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On the incommensurate phase in modulated Heisenberg chains*

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Abstract. Using the density matrix renormalization group method (DMRG) we calculate the magnetization of frustrated $S = 1/2$ Heisenberg chains for various modulation patterns of the nearest neighbour coupling: commensurate, incommensurate with sinusoidal modulation and incommensurate with solitonic modulation. We focus on the order of the phase transition from the commensurate dimerized phase (D) to the incommensurate phase (I). It is shown that the order of the phase transition depends sensitively on the model. For the solitonic model in particular, a k-dependent elastic energy modifies the order of the transition. Furthermore, we calculate gaps in the incommensurate phase in adiabatic approximation.

PACS. 71.27.+a Strongly correlated electron systems; heavy fermions – 75.10.-b General theory and models of magnetic ordering – 75.10.Jm Quantized spin models

1 Introduction

Low dimensional magnetic systems have attracted considerable attention in recent years. Various theoretical and experimental efforts have been made to understand the fascinating low energy physics of quasi-one dimensional gapped spin systems, such as spin-Peierls systems ($CuGeO_3$ [1] or NaV_2O_5 [2,3]), Haldane systems (*e.g.* $Ni(C_3H_{10}N_2)_2N)_2ClO_4$ [4]) and spin ladders (*e.g.* $SrCu_2O_3$ [5] or $Cu_2(C_5H_{12}N_2)_2Cl_4$ [6]). Even if questions still remain open, many of the experimentally observed features can be already understood within the framework of one dimensional Heisenberg chains with various couplings (this includes also spin ladders [7]).

Some of these systems exhibit interesting features in external magnetic fields, for instance, a transition from a commensurate to an incommensurate phase. At this transition weak hysteresis effects are observed in $CuGeO_3$ at low temperatures [8,9] and Kiryukhin *et al.* found a small jump in the incommensurability measured by X-ray scattering [10–12]. These features are characteristic for a first order phase transition. From the theoretical point of view, no consensus has been reached so far on the order of the transition. The phase transition was predicted to be of first order by Cross [13]. Bhattacharjee *et al.* obtained the same conclusion using a phenomenological Landau expansion [14]. But mean-field calculations of Fujita and Machida for a renormalized XY-model display a second order phase transition [15] while Buzdin *et al.* [16] find a second order phase transition only at $T = 0$ and a first order one for $T > 0$ using essentially the same model as Fujita-Machida. Horovitz underlines the importance of the correct treatment of cutoffs when passing to the continuum limit [17,18].

In this paper, we propose to clarify which parameters influence the properties of the I phase with the help of the DMRG method for finite systems. In Section 2 we calculate magnetizations for different types of modulations and show that the order of the D–I phase transition is model dependent. In the I phase we calculate the magnetization dependence of the two gaps $\Delta_{+/-}$ corresponding to the increase-decrease of the z component of the total spin by unity [19].

For all calculations we have chosen parameter sets which are convenient for the numerical calculations, *i.e.* displaying small finite size effects. Computational aspects are given in Section 3. In Section 4 we summarize the results.

2 Magnetization

In the adiabatic approximation for the phonons the modulation of the exchange couplings can be described by parameters δ_i which are linked to the lattice distortion. Thus the Hamiltonian includes an elastic energy which is a positive quadratic form of the $\{\delta_i\}$. In a first step we take the elastic energy to be dispersionless, *i.e.* diagonal in real

* Dedicated to J. Zittartz on the occasion of his 60th birthday

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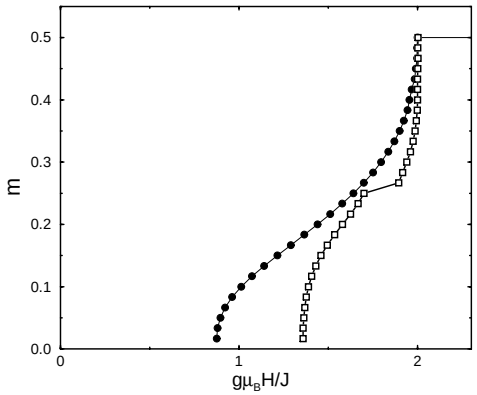

Fig. 1. Magnetization as a function of the magnetic field for $\delta = 0.3$, $\alpha = 0.1$ (filled circles) and $\delta = 0.5$, $\alpha = 0.2$ (open squares) for a 60 site chain. The lines are guides to the eye.

