Magnetization plateaux induced by a coupling to the lattice

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We investigate a simple model of a frustrated spin-1/2 Heisenberg chain coupled to adiabatic phonons under an external magnetic field. Using field theoretic methods complemented by extensive Density Matrix Renormalisation Group techniques generalized to include self-consistent lattice distortions, we show that magnetization plateaux at non-trivial rational values of the magnetization can be stabilized by the lattice coupling. We suggest that such a scenario could be relevant for some low dimensional frustrated spin-Peierls compounds.

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The field of quantum spin chains offers a wonderful playground for both theorists and experimentalists to investigate a variety of exotic phases cooperatively induced by frustration and magnetic field. The so-called zig-zag chain with nearest neighbor (NN) and next nearest neighbor (NNN) Heisenberg couplings $J_1$ and $J_2$ is a fundamental and simple model of a quantum (S=1/2) spin system exhibiting a quantum (i.e. $T = 0$) phase transition (at zero magnetic field) between a quasi-ordered antiferromagnetic phase (so-called Tomonaga-Luttinger liquid (TL)) and a spontaneously dimerized gapped phase $\mathcal{H}$. The related quantum critical point is known accurately to be located around $(J_2/J_1)_{\text{crit}} = 0.2411 \pm 0.0002$. Interestingly enough, SrCuO$_2$ $\mathfrak{R}$ and copper germanate (CuGeO$_3$) $\mathfrak{A}$ are fairly good experimental realizations of the zigzag chain in the uniform and dimerized phases respectively.

The underlying richness of the zig-zag chain physics is also manifest under an external magnetic field $\mathfrak{R}$. The magnetic phase diagram shows, besides the previously discussed dimerized phase (at sufficiently low field) and several types of TL phases including a chiral phase $\mathfrak{A}$ (with spontaneously broken parity), a new phase which exhibits (i) a spontaneous breaking of the lattice symmetry of period $q = 3$ and (ii) a magnetization plateau at 1/3 of the full moment, $M = 1/3$ (we normalize the magnetization $M$ as being 1 at saturation). Note that both features (i) and (ii) are expected simultaneously from the quantization condition $qS(1-M)$ integer $\mathfrak{R}$. Note that the 1/3 plateau state is only stable in the range $0.56 \leq J_2/J_1 \leq 1.25 \mathfrak{R}$. Recent Density Matrix Renormalization Group (DMRG) computations suggest also that this state supports fractional magnetization $S_Z = \pm 1/3$ domain-wall type excitations $\mathfrak{R}$.

Although its large variety of different phases the magnetic phase of the simple zig-zag chain model does not show other plateau phases besides the 1/3 plateau state. In this Letter, supported by both analytical and numerical calculations, we argue that a moderate lattice coupling can generate an extremely rich magnetic phase diagram with a zoo of new $M = p/q$ (rational) plateau states. Experimentally, the lattice coupling is known to be crucial in spin-Peierls materials like CuGeO$_3$ $\mathfrak{A}$. It has also been proposed to be responsible for a spontaneous tetramerization $\mathfrak{A}$ in the spin-1/2 LiV$_2$O$_5$ chain compound $\mathfrak{A}$. A cooperative effect of the magnetic field and the coupling to an adiabatic lattice was shown to produce in 2-leg spin ladders long-range modulated structures $\mathfrak{A}$ for several rational values of the magnetization M. Although the quantization condition $\mathfrak{R}$ suggests that the modulated states of Ref. $\mathfrak{A}$ could give rise to magnetization plateaux, a theoretical investigation of lattice-induced plateau phases in quantum spin systems has not been carried out so far $\mathfrak{A}$. In this Letter such an investigation is performed in the case of the zig-zag chain geometry (which can be smoothly connected to the ladder geometry).

The Hamiltonian of a frustrated spin chain coupled to adiabatic phonons in a magnetic field $H$ is written as,

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

$H$ is measured in units where $g \mu_B = 1$, $\delta_i$ 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 energy scale and we fix $J_1 = 1$ in what follows.

