Mixing of magnetic and phononic excitations in incommensurate spin-Peierls systems

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We analyze the excitation spectra of a spin-phonon coupled chain in the presence of a soliton. This is taken as a microscopic model of a spin-Peierls material placed in a high magnetic field. We show, by using a semiclassical approximation in the bosonized representation of the spins, that a trapped magnetic state obtained in the adiabatic approximation is destroyed by dynamical phonons. Low-energy states are phonons trapped by the soliton. When the magnetic gap is smaller than the phonon frequencies, the only low-energy state is a mixed magnetophonon state with the energy of the gap. We emphasize that our results are relevant for the Raman spectra of the inorganic spin-Peierls material $CuGeO_3$.

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The discovery in 1993 by Hase, Terasaki, and Uchinokura[1] of the first inorganic spin-Peierls compound $CuGeO_3$ has opened the possibility of study of the physics of this collective phenomena in a deep way. Several experimental proofs have given exhaustive information about the excitation spectra of this system and its evolution with an applied magnetic field. The effect of nonmagnetic impurities has been investigated also.

Theoretical studies have focused on a simplified magnetic model. The excitation spectra in the low-temperature phase have been analyzed using a dimerized and frustrated Heisenberg chain as a minimal model for this material.[3–5] The logic underlying these studies are: the competition between magnetic and elastic energies resolves in the low-temperature phase in the dimerization of the lattice. Once this process takes place, phononic and magnetic excitation completely decouple, and the magnetic excitations are the same as the chemical dimerized system. This point of view is based on an adiabatic approximation supposing that the energy scale of the magnetic process is high enough with respect to the phononic ones. As it has been recently emphasized,[6] this relation is not fulfilled for $CuGeO_3$ where the phonons relevant for the dimerization process are about one order of magnitude more energetic than the magnetic gap. The adiabatic approximation is questionable for this system. An antiadiabatic approach has been developed. The frustrated interaction arises, in this context, from the integration of the in-chain phonons and the explicit dimerization from the interchain interaction treated in a mean-field approximation.[7] The same frustrated-dimerized Hamiltonian is therefore obtained, but with a reinterpretation of the parameters. What is clearly missed in these studies is a general understanding on how spin and phonons mix as elementary excitation and how the spectra of spin-Peierls systems is built as a result of this mixing. Some recent numerical results have partially addressed this question.[8]

In this paper, we analyze the excitation spectra of a one-dimensional spin-phonon system by semiclassical techniques on the bosonized representation of the spin subsystem. We focus on the properties of this system in a high magnetic field. In the dimerized phase, the system is in a singlet ground state. Coupling with a magnetic field is not effective up to a critical field value where some dimer break and their spins are freed from their singlet. The lattice also relaxes in this process forming the so-called soliton lattice. This relaxation is a first indication that spin and phonons do not act as independent excitation. It has been experimentally shown by x-ray measurements that the lattice becomes incommensurate following a soliton pattern.[9] The magnetic profile of the soliton has been analyzed by NMR measurement.[10]

More recently, optical proofs have shown the spectral signature of the incommensurate phase. In the uniform dimerized phase, a low-energy resonance appears at $30\,\mathrm{cm}^{-1}$, which is a smaller energy than two times the magnon gap.[11] This peak has been adjudicated to a bound state of two triplet.[5] When the incommensurate phase appears, the spectral weight is transferred from this state to a lower-energy peak at the position of the magnon gap.[2] Direct magnon process could not be seen in the optical response due to spin conservation. Soliton-assisted one-magnon excitation was recently proposed as the origin of this peak,[2] in similarity with the situation in the presence of nonmagnetic impurities.[12]

This approach is based on the image of the soliton as an isolated spin in the externally dimerized chain so that an adiabatic approximation is supposed. We will show that this state in fact disappears when the dynamics of the phonons is included. We will also show that a trapped magnetophonon state with the energy of the gap appears in the antiadabatic regime, so explaining the optical data.

