Excitations with fractional spin less than $\frac{1}{2}$ in frustrated magnetoelastic chains

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We study the magnetic excitations on top of the plateaux states recently discovered in spin-Peierls systems in a magnetic field. We show by means of extensive density matrix renormalization group (DMRG) computations and an analytic approach that one single spin-flip on top of $M=1-\frac{2}{N}$ $(N=3,4,\ldots)$ plateau decays into N elementary excitations each carrying a fraction $\frac{1}{N}$ of the spin. This fractionalization goes beyond the well-known decay of one magnon into two spinons taking place on top of the $M=0$ plateau. Concentrating on the $\frac{1}{3}$ plateau $(N=3)$ we unravel the microscopic structure of the domain walls which carry fractional spin-$\frac{1}{3}$, both from theory and numerics. These excitations are shown to be noninteracting and should be observable in x-ray and nuclear magnetic resonance experiments.

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Constitutive elements of condensed systems and their interaction laws are all well known and in spite of this, modern condensed matter physics is a field where new fundamental concepts arise continuously, mainly due to strong correlation effects. The clue is that the emergent laws governing a system of many interacting bodies could have no direct relationship with the behavior of each individual member. In other words, the interaction processes could wash out the individual properties of the constituents and give rise to excitations of fundamentally new character.[1] Specifically, a new paradigm is now arising in the field of strongly correlated electron systems, where the concept of Fermi liquid theory is not applicable any more. Collective excitations with quantum numbers essentially different than those of the individual electrons are now predicted and observed in a variety of systems.

The earliest example arose in the 1970s in the study of conducting polymers as polyacetylene. For this system, it was proposed that conduction was due to solitons carrying the electronic unit charge but no spin. The emergence of these quasiparticles carrying different quantum numbers than the original constituent, was understood as a consequence of electron-phonon interactions.[2] Another example is provided by a two-dimensional layer of electrons in a high magnetic field. In the so-called fractional quantum Hall effect regime at a certain filling fraction corresponding to a plateau in the conductivity, the charge of the elementary excitations is a fraction of the electronic charge. The statistical properties of these quasiparticles are intermediate between fermionic and bosonic and they are termed "anyons."[3]

Understanding the mechanisms through which collective processes could produce excitations different in character than the original constituents of a solid state system is currently under intense study. In particular, making specific predictions of the effects of these excitations on the experimental observations is a very important issue of modern condensed matter physics.

In studying the properties of many-body systems, magnetic systems have provided a fertile playground especially for elucidating very important aspects of reduced dimensionality and strong correlations. When one flips the spin of an individual electron (say $S^z=-\frac{1}{2}\rightarrow S^z=\frac{1}{2}$) the total spin of the system changes by one unity, $\Delta S^z=1$, so one has created an excitation carrying spin $S^z=1$. In a three-dimensional system this excitation was ascribed to be carried by a bosonic particle called a magnon, a quantum of a spin wave. It came as a big surprise when Fadeev and Takhtajan identified the elementary spin quantum number of a spin wave as $S^z=\frac{1}{2}$ in the one-dimensional world, calling them spinons.[4] One can "have a look" at these spinons if one introduces sufficiently strong frustration in the one-dimensional Heisenberg chain so that the ground state becomes dimerized. Then the spinon acquires a finite gap and it is visualized as a free spin separating the different domains of dimerization as depicted in Fig. 1.

Apart from the natural $S^z=\frac{1}{2}$ value (which could still be ascribed to the individual electron) no other fractional values were observed in experiments.

The present paper is devoted to the study of fractional spin excitations that go beyond the usual fractionalization of a magnon into two spinons discussed above. For example, as we discuss below, the excitations on top of the $M=\frac{1}{3}$ plateau carry a fractional spin $S^z=\frac{1}{3}$, which we dub "tertions." This fractionalization takes place due to collective effects in certain magnetoelastic systems under a strong magnetic field. These excitations should be observable in spin-Peierls sys-

FIG. 1. Deconfined spinons in dimerized chain, connected black dots represent dimers - spin singlet combination of two neighboring spins, arrow is for free spin.

tems like $CuGeO_3$ and in Ising antiferromagnetic chains susceptible to lattice deformations. These tertions should condense as a soliton lattice in the ground state of a system under a magnetic field greater than the value corresponding to the $M=\frac{1}{3}$ plateau. This would allow to directly observe these objects in nuclear magnetic resonance (NMR), x-ray or neutron scattering experiments as has been the case with closing the zero magnetization gap.[5,6]

