) \right] c_{n-1} \end{aligned} \quad (12)$$

where dot symbols refer to time derivatives. However, excitations of the electronic states are best described by means of the wavefunctions $\psi_n(t)$ of the fermion occupation probabilities $\langle c_n(t) \rangle$ for each given lattice site n , where the mean value is taken from the groundstate of

the free-fermion spectrum. In terms of these new variables and making the assumption that each electronic state has a coherent dynamics, the above set of coupled discrete equations becomes:

$$M\ddot{u}_n = K(u_{n+1} - 2u_n + u_{n-1}) - \lambda_1 e^{i\alpha_1} (\psi_n^* \psi_{n+1} - \psi_{n-1}^* \psi_n) + \lambda_1 e^{-i\alpha_1} (\psi_{n+1}^* \psi_n - \psi_n^* \psi_{n-1}), \quad (13)$$

$$i\hbar\dot{\psi}_n = - [\epsilon e^{i\alpha} + \lambda_1 e^{i\alpha_1} (u_n - u_{n+1})] \psi_{n+1} - [\epsilon e^{-i\alpha} + \lambda_1 e^{-i\alpha_1} (u_{n-1} - u_n)] \psi_{n-1} \quad (14)$$

where the star denotes complex conjugate.

3 Polaron dynamics in the continuum limit

The point of focus of our attention is the dynamics of electronic excitations localized at the bottom of the Fermi sea. Although these modes put into play low-energy or long-wavelength fluctuations, the robustness of polaronic excitations of the soliton type can turn to be advantageous in field-induced transport phenomena. For these low-lying objects, the long-wavelength approximation $na \rightarrow x$ (where a is the lattice parameter) can readily be envisaged which in the weak dispersion regime expresses:

$$\psi_{n\pm 1} \approx \psi \pm a\psi_x + \frac{a^2}{2}\psi_{xx} \pm 0(a^3). \quad (15)$$

Applying the same approximation to the displacement fields $u_{n\pm 1}$, the following set of coupled continuum equations arises:

$$\ddot{u} - c_o^2 u_{xx} + 2a\lambda_1 \cos \alpha_1 (|\psi|^2)_x = 0, \quad c_o^2 = \frac{a^2 K}{M}, \quad (16)$$

$$i\hbar\dot{\psi} + 2a^2\epsilon \cos \alpha \psi_{xx} + 2ia\epsilon \sin \alpha \psi_x + 2(\epsilon \cos \alpha + a\lambda_1 \cos \alpha_1 u_x) \psi = 0, \quad (17)$$

where c_o is the speed of sound. As one can remark, in spite of apparent resemblance with the set commonly obtained in the studies of acoustic polarons [15], the two coupled equations (16, 17) are actually unusual and therefore absolutely specific to the Hamiltonian (10). Essentially, the difference with previous equations resides in the second equation which carries an extra term proportional to ψ_x . This term clearly reflects changes in the coordinate space of the fermion-lattice system with respect to the XY model due to the account of Dzyaloshinsky-Moriya interaction. In connection with this last remark, as well as the fact that the Bloch theorem still holds such that the periodicity properties of the Bloch wavefunctions $\psi(x, t)$ are invariants with respect to the renormalization of the fermion spectrum by the shift α , we can substitute $\psi(x, t)$ in (16)–(17) with a new wavefunction defined as:

$$\psi(x, t) = \phi(x, t) e^{-i\kappa(\alpha)x}, \quad (18)$$

which is supposed to be consistent with the new path followed by the system states for nonzero values of the phase factor α . From this last point of view the parameter $\kappa(\alpha)$ must be entirely determined by the free-fermion phase factor α and should not depend on time and space. When (18) is replaced in (17) this yields the gauge condition:

$$\kappa(\alpha) = \frac{1}{2a} \operatorname{tg} \alpha \quad (19)$$

and it follows:

$$\ddot{u} - c_o^2 u_{xx} + 2a\lambda_1 \cos \alpha_1 (|\phi|^2)_x = 0, \quad (20)$$

$$i\hbar\dot{\phi} + 2a^2\epsilon \cos \alpha \phi_{xx} + \frac{\epsilon}{2} (4 \cos \alpha + \sin \alpha \operatorname{tg} \alpha) \phi + a\lambda_1 \cos \alpha_1 u_x \phi = 0. \quad (21)$$