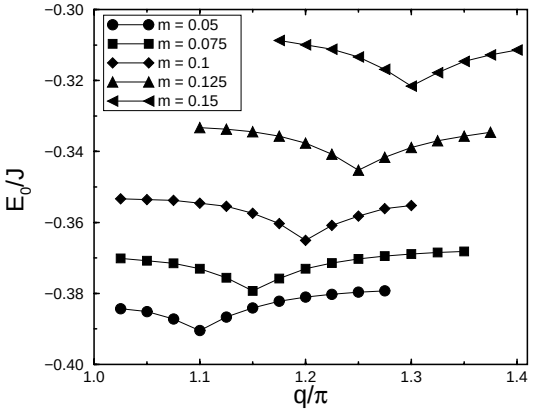

Fig. 2. Ground state energy per site of an 80 site chain as a function of the wave vector q for various magnetizations m, $\alpha = 0.35$ and $\delta = 0.1$.

space

$$\hat{H} = \hat{H}_{chain} + \hat{H}_{Zeeman} + E_{elast} \tag{1}$$

$$\hat{H}_{chain} = \sum_{i=1}^{L} (J(i)\mathbf{S}_i \cdot \mathbf{S}_{i+1} + J\alpha\, \mathbf{S}_i \cdot \mathbf{S}_{i+2})$$

$$\hat{H}_{Zeeman} = g\mu_B H S_z \ ,$$

$$E_{elast} = \frac{K_0}{2} \sum_i \delta_i^2 \ ,$$

$$J(i) = J(1 + \delta_i) \ ,$$

where α denotes the relative frustration and S_z is the z component of the total spin of the L-site chain. The last two terms in (1) are the Zeeman energy and the elastic energy associated to the lattice distortion.

2.1 Fixed modulations

As a starting point let us consider the simple case where the lattice distortion is kept frozen as in the D phase even in the presence of a magnetic field.

$$\delta_i = (-1)^i \delta. \tag{i}$$

The amplitude δ is treated as a fixed parameter. The constant elastic energy is not taken into account for the moment. Chitra and Giamarchi [20] calculated the magnetization of frustrated *or* dimerized spin chains in a magnetic field using bosonization techniques. Within this continuum-limit approach the frustration and dimerization cannot be treated simultaneously (double sine-Gordon model). For $\alpha < \alpha_c$ and $\delta > 0$ the contribution of the frustration is assumed to be irrelevant and the model reduces to an integrable sine-Gordon model. However, recently it has been shown by Bouzerar *et al.* that this is not the case [21]. The magnetization increases just above the lower critical field H_c like $m \propto \sqrt{H - H_c}$ [20,22]. The same power law is found for $\alpha > \alpha_c$ and $\delta = 0$. In particular, the transition to finite magnetization is of *second order* in both cases. With the DMRG method, we find this square root behavior in presence of both dimerization and frustration. But as shown recently by Tonegawa *et al.* by means of exact diagonalization [23] an additional remarkable difference appears in some parameter range of dimerization and frustration, *i.e.* a plateau at $m = 1/4$, as indicated in Figure 1.

In the case of finite magnetization, it is known that the commensurate dimerization pattern (i) is not appropriate for describing spin-Peierls systems. For instance X-ray measurements on $CuGeO_3$ clearly show that the structure of the lattice distortion becomes incommensurate under a sufficiently large magnetic field [10–12]. Thus a more appropriate choice for the modulation is,

$$\delta_i = \delta \cos(q r_i) \tag{ii}$$

as it was suggested in [19,24]. To begin with, q is considered as a free parameter which is fixed by minimizing the total (free) energy. Note that for $q \neq \pi$ the elastic energy is q independent for the ansatz (ii) yielding only a constant contribution at given amplitude which will be dropped for the following consideration.

Using the Jordan-Wigner transformation the applied magnetic field corresponds to a shift of the chemical potential. For the XY-model with a finite magnetization $m = S_z/L$, it is straightforward to show that an infinitesimal spin-lattice coupling leads to an instability at momentum $q = 2k_F = \pi(1 + 2m)$. In the case of the Heisenberg model, this relation is expected to hold true as well [13,19,20,25,26]. We have confirmed numerically for various sets of parameters δ, α and various system sizes that the energy is minimum at $q = \pi(1 + 2m)$ for a given m. The ground state energy per site for $H = 0$ as a function of q is plotted in Figure 2, for various magnetizations m at fixed $\delta = 0.1$ and $\alpha = 0.35$. The positions of the cusps correspond exactly to $q = \pi(1 + 2m)$. The fact that one observes cusps and not smooth quadratic