Let us proceed more formally. Our starting Hamiltonian for a spin-Peierls compound is

$$H = H_{ph} + H_{mg}, \tag{1}$$

$$H_{ph} = \sum_i \frac{P_i^2}{2M} + \frac{K}{2}(u_{i+1} - u_i)^2, \tag{2}$$

$$H_{mg}=\sum_i J\left[1+\frac{\alpha}{2}(u_{i+1}-u_i)\right]\mathbf{S}_i\cdot\mathbf{S}_{i+1}. \tag{3}$$

$\mathbf{S}_i$ are spin-1/2 operators of the i ion and α the magnetoelastic coupling. H_{ph} represents our simplified model for the phonons. It contains a scalar coordinate u_i and its conjugate momentum P_i that are supposed to be the relevant ion coordinates for the dimerization process. As we will only retain the phonons relevant for spin-Peierls (SP) transition, the specific dispersion of the phonons is not important in our approach. The tridimensional character of the phonons field is essential to account for the finite spin-Peierls temperature and the excitations in the low-temperature dimerized phase.[13] We will discuss later its effect on the incommensurate phase.

The low-energy spectrum could be studied by bosonization. The spin variables are approximately represented by the bosonic field $\phi(x)$ and its conjugated momentum $\Pi(x)$.[14] In addition, we retain only the phonon modes producing a smooth deviation of the dimerized pattern. So, we make the replacement $(-1)^i u_i \rightarrow u(x)$. The low-energy Hamiltonian becomes:

$$H_{ph}=\int dx\left\{\frac{aP(x)^2}{2M}+\frac{2K}{a}u(x)^2\right\},$$

$$H_{bos}=\int dx\left\{\frac{1}{2\pi}\left[\frac{v_s}{\eta}[\partial_x\phi(x)]^2+v_s\eta[\pi\Pi(x)]^2\right]+\frac{J\alpha u(x)}{\pi a_0}\sin\phi(x)\right\}, \tag{4}$$

where a is the lattice constant of the original chain and a_0 a short range cutoff introduced in the bosonization procedure. v_s is the spin-wave velocity and η is related with the exponent of the correlation functions. For the isotropic Heisenberg model with nn interaction we have $v_s=Ja\pi/2$ and $\eta=2$.

We use a semiclassical approach in the form of a self-consistent harmonic approximation (SHA) as it has been originally proposed by Nakano and Fukuyama (NF).[15] In this approach, the boson field ϕ is split in a classical component ϕ_{cl} and the quantum fluctuation $\hat{\phi}$. The last term of Eq. (4) is developed up to second order around ϕ_{cl} and then treated self-consistently by the following replacement:

$$\sin\phi\rightarrow e^{-\langle\hat{\phi}^2\rangle/2}\left[\sin(\phi_{cl})\left\{1-\frac{(\hat{\phi}^2-\langle\hat{\phi}^2\rangle)}{2}\right\}+\cos(\phi_{cl})\hat{\phi}\right]. \tag{5}$$

$\langle\hat{\phi}^2\rangle$ is the ground-state expectation value.

In their original work, NF have fixed the displacement field u to its equilibrium classical value (u_{cl}), so that an adiabatic approximation was assumed. Let us summarize the main results of this study and its consequence for the spectra:

(i) The classical equations for ϕ and $u(x)$ have a soliton solution of the form: $\sin(\phi_{cl})=\tanh(x/\xi)$, $u_{cl}(x)=u_0\tanh(x/\xi)$. ξ, the soliton width, is v_s/Δ and Δ is the gap over the homogeneous dimerized state (the ''magnon'' gap) and u_0 are the displacements in this homogeneous dimerized state. The soliton carries $S_z=1/2$ spin. In the presence of an external magnetic field, these solitons will condense in the ground state and accommodate in a soliton lattice structure.