The lattice Hamiltonian of a frustrated spin chain coupled to frozen phonons in a magnetic field reads as[7]

$$\mathcal{H} = \frac{1}{2}K\sum_i \delta_i^2 + J_1\sum_i (1 - A_1\delta_i)\vec{S}_i \cdot \vec{S}_{i+1} + J_2\sum_i \vec{S}_i \cdot \vec{S}_{i+2} - H\sum_i S_i^z, \quad (1)$$

H is measured in units where $g\mu_B=1$, δ_i is the distortion of the bond between site i and $i+1$, K the spring constant and the first term corresponds to the elastic energy loss. J_1 sets the overall energy scale, and $\sqrt{\frac{J_1}{K}}$ a corresponding distance scale. From now on, we fix $J_1=K=1$ to get dimensionless energies and distances.

Recently we have shown that plateaux can be present for magnetization values $M=1-\frac{2}{N}$, with $N=2,3,4,\ldots$ being the length of the periodic cell of the ground state in units of the lattice constant. The actual presence of these plateau depends on the strength of frustration, except for the $M=0$ plateau ($N=2$) which is always present. The simplest nontrivial ones, at $M=\frac{1}{3}$ ($N=3$) and $M=\frac{1}{2}$ ($N=4$), have been observed clearly in numerical simulations for moderate values of frustration J_2 and spin-lattice coupling A_1.[7]

We have found that these plateaux are due to the next-to-leading transfer processes becoming commensurate, in first order of the spin-phonon interaction, and they appear at special rational magnetization values in accordance with Ref. 8. For the $M=\frac{1}{3}$ plateau this corresponds to the process of transferring two particles from, say, the left to the right Fermi point, and for the $M=\frac{1}{4}$ plateau, a process involving the transfer of three particles from the left to the right Fermi point. Those plateaux are generically less wide than the zero magnetization plateau which is caused by the doubling of the amplitude of the basic transfer process at $M=0$.

Close to the zero magnetization plateau, the modulation of the lattice distortions breaks into domains corresponding to a soliton lattice.[9] Domain walls carry spin $S^z=\frac{1}{2}$ and are deconfined. In analogy to the above picture our purpose is to study the excitations on top of the nontrivial magnetization plateaux at $M=1-\frac{2}{N}$, $N=3,4,\ldots$ to show that one spin-flip decays into N free fractional spin excitations, with spin $S^z=\frac{1}{N}$. To this end, we analyze the formation of a soliton lattice on top of the $\frac{1}{3}$ plateau state, which is an up-up-down (*uud*) modulated structure in the frustrated antiferromagnetic spin chain coupled to adiabatic phonons.

Fractionally charged excitations in the systems with commensurability 3 were studied in the early 1980s in one-dimensional electron- phonon systems numerically[10] and by bosonization.[11] In the case of 1/3 electron filling these works identified elementary excitations carrying charge and spin

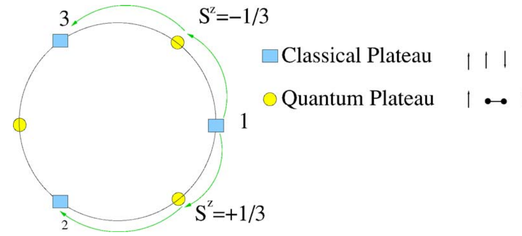

FIG. 2. (Color online) Values of the (periodic) bosonic field for different $M=\frac{1}{3}$ ground states. Squares correspond to the three (classical) configurations and circles to the quantum counterpart (Ref. 19).

values (in addition to polaronic excitation with ordinary electronic quantum numbers): $\Delta Q=\pm e/3$, $\Delta S=1/2$ and $\Delta Q=\pm 2/3$, $\Delta S=0$, respectively. Our case corresponds to 1/2 electron filling, with completely frozen charge fluctuations. As we will show in this case spin excitations will be fractionalized in the units of 1/3. Since the charge field is suppressed there is no direct analogy between the quantum numbers of the excitations for electronic systems and our magnetic system which is equivalent to the system of spinless electrons.