The spin-lattice coupling $A_1$ is dimensionless so that the distortions $\delta_i$ are given in units of the lattice spacing. Following $\mathfrak{A}$ we redefine the coupling strengths as $\tilde{A}_1 =$...
At zero field this modulation produces a total energy gain given by
\[ E_{\text{mod}}(\{\delta(x)\}) = K\delta_0(0)^2 - \beta A_1\delta_0(0) \int dx : \cos(\sqrt{2\pi}\phi) : \]
while for non-zero field we have
\[ E_{\text{mod}}(\{\delta(x)\}) = \frac{K}{2}\delta_0(M)^2 - \frac{\beta}{2}A_1\delta_0(M) \int dx : \cos(\sqrt{2\pi}\phi) : -\hbar^2 M. \]

If we assume a smooth variation of \( \delta_0(M) \) with \( M \), we can conclude that we need a finite magnetic field to start increasing \( M \) from zero. In that case we have a plateau at \( M = 0 \) up to a critical field \( h_c \), after which the magnetization jumps to the value \( M_s \) such that the product \( -h_c M_s/2 \) is of the order of the contribution to the energy due to the modulation \( E_{\text{mod}} \), Eq. (7). Due to the presence of the relevant term \( \propto \cos(\sqrt{2\pi}\phi) \), the system has a spin gap for all magnetizations. However, the situation described above (plateau and jump) occurs only around \( M = 0 \) and there are no further plateaux in the magnetization curve, in accordance with the numerical results. The ground state structure above the \( M = 0 \) plateau has been studied extensively (see e.g. \[18\] and references therein) and it comes out that a soliton lattice with a periodicity \( 2k_F \) starts to develop. The only difference found in the magnetization curve between simulations with fixed and adaptive modulation (when the lattice deformation is determined from minimizing the total energy in a self-consistent iterative form) is a change in the order of the transition from \( M = 0 \), that changes from first to second order.

If we add \( J_2 \) a different situation can occur, and in particular non-trivial plateaux can appear in certain regions of the parameter space. Let us analyze the case of \( M = 1/3 \) with a modulation of the form \( \delta(x) = \delta_0(1/3) \cos(\frac{\pi}{3}x) \). Combining this modulation with the second harmonics of the energy density \( \gamma : \cos(4k_F x + 2\sqrt{2\pi}\phi) : \) we obtain an interaction energy given by
\[ -A_1\delta_0(1/3) \int dx \left( \beta : \cos(\sqrt{2\pi}\phi) : + \gamma : \cos(2\sqrt{2\pi}\phi) : \right). \]

To minimize the energy, the second cosine interaction is pinned at the minimum of the first one and hence we have again a particular situation for \( M = 1/3 \) since the second harmonics becomes commensurate only for this value of the magnetization. The presence of a plateau at \( 1/3 \) depends on the scaling dimension of the second cosine interaction, which depends on \( J_2 \), and from a first order analysis one can estimate that it will be relevant for values of \( J_2 \) close to the couplings in \( CuGeO_3 \), in which \( J_2 \sim 0.24 - 0.36 J_1 \).
This is a new generic mechanism for the appearance of a plateau due to the spin-phonon coupling. The novelty is that the plateau is not produced by the commensurability of the main (relevant) harmonics (as for the zero magnetization case) but it is due to the commensurability of the next-to-leading harmonics, whenever it is relevant.

Note that a plateau at $M = 1/3$ is present in the $J_1 - J_2$ chain without phonons, but in that case, the plateau mechanism is the usual one (so called classical, since it is well visualized in the Ising limit $[9]$) and it is driven by the operator $:\cos(3\sqrt{2}\pi\phi):$ which needs larger values of $J_2/J_1$ than in the present case to become relevant. The present situation is thus much more favorable, making it potentially observable in experiments. Moreover, this plateau can be present also in the extreme anisotropic $XY$ case.

To study the transition from and to the plateau at $M = 1/3$, we are in a similar situation as for the $M = 0$ case in the normal chain discussed above from which we conclude that we have jumps in $M(h)$ at both ends of the $M = 1/3$ plateau. It would be interesting to analyze the formation of a soliton lattice similar to that appearing above $M = 0$ in the present case. We expect that the only modification from fixed to adaptive modulations will be again in the order of the transition.

This analysis can be applied to more general situations, e. g. for a single $XXZ$ chain where one can also expect a $1/3$ plateau in the Ising regime. In this case one would need a rather big Ising anisotropy $\Delta \gtrsim 10$ for the second harmonics to be relevant $[14]$.