(ii) The creation energy of the soliton, as well as the excitations over this solitonic vacuum, could be evaluated once the eigenvalues of the fluctuation operator are known. This eigenvalue problem corresponds to a one of a Schrödinger-like equation that reads as

$$\{-\nabla^2_{\hat{x}}+\tanh^2(\hat{x})\}\psi_\lambda=\frac{\Omega(\lambda)^2}{\Delta^2}\psi_\lambda(\hat{x}),$$

$$\hat{x}\equiv\frac{x}{\xi}. \tag{6}$$

$\Omega(\lambda)$ are the frequency oscillations in the presence of the soliton. Eq. (6) has one bound state at $\Omega_b/\Delta=\sqrt{\sqrt{5}-1/2}\sim 0.786$ and a continuum started at $\Omega=\Delta$. The excitation spectra of the theory is spanned by the following state:

(iii) The ground state of the quantum soliton builded around ϕ_{cl}. Their creation energy (E_s) is given by its classical energy plus the difference between the sum of the zero point energies of the oscillators $[\Omega(\lambda)]$ and the ones in absence of the soliton. This creation energy measures the critical field for the commensurate-incommensurate transition.[15]

(iv) The excited state of the soliton with energy $E_s^*=E_s+\Omega_b$. It is related with the bound state of Eq. (6).

(v) Labeling by q the continuum of level of Eq. (6), they are $\Omega(q)=v_s\sqrt{q^2+1/\xi^2}$. This is just the kinetic energy of a particle in the soliton-free sector. In terms of the original spin chain, this is the low-energy dispersion of the $S_z=0$ component of a magnon. Therefore, this state corresponds to the scattering of a magnon in the presence of the soliton. Moreover, when one of the continuum modes is excited once, we get a two-particle magnon-soliton state.

The two last adjudication of states have not been done in the original analysis of the NF work. As our formalism breaks SU(2) symmetry at an intermediate stage, the total spin of each state is not directly accessible and should be carefully reanalyzed. We have previously stated that the states below the continuum correspond to the emission of a magnon in the presence of the soliton. Therefore they have total spin 3/2. The bound state has the same total spin as the soliton. Then, it is an optical active mode and it is the analogue in our formalism of the so-called soliton-assisted magnon process founded in the strong dimerization limit.[12]

Moreover, the previous predicted spectra could be tested by numerical exact diagonalization on a finite chain. To this end, we solve iteratively the adiabatic equations for u_i arising from Hamiltonian Eq. (1). The ground state of the spin system was recalculated at each iteration step by Lanczos diagonalization. We considered chains of an odd number of sites up to $L=23$ sites with periodic boundary conditions and look for the equilibrium positions in the subspace $S_z=1/2$. The numerical details of the method was given in Refs. 17,18.

Once the ionic coordinate converge, we diagonalize the spin Hamiltonian, with fixed u_i, to obtain the low-lying ex-

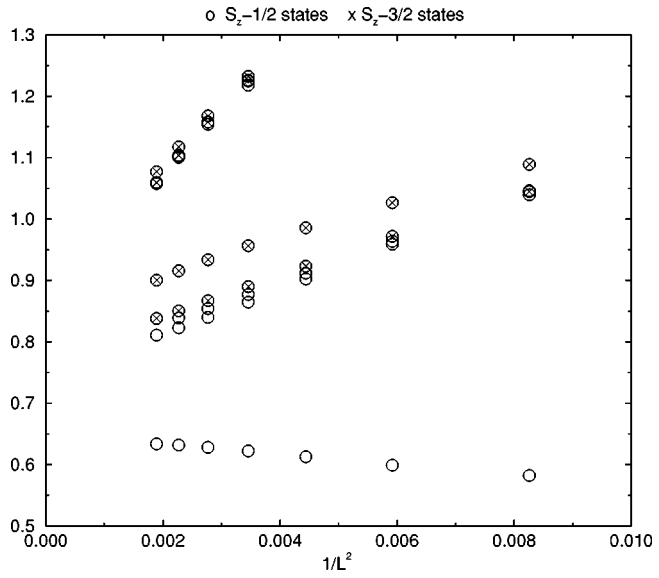

FIG. 1. The excitation spectrum calculated by Lanczos diagonalization in the presence of an adiabatic soliton. Circles are for states of $S_z=\frac{1}{2}$ and crosses for $S_z=\frac{3}{2}$. The zero of the energies is chosen at the soliton ground state. Energies are in units of J.