We developed a self-consistent harmonic approximation (SCHA) in analogy to the zero magnetization case and our findings are fully confirmed by extensive DMRG computations.

The bosonized version of Eq. (1) reads like

$$H = H_0 + H_{ph} + H_{sp}, \quad (2)$$

where H_0 is a Gaussian part, H_{ph} is the adiabatic phonon part, and H_{sp} is the spin-phonon interaction term which, around $M=\frac{1}{3}$ is given by[7]

$$-A_1\int dx\,\delta(x)[\beta{:}\cos(\sqrt{2\pi}\phi){:} + \gamma{:}\cos(2\sqrt{2\pi}\phi){:}], \quad (3)$$

where $\delta(x)$ is the smooth part of the displacement field in the continuum limit and columns $:\cdots:$ indicate normal ordering of the vertex operators with respect to the ground state with magnetization M. For $k_F=\frac{\pi}{3}$ there are three inequivalent minima which are degenerate, which correspond to the three different *uud* arrangements. In terms of the phonon and bosonic fields, they correspond to $\delta_p(x)=\delta_0\cos[2k_F(x+p)]$ ($p=0,1,2$) and $\sqrt{2\pi}\phi=0, \pm\frac{2\pi}{3}$, respectively. These three structures are clearly observed in the numerical simulations.

An interesting observation is that singlets can always appear in domain walls because when tunnelling from the first vacuum to the second or third, the field rests on the intermediate pseudominimum in between (which turns out to be a portion of the quantum plateau indicated by yellow circles in Fig. 2).

Let us now analyze the excitations on top of the $M=\frac{1}{3}$ plateau. In the pure spin case, the potential energy is given simply by $V[\phi]\propto\int dx\cos(3\sqrt{2\pi}\phi)$, which also has three degenerate minima.[12] From this potential, one immediately concludes that the excitations on top of the plateau correspond to massive kinks (whenever $V[\phi]$ is a relevant perturbation) interpolating between these inequivalent minima, and carry fractionalized spin-$\frac{1}{3}$.[12]

In the spin-phonon case, the situation is more subtle, since now the three minima correspond to combined magnetoelastic configurations as we discussed above. To see how fractional spin kinks arise in that case, we resort to a SCHA along the lines of Refs. 13–15.

Following Refs. 13–15 we split ϕ into classical and quantum components, $\phi = \phi_c + \phi_q$. Using the value of k_F for $M = \frac{1}{3}$ and keeping only commensurate terms, we arrive at the following potential for the classical bosonic field:

$$V[\phi_c] \sim -\int dx \cos(3\sqrt{2\pi}\phi_c) \tag{4}$$

which led us to conclude that kinks are similar to those in the pure spin case, though now both spin and phonon modulations must combine appropriately. Below we find the explicit expression for the local magnetization and bond modulations and compare them with our numerical results obtained by DMRG.

Let us start discussing how ϕ_c evolves as we walk around a chain with periodic boundary conditions (PBC). We start from the vacuum corresponding to $\sqrt{2\pi}\phi_c = 0$, then we have a tunnelling of $\sqrt{2\pi}\phi_c$ from $0 \to \frac{2\pi}{3}$, at the position of the first domain wall (let us call this point x_1), then a tunnelling process from $\frac{2\pi}{3} \to \frac{4\pi}{3}$ takes place (at x_2) and at the position of the third domain wall (x_3) the initial vacuum is restored by tunnelling $\frac{4\pi}{3} \to 0$. An analytic expression for ϕ_c can be built up as a product of three soliton solutions of the sine-Gordon model[16] centered at x_1, x_2, and x_3. It reads

$$\begin{aligned} 3\sqrt{2\pi}\phi_c(x) = \frac{1}{8\pi^2}\Big[& 4\arctan\{\exp[(x-x_1)/\xi]\} \\ & \times(2\pi + 4\arctan\{\exp[(x-x_2)/\xi]\}) \\ & \times(4\pi + 4\arctan\{\exp[(x-x_3)/\xi]\})\Big] \end{aligned} \tag{5}$$

with ξ being the soliton width. From Eq. (5) and the bosonization formulas connecting $\phi(x=ia)$ with S_i^z (Ref. 17) we extract the local magnetization of every three sites,

$$\begin{aligned} \langle S_\alpha^z(3x)\rangle = {} & \frac{1}{6\pi}\partial_x\phi_c(x) - B_1\cos\left(\sqrt{2\pi}\phi_c(x) + \frac{4\pi}{3}\alpha\right) \\ & - B_2\cos\left(2\sqrt{2\pi}\phi_c(x) + \frac{8\pi}{3}\alpha\right) + \frac{1}{6}. \end{aligned} \tag{6}$$