A similar situation is found for $M = 1/2$ for the $J_1 - J_2$ case, where the second cosine in $\delta_i$ is now replaced by $:\cos(3\sqrt{2}\pi\phi):$ and is hence less relevant. In the present case a first order estimate hints that the $1/2$ plateau could occur at moderate values of $J_2$. Notice that this third harmonics is responsible for the plateau at $1/3$ in the $J_1 - J_2$ case without phonons $[9,14]$.

We now turn to a numerical analysis of the magnetization process of Hamiltonian $H$. We have used the DMRG method to obtain the ground state energy $E(S_z)$ in each subspace of the $S_z$ operator (the $z$-component of the total spin of the chain) on a finite chain of $N$ sites with open or periodic boundary conditions (OBC or PBC). Furthermore, minimizing $E = E(S_z) - H S_z$ we have found the magnetization $M = \frac{E}{\delta M_S}$ as a function of the applied magnetic field $H$.

To begin with, we assume a phonon field $\delta_i$ with a fixed periodic modulation $\delta_i = \delta_0 \cos(\pi(1 + M)i)$, as in the previous analytic treatement. In Fig. 1 we show the magnetization as a function of $H$ for three different system sizes and open boundary condition. Parameters are $\delta_0 = 0.4$ (for which no plateau is present in the pure $J_1 - J_2$ chain $[5]$) and $A_1 \delta_0 = 0.4$. A finite size scaling study of the critical fields is shown in the inset of this figure. The plateaux widths at $M = \frac{1}{3}$ and $M = \frac{1}{2}$ extrapolate to finite (although small) values in the thermodynamical limit, in agreement with the bosonization analysis. Let us proceed in a more general way, assuming periodic boundaries and minimizing the total energy with respect to all non-equivalent lattice coordinates $\delta_i$. We use the iterative procedure proposed by Feiguin et al $[17]$ and implemented within a DMRG approach by Schönfeld et al $[21]$. The algorithm has been constructed by using an initial (periodic) ansatz for the $\delta_i$ parameters and obtaining a new set of $\delta_i$ from the adiabatic equation,

$$\delta_i = \tilde{A}_i < S_i S_{i+1} >$$  \hspace{1cm} (10)

with the constraint $\sum \delta_i = 0$. The procedure is iterated until convergence for the energy and the distortions. Obtaining the distortion pattern in all $S_z$ subspaces the magnetization curve is then generated. In Fig. 2 we show $M(H)$ for $J_2 = 0.5$ and $A_1 = 0.8$. The plateaux at $M = \frac{1}{3}$ and $M = \frac{1}{2}$ and is clearly seen. A finite size
Peierls systems, like CuGeO$_3$, are supported by both analytical and numerical calculation leading to the formation of rational magnetization plateaus. It involves a subtle interplay between magnetic frustration and lattice coupling. Our claims plateau phases. It involves a subtle interplay between small clusters.

Finally we performed a careful finite size scaling analysis of the regions of stability of the two most robust plateaux. For that purpose, it is only necessary to consider the $S_z$ values around magnetizations 1/3 and 1/2. Although we have applied the same iterative procedure as discussed previously, here we have restricted ourselves (at each step) to distortion patterns which fit within the expected supercell, a procedure which greatly improves the convergence towards the optimum configuration. The “phase diagram” representing the region of stability of the $M = 1/3$ and $M = 1/2$ plateaux with $\frac{J_1}{J_2}$ is shown in Fig. 3. Note that stability of other rational plateau phases suggested by the bosonisation approach or by the naive fixed modulation calculation (see Fig. 1) are at all excluded. However, such phases which probably have quite narrow widths are difficult to identify on small clusters.

In conclusion, we have described a new mechanism leading to the formation of rational magnetization plateau phases. It involves a subtle interplay between magnetic frustration and lattice coupling. Our claims are supported by both analytical and numerical calculations. We suggest that quasi-one dimensional spin-Peierls systems, like CuGeO$_3$ and Tetrathiafulvalene-Au$_4$C$_4$$_4$(CF$_3$)$_4$$_4$, where both phonons and frustration play a role, would be the most natural candidates to observe such a phenomenon.

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