citation in the $S_z=1/2$ and $S_z=3/2$ subspaces. The results are shown in Fig. 1 as a function of the $1/L^2$. Parameter $K/(\alpha J)^2=\frac{1}{4}$ has been chosen in order to have a thin soliton and to reduce the finite-size effect. The bound state predicted by the bosonized theory is clearly seen. The higher-energy states collapse in a continuum of total spin 3/2 in the thermodynamical limit. By linear extrapolation, we found for $L\rightarrow\infty$ the ratio 0.84 between the bound state and the border of the continuum. This value compares well with our previous prediction of 0.786. We conclude that the method gives at least a qualitative feature of the low-energy spectra. The states appearing in the border of the continuum in Fig. 1 are an artifact of the strongly thin soliton we are considering. We have checked that for bigger values of $K/(\alpha J)^2=\frac{1}{4}$, these states in fact disappear.

We discuss in the following, two effects that could change our estimated value of the bound state from the SHA method:

(1) Going from Eq. (1) to Eq. (4), we have neglected, as did NF in their original work, a term proportional to $\cos(2\phi)$ in the bosonized theory. Even though this operator plays an important role in the case of Ising anisotropy, it is a marginally irrelevant operator in the Heisenberg case and therefore it should not change the qualitative features previously discussed. Moreover, NF have studied in a further contribution[16] the effect of this term. Unfortunately, the estimation of the bound-state value is strongly dependent on the value of the cutoff in the bosonization procedure (a_0) in this situation. If we assume, as NF did, that $\pi a_0=a$, the bound state becomes $\Omega_b\Delta=\sqrt{\sqrt{3}/2}\sim 0.93$. We can conclude as a general fact that the presence of this term tends to increase the bound-state value.

(2) It has been recently noted[19,20] that a full self-consistent treatment (where $\langle\phi^2\rangle$ in Eq. (5) is not fixed to its value in the ground state) changes the form of the soliton. Moreover, it has been shown in Ref. 20 that this treatment produces a smoother soliton than the one considered here. Therefore, we conclude that this treatment will reduce the bound-state value.

In the following, we analyze the evolution of the spectra when nonadiabatic effects are included. For simplicity, we do not introduce the two additional effects previously discussed. These effects will not affect the prediction of the trapped magnetophonon state we will find.

Inclusion of nonadiabatic effects. To go beyond this static adiabatic approximation in this semiclassical calculation it is necessary to include fluctuations in the displacement field $u(x)$. Therefore, we split $u(x)$ as $u_{cl}+\hat{u}$ and replace it in Eq. (4). This approach was already used by Takano, Nakano, and Fukuyama (TNF)[21] to study the translational mode of the soliton lattice in a nearly half-filled Peierls system with interaction between the parallel spin electrons.

The classical equations are the same as before. The fluctuation operator is now a 2×2 differential operator with a component over u and ϕ. The eigenvalue problem is now given by:

$$\Delta^2[-\nabla_{\hat{x}}^2+\tanh^2(\hat{x})]\psi_1+\frac{u_0}{a}\,8\pi K v_s\,\mathrm{sech}(\hat{x})\,\psi_2=\Omega^2\psi_1,$$

$$\omega^2 u_0\,\mathrm{sech}(\hat{x})\,\psi_1+\omega^2\psi_2=\Omega^2\psi_2. \tag{7}$$

ψ_1 and ψ_2 are the component of the fluctuation eigenvector over ϕ and u, respectively. $\omega=\sqrt{4K/M}$ is the phonon frequency at $q=\pi$. The eigenfrequency are as previously given by Ω.

Equation (7) is the same as Eqs. (4.13) and (4.14) of Ref. 21. However, as we work in the one soliton sector the elliptic functions of Ref. 21 become the hyperbolic functions of Eq. (7) and the relevant electronic degree of freedom that were the charge fluctuation in Ref. 21 is the bosonized spin variable ϕ in our purely magnetic spin-Peierls system.