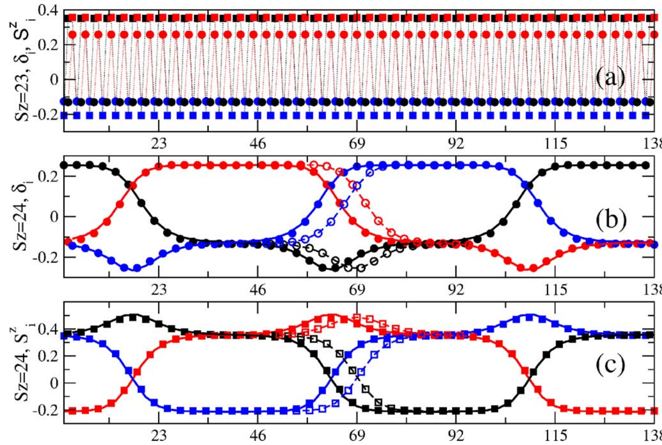

FIG. 3. (Color online) DMRG solution for $N_s = 138$, $J_2 = 0.5$, and $A_1 = 0.6$. We represent with circles (squares) symbols δ_i ($\langle S_i^z\rangle$), using different colors for each of the three sublattices. (a) Results for $M = \frac{1}{3}$ in our system. (b) and (c) show the results for the next magnetization over $M = \frac{1}{3}$. Solid lines in (b) and (c) correspond to the modulations obtained within the SCHA (Ref. 14). Three well-defined excitations are seen as what we call tertions. Open symbols and dotted lines correspond to DMRG and bosonization results for a second pattern where the central tertion is shifted. Both patterns have the same energy, showing that tertions are noninteracting.

As anticipated, singlets indeed appear within domain walls. This is because when tunnelling from one vacuum to another, the field passes through the intermediate pseudominimum in between, which is exactly a portion of the quantum plateau[18,19] (see Fig. 2). Here we would like to note that in the absence of the spin phonon coupling the $\frac{1}{3}$ magnetization plaetau in the J_1-J_2 model was for the first time identified for stronger values of J_2 by Okunishi and Tonegawa[20] who also identified similar fractionalized spin-$\frac{1}{3}$ excitations around it.[21] They connected this excitation with a domain wall in the Ising limit, microscopically different from a singlet-core excitation that is realized in our case of additional spin phonon interaction and SU(2) symmetric spin exchange.

We now undertake a numerical analysis of the lattice deformations (δ_i) and the local magnetization ($\langle S_i^z\rangle$) around the plateau at $M = \frac{1}{3}$. We have used an iterative method based on a DMRG procedure to solve the adiabatic equation corresponding to Hamiltonian (1) along the lines stated in Ref. 7. To compare with the previous analytical study, we consider PBC, and the calculations were carried out keeping $m = 200$ states, with a truncation error of order 10^{-11}.

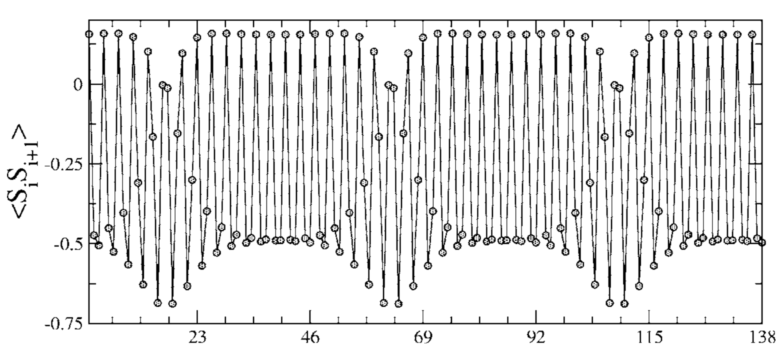

FIG. 4. DMRG results for the same set of parameters used in Fig. 3 for the local spin-spin correlation function.