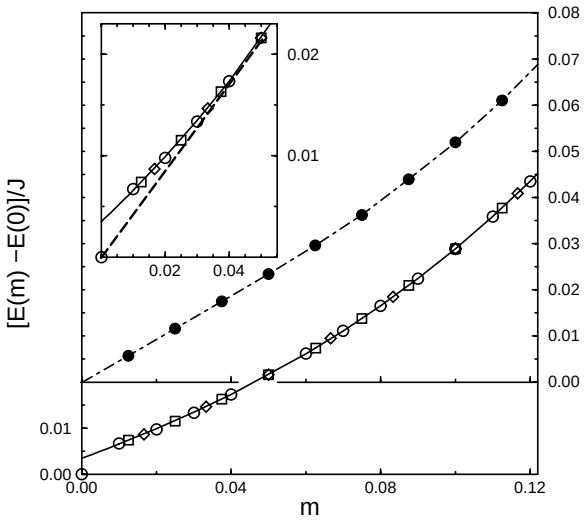

Fig. 3. Open symbols (left scale): ground state energies $E(m) - E(0)$ as a function of the magnetization for the sinusoidal modulation (ii) ($\delta = 0.2$, $\alpha = 0.35$) for chains of 100 (circles), 80 (squares) and 60 (diamonds) sites. To highlight the discontinuity at $m = 0$ a cubic fit for $m > 0$ is depicted with a solid line. The inset shows an enlargement and the tangent for $m = 0.05$ as described in the text. Filled circles (right scale): ground state energies $E(m) - E(0)$ for the adaptive modulation from (iii), $K_0 = 1.7$ ($\delta \approx 0.2$ in the D phase) and $\alpha = 0.35$. The dot-dashed line is just a guide to the eye.

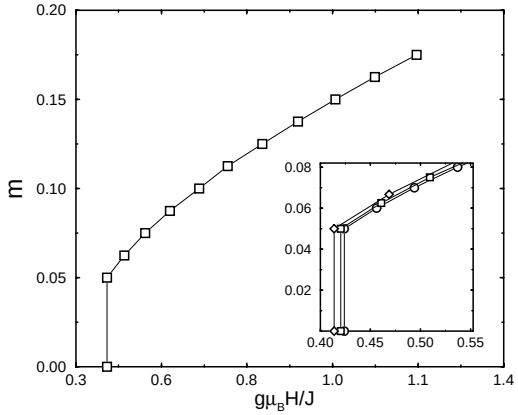

Fig. 4. Magnetization as a function of the applied magnetic field for $\alpha = 0.35$ and $\delta = 0.2$ of an 80 site chain as deduced from the open squares in Figure 3. The inset shows an enlargement near H_c for 100 (circles), 80 (squares) and 60 (diamonds) site chains.

minima is linked to the divergence of the susceptibility at $q = \pi(1 + 2m)$, *i.e.* an instability even for infinitesimal coupling. At least for $\alpha < 0.5$ and arbitrary δ this is the generic behavior, and confirms the relation between the wave vector and the magnetization.

Henceforth, we fix $q = \pi(1 + 2m)$ and investigate the magnetization as a function of the applied field. We find that the incommensurate exchange coupling (ii) has a rather strong effect on the magnetization leading to a *first order* phase transition. To elucidate this we present the magnetic ground state energy per site $E(m) = (\langle \hat{H}_{chain} \rangle + E_{elast})/L$ as a function of the magnetization in Figure 3. Results for several chain lengths are included to show the absence of finite size effects.

The salient feature of $E(m)$ for sinusoidal modulation is the discontinuous jump at $m = 0$. To understand this jump it is helpful to look at the averaged squared distortion $\frac{1}{L}\sum_i \delta_i^2$ which takes the value δ^2 at $q = \pi$ and $\delta^2/2$ otherwise. We see that in the D phase all δ_i are maximally distorted whereas in the sinusoidally modulated phase there are also large regions with weaker distortion. So neither the elastic energy is continuous in the limit $q \to \pi$ nor is the magnetic energy since it reacts to the distortions.

To deduce the dependence $m(H)$ from Figure 3 we have to resort to Maxwell's construction, *i.e.* we compute the convex hull. The magnetic field defines the slope $g\mu_B H = \partial E/\partial m$ of the tangent which touches the convex hull at the value m (Legendre transformation). So one obtains $m(H)$. The jump in $E(m)$ leads to a first order transition with a jump in $m(H)$. The resulting $m(H)$ deduced from Figure 3 is depicted in Figure 4.

Calculating the corresponding local magnetizations [19] one finds that there is a large alternating local magnetization close to each zero of the modulation. Summing the local magnetizations around each zero one finds a contribution of $S_z = 1/2$, *i.e.* of one spinon.

2.2 Adaptive modulations

In the previous section we chose a sinusoidal modulation and found that $q = \pi(1 + 2m)$ minimizes the total energy. We now proceed in a more general way by minimizing the total energy including the elastic energy term with respect to all the parameters δ_i. In other words, we allow the lattice distortion to adapt to the spin system. Within our DMRG approach we follow the iterative procedure proposed by Feiguin *et al.* [28] who applied exact diagonalization and Monte-Carlo-Simulations to a slightly different model. The dimerization amplitudes δ_i are calculated self-consistently by minimizing $\langle \hat{H}_{chain} \rangle + E_{elast}$ which leads to

$$J\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle + K_0 \delta_i - \frac{J}{L} \sum_i \langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle = 0 \,, \qquad \text{(iii)}$$

where the last term ensures that the δ_i satisfy the constraint $\sum_{i=1}^{L} \delta_i = 0$. Following [28] this equation is used to improve iteratively the local distortions δ_i. The expectation values are taken with respect to the lowest-energy state of the previous iteration. Starting from the sinusoidal modulation (ii) we find that four to five iterations are enough to achieve a stable pattern that does not change significantly on further iterations as shown in Figure 5.