We obtain from the second equation of Eq. (7):

$$\psi_2=\frac{u_0\omega^2\,\mathrm{sech}(\hat{\mathrm{x}})}{\Omega^2-\omega^2}\psi_1. \tag{8}$$

Replacing in the first equation, we have a kind of Schrödinger equation where the potential depends on the energy. This equation reads:

$$\{-\nabla_{\hat{x}}^2+\tanh^2(\hat{x})\}\psi_1+\left(\frac{\omega}{\Delta}\right)^2\frac{\mathrm{sech}^2(\hat{x})}{\left(\frac{\Omega}{\Delta}\right)^2-\left(\frac{\omega}{\Delta}\right)^2}\psi_1=\left(\frac{\Omega}{\Delta}\right)^2\psi_1. \tag{9}$$

It is worthy to note that the only relevant parameter is ω/Δ. Then, we can follow the evolution of the spectra from the adiabatic to the antiadiabatic limit by moving this parameter.

We have numerically solved Eq. (9). In Fig. 2, we show the evolution of the excitation spectra as a function of ω/Δ. The soliton creation energy has been taken as the zero of the energy.

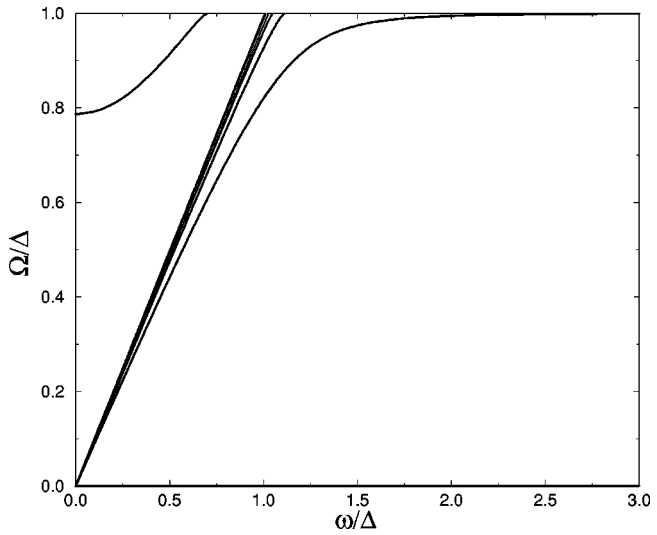

FIG. 2. The excitation spectrum as a function of the phonon frequency. Both energy scales are given in units of the magnon gap (Δ).

The main results are:

• There is a zero-energy solution that was not present in the adiabatic calculation. This mode was originally found by TNF and it is a consequence of the translation invariance of the theory. It is nothing but the translational mode of the soliton. In a realistic situation, solitons are not isolated, they form a soliton lattice. This zero mode will acquire some dispersion giving rise to the so-called phason modes of the soliton lattice. The dispersion of this mode was in fact studied by TNF in Ref. 21. If the magnetic field is not much higher than the critical one, the solitons will be rather separate and we can neglect their interference.

• In the direction perpendicular to the magnetic chains, solitons will accommodate in a domain wall, i.e., they form an array of parallel solitons. Their coherency is assured by the interchain elastic coupling. The zero mode, as well as all the states of the spectra, will have a transversal dispersion, they will depend on the momentum perpendicular to the chains. The spectrum shown in Fig. 2 gives the $q=0$ excitations. We will analyze their dispersive character in a forthcoming work.

• The upper branch corresponds to the excited state of the soliton previously found in the adiabatic approximation. Its energy increases with ω up to a critical value $\omega^2/\Delta^2=\frac{1}{2}$ where this state disappear. For this ω and $\Omega=\Delta$, the energy-dependent potential vanishes. The lattice soliton produces an harmonic potential over the magnetic soliton where it oscillates. In the adiabatic approximation, the lattice soliton is frozen and the magnetic one oscillates. For finite ω, the lattice soliton can also move and vibrate with respect to the magnetic deformation. Finally, at the critical value of ω, there is no more a localized vibration and the soliton becomes an unique entity both for the lattice and for the spins. This explains the disparition of the trapped state at a critical phonon frequency.