With $M=\frac{2S^z_{\rm tot}}{N_s}$, we want to study the states for $M=\frac{1}{3}$ and one unit of magnetization above it. The iterative procedure for the δ_i, takes around 100 iterations to achieve convergence in a particular N_s. Note however that a periodic pattern with a wavelength $\lambda=n\frac{2}{1+M}$ (n integer) is expected for each magnetization M.[7] Therefore, to reduce the CPU time we impose such a periodicity for both M, on the δ_i pattern in our numerical calculation, choosing $N_s=138$. Then we study for values of $S^z_{\rm tot}=23$ and 24, and this enforcement helps us to obtain very accurate results for the states we are interested in. In Fig. 3 we show the results of δ_i and S^z_i for a particular set of parameters where the plateau at $M=\frac{1}{3}$ is present. In Fig. 3(a), for $S^z_{\rm tot}=23$, $\lambda=3$ the up-up-down structure is clearly seen, corresponding to a weak-weak-strong structure for the bonds. Figures 3(b) and 3(c) show magnetization and distortion, respectively, for $S^z_{\rm tot}=24$, $\lambda=46$.

The patterns obtained for δ_i and S^z_i are oscillatory on the scale of the lattice constant. We separate the lattice in three different sublattices to extract the smooth variations of the relevant quantities. Three different excitations are clearly identified which are characterized as domain walls of the *uud* order. As the total spin of this state is $S^z=1$ above the $M=\frac{1}{3}$ state, each excitation carries $S^z=\frac{1}{3}$ and for this reason we term them tertions. Moreover, a very accurate fitting could be found between the DMRG results and the analytic form given in Eq. (6). Lines on Fig. 3(c) were obtained from this expression with parameters $B_1=0.35$, $B_2=0.03$, and the soliton width in units of three lattice sites, $\xi=4.5$.

In Figs. 3(b) and 3(c), we added further DMRG results and the analytical fitting, now shifting the position of the second domain wall, and running the code again without forcing the periodicity. The overall coincidence between the bozonization and DMRG results and the fact that both states have the same energy confirm that the excitations correspond to noninteracting solitons with fractionalized spin $S^z=\frac{1}{3}$. DMRG results for other lattice sizes not shown here lend further support to this conclusion of independence, in particular since Eq. (6) perfectly fits in all cases the numerical results using the same set of constants B_1, B_2, and ξ. We also checked that excitations behave similarly for different sets of parameters where the $M=\frac{1}{3}$ plateau is present.

Finally, let us analyze the internal structure of these tertions. Looking at the tertion placed at the center of the lattice, it can be seen in Fig. 3(c) that S^z has greater value at position 63, and almost vanishes at sites 61–62 and 64–65. This fact points towards singlet formation as we have predicted theoretically. In fact, we have calculated the spin-spin correlation $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle$ shown in Fig. 4, and we obtain that the value $\sim -\frac{3}{4}$ at the bonds around each tertion is centered. Depending on the system size, the quantum plateau portion can be longer or shorter.

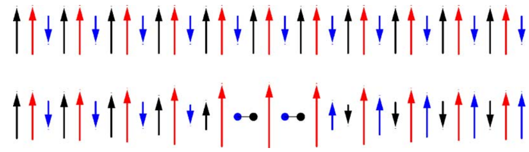

FIG. 5. (Color online) Scheme of the magnetic structure of the state at $M=\frac{1}{3}$ (upper panel) and a tertion (lower panel) as given by DMRG calculation for the same parameters of Fig. 3. The length of the arrows is proportional to $\langle S^z_i \rangle$.

In conclusion we have shown that plateaux in magnetoelastic systems, independently of the mechanism that produce them, involve the development of a soliton lattice at the threshold. We have also shown that solitons-domain walls carry fractional spin values which are generically smaller than $\frac{1}{2}$, in particular for the excitations around the $M=\frac{1}{3}$ plateau, noninteracting quasiparticles with fractional spin $S^z=\frac{1}{3}$ arise. We have also identified the core of the domain wall as singlets in the case of the $M=\frac{1}{3}$ plateau (Fig. 5). We hope that our predictions will stimulate further high field experiments on spin-Peierls compounds. Like for the case near $M=0$ in the spin-Peierls material $CuGeO_3$,[5] the lattice deformation we predict could be measured in x-ray or neutron scattering experiments. The local magnetic texture could otherwise be seen in NMR experiments as in Ref. 6.

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