Solving the last system, we first carry out the coordinate change $z = x - vt$ where v is the propagation velocity of the lattice distortion $u(x, t)$. With this new coordinate the last system transforms to:

$$u_{zz} = \frac{2a\lambda_1 \cos \alpha_1}{c_o^2 (1 - v^2/c_o^2)} (|\phi|^2)_z, \quad (22)$$

$$\left[i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m_e} \frac{\partial^2}{\partial z^2} + \epsilon_\alpha + g_0 |\phi|^2 \right] \phi = 0, \quad (23)$$

with

$$\epsilon_\alpha = (4 \cos \alpha + \sin \alpha \operatorname{tg} \alpha) \frac{\epsilon}{2}, \quad m_e = \frac{\hbar^2}{4a^2\epsilon \cos \alpha} = \frac{\hbar^2}{2a^2 J}, \quad (24)$$

and where

$$g_0(v) = \frac{4a^2\lambda_1^2 \cos^2 \alpha_1}{c_o^2 (1 - v^2/c_o^2)} = \frac{a^2\lambda^2 J^2}{c_o^2 (1 - v^2/c_o^2)} \quad (25)$$

represents the effective fermion-lattice coupling. Equation (23) admits the single-soliton solution:

$$\phi(z, t) = \phi_0 \operatorname{sech} [\nu (z - z_o - \vartheta_0 t)] e^{i\theta_k(x, t)}, \quad \theta_k(z, t) = k(z - z_o) - \frac{E_\alpha(k)}{\hbar} t. \quad (26)$$

A sketch of the spatial shape of the fermionic polaron occupation density as well as of the lattice distortion it induces are shown in Figure 1. We see that the polaron is a localized pulse and the induced lattice distortion has a kink shape. The pulse amplitude ϕ_0 and inverse half width ν are given by:

$$\phi_0 = \frac{g_0}{2\hbar} \sqrt{m_e}, \quad \nu = 2\phi_0^2, \quad (27)$$

while

$$E_\alpha(k) = \frac{\hbar^2 k^2}{2m_e} - \epsilon_\alpha - \frac{g_0^2(v)}{8\hbar^2}. \quad (28)$$

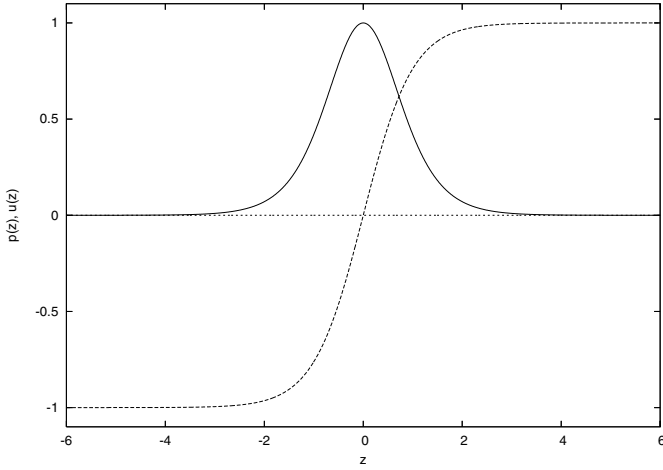


Fig. 1. Spatial shapes of the fermionic polaron occupation density $P(z) = |\phi(z)|^2$ and of the accompanying lattice kink distortion $u(z)$, plotted in units of the polaron amplitude squared ϕ_0^2 .