• The straight line of slope one in Fig. 2 corresponds to $\Omega=\omega$. The eigenstate with this energy corresponds to the excitation of a phonon in the presence of the soliton. The eigenvalues near above are satellite phonons corresponding to phonons trapped by the soliton (i.e., particle vibrations near the soliton). They have only spectral weight on the phonons as it can be seen putting in Eq. (8) $\Omega\sim\omega$. For increasing phonon frequency, most of these eigenvalues lose, but the lowest survives acquiring the energy of the magnetic gap. This state is a mixing of a magnetic and a phononic excitation, as we show in the following.

• Four Peierls active phonons have been identified for $CuGeO_3$.[22] They have frequencies of 3.12, 6.53, 11.1, and 24.6 THz, i.e., the smaller one is about 150 K. The spin gap is rather small for this system $\Delta=24$ K. As we previously stated, the real parameter regime where this material lives is $\omega>\Delta$ and the only survival bound state has the energy of the gap. This is a singlet state that we associate with the low-energy peak seen in Raman scattering in the incommensurate phase.[2] The ψ_1 and ψ_2 components of the corresponding eigenfunction are different from zero for this state.

Their mixed character could be advocated by analyzing separately the magnetic and phononic spectral response. The magnetic Raman operator of a dimerized chain is given by $\mathcal{R}_{mg}=\Sigma_i[1+\gamma_{mg}(-1)^i\mathbf{S}_i\cdot\mathbf{S}_{i+1}]$ (Ref. 23) γ_{mg} is a microscopic parameter. In our bosonized formalism, the most relevant contribution comes from the staggered part and it is given by $(\gamma_{mg}/\pi a_0)\sin(\phi)$. By using the SHA given by Eq. (5), retaining the term linear in $\hat{\phi}$ and developing in the basis of the eigenvalues of the fluctuation operator the magnetic spectral weight (M_n) of an state of energy Ω_n is given by:

$$M_n=\frac{\gamma_{mg}^2}{2\Omega_n}\left\{\frac{4K}{J\alpha a}\,\frac{\Omega_n-\omega^2}{\omega^2}\int\psi_2 dx\right\}^2, \tag{10}$$

where we have used Eq. (8) to write ψ_1 as a function of ψ_2. Phonons contribution to Raman scattering is proportional to the square of the transition elements of the normal coordinates $\mathcal{R}_{ph}=\gamma_{ph}\int(dx/a)u(x)$, the phonons spectral weight of the n state is given by:

$$P_n=\frac{\gamma_{ph}^2}{2\Omega_n}\left\{\int\psi_2\frac{dx}{a}\right\}^2. \tag{11}$$

The relation between the magnetic and phononic contribution to the nth peak of the spectra is

$$\frac{M_n}{P_n}=\frac{\gamma_{mg}^2}{\gamma_{ph}^2}\left\{\frac{4K}{J\alpha}\right\}^2\left\{\frac{\Omega_n-\omega^2}{\omega^2}\right\}^2. \tag{12}$$

We take the first two factors as a measure of the spin-phonon coupling, we fix this parameter when moving ω. Equation (12) shows that the magnetic component of a given Raman peak increases when its position shifts from a phonon frequency. The lower-energy eigenvalue of Fig. 2 starts being a trapped phonons for $\omega/\Delta<1$ and transmutes in a magneto-phonon in the opposite limit where the real material lives. Its existence is a consequence of the quasi-one-

dimensional character of our system because a one-dimensional well has always one bound state.

In summary, we have shown that nonadiabatic effects are relevant for an incommensurate spin-Peierls system. In the antiadiadatic limit applicable to $CuGeO_3$, we show the apparition of a trapped mixed state with the energy of the magnon gap. It gives an alternative explanation of the Raman-induced peak found in the incommensurate phase of $CuGeO_3$.

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