is the energy of the k excited state of the fermionic polaron. Note that the last formula has been derived by defining:

$$\vartheta_0 = \frac{\hbar k}{m_e}, \quad (29)$$

which, according to (26), contributes to the velocity of translation of the polaron along the one-dimensional lattice. It is also interesting to remark that the ways we defined the polaron dispersion energy $E_\alpha(k)$ and velocity ϑ_0 bring to the fore an effective mass m_e , which is nothing else but the effective mass of the free charge particle in the renormalized fermion spectrum. In this respect we see that the effective mass of free-fermion particles is not affected by the Dzyaloshinsky-Moriya interaction. However, the polaron excitation energy $E_\alpha(k)$ as defined in (28) involves not only the energies of the k excited states of the free fermion, also present are contributions from the tight-binding spectrum and the coupling to the lattice. The total binding energy of the polaron is:

$$E_\alpha = -\epsilon_\alpha - \frac{g_0^2(v)}{8\hbar^2}. \quad (30)$$

and is a quantity dependent on the ratio D/J as well as on the fermion-lattice coupling parameter λ . In Figure 2, we display a sketch of the variation of the polaron binding energy with the ratio D/J . It is easy to check that (30) does not depend on β . Although this is a surprising result given previous predictions [19–21] of a relevant contribution of the Dzyaloshinsky-Moriya parameter β to the spin-Peierls instability, it can easily be understood from the continuum limit approximation which involves fermions of a very long wavelength i.e. $k \ll k k_F^\alpha$, where effects of the Dzyaloshinsky-Moriya interaction parameters D and β are found to have drastic incidence [27] on the process of gap formation in the fermion dispersion spectrum.

Before ending, it would be enriching for a global understanding of the physics of polarons in the current model, to also examine the polaron parameters now in terms of the

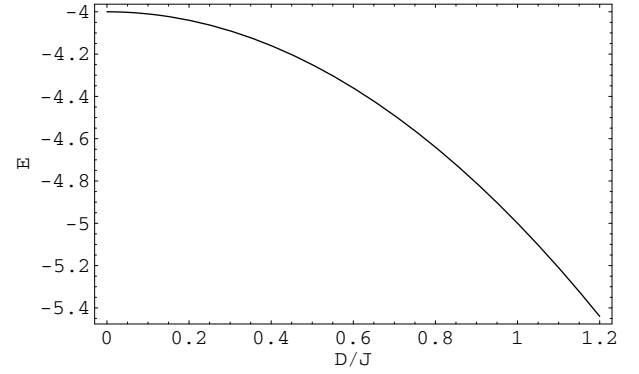


Fig. 2. The polaron binding energy (at fixed velocity v of the lattice soliton) versus the ratio D/J of the Dzyaloshinsky-Moriya interaction D and the isotropic XY exchange interaction J .

original wavefunction $\psi(x, t)$. Indeed, if we substitute (26) in formula (18) we obtain that the binding energy of the ψ polaron is instead:

$$E_\alpha = \frac{\hbar^2 \kappa^2}{2m_e} - \epsilon_\alpha - \frac{g_0^2(v)}{8\hbar^2}. \quad (31)$$

This means that the dispersion energy of the ψ polaron can be approximated by:

$$E_\alpha(k) = \frac{\hbar^2(k - \kappa)^2}{2m_e} - \epsilon_\alpha - \frac{g_0^2(v)}{8\hbar^2}, \quad (32)$$

which shows that excited states of the ψ polarons are uniformly shifted down by κ with respect to the excited states of the ϕ polarons, and consequently are of lower energies.

4 Conclusion

We have investigated the effects of the Dzyaloshinsky-Moriya interaction on polaron shape and dynamics in the microscopic version of the spin-1/2 quantum chain with an isotropic XY exchange and the Dzyaloshinsky-Moriya interaction. We found an explicit expression of the polaron shape reflecting the relevant dependence on the Dzyaloshinsky-Moriya interaction parameters. However, it appeared that the continuum limit approximation favours the XY exchange against the Dzyaloshinsky-Moriya interaction in the formation process of the fermion polaron, especially when polaronic processes involve fermion states far below the Fermi level. The last result is quite relevant to the physics of the system and in particular transport properties of cooper benzoate to which the present study addresses in primary. Note also that a spin-Peierls instability in this system is fully consistent with the one-dimensional anisotropy of its electronic structure resulting from the Jordan-Wigner transformation as predicted in the general case of quasi-one-dimensional quantum spin chains coupled to the lattice. For this spin-Peierls instability, important contributions from the Dzyaloshinsky-Moriya interaction parameters D and β are expected in the opening of the gap at the Fermi level k_F^α of the one-dimensional fermion spectrum.

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