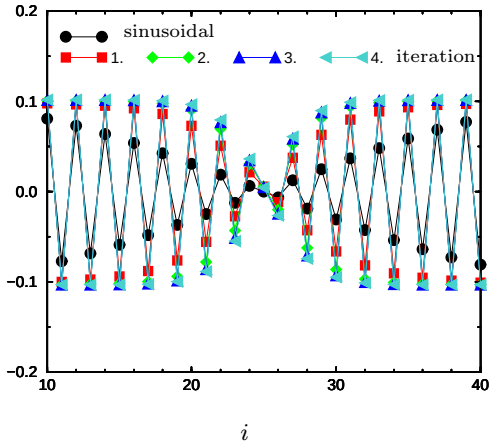

Fig. 5. Incommensurate modulation: local distortions δ_i *versus* site index i for the first four iterations starting from a sinusoidal modulation (filled circles); 100 sites, $\alpha = 0.35$, $K_0 = 3.3$, and $S_z = 1$.

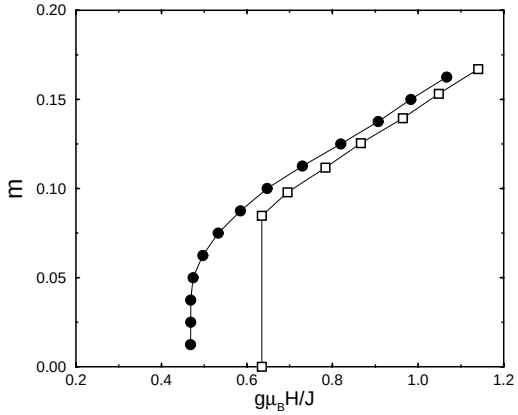

Fig. 6. Filled circles: Magnetization for the adaptive modulation ($K_0 = 1.7$, $\alpha = 0.35$) as deduced from the corresponding curve in Figure 3. Open squares: magnetization with a dispersive elastic energy as discussed in the text. $\tilde{K} = 6K_0$, K_0 and α unchanged.

The envelope of the final modulation can be fitted by a product of complete Jacobi elliptic functions of modulus k as predicted analytically [17,16,15]. For very low magnetization, *i.e.* low concentration of solitons, the vicinity of each zero resembles a tanh [27].

Within the self-consistent approach we calculate $E(m)$ per site as plotted in Figure 3 (filled circles). $E(m)$ is convex but in contrast to the curves with fixed sinusoidal modulation it is continuous. The convexity will be shown more clearly below in a modified representation. Thus we have a continuous, *second order* transition from the D phase to the adaptive I phase. The corresponding magnetization $m(H)$ is shown in Figure 6 (filled circles).

The enormous steepness of the continuous magnetization is explained by the following argument. For non-interacting spinons which are far enough from each other, the energy per site $E(m) - E(0)$ is proportional to the number of spinons and hence to the magnetization m (see also filled circles in Fig. 3 for small m). The proportionality constant e_0 is the energy of a single spinon and determines the critical field $2e_0 = g\mu_B H_c$, since two spinons are created by breaking one singlet. Because the spinons are exponentially localized (*cf.* Fig. 5) two spinons at mutual distance l have additionally an exponential interaction $w(l) = w_0 \exp(-cl)$. Here c is a constant of the order of the inverse correlation length and w_0 is a proportionality constant which is positive for repulsion and negative for attraction. The typical distance of the spinons is $l = 1/(2m)$ since each spinon carries spin $S = 1/2$. Hence for not too large values of m the total energy in an external magnetic field H equals

$$E(m) - E(0) = g\mu_B(H_c - H)m + w_0 2m e^{-\frac{c}{2m}} . \qquad (2)$$

By minimizing this expression for repulsion ($w_0 > 0$) one derives $H(m)$ which increases exponentially slowly just above H_c. This in turn leads to the drastic increase of m as depicted in Figure 6.

To present the effects of soliton interaction more clearly we pass to an affine representation of the ground state energy $E(m)$ by investigating

$$E_{eff}(m) := E(m) - E(0) - g\mu_B H_c m \qquad (3)$$

which would be constantly zero if no interaction between the solitons existed. Note that $E_{eff}(m)$ is convex if and only if $E(m)$ is. In Figure 7 the generic resulting curves are shown with filled symbols (solid line) for the XY-model and the spin isotropic XXX-model. The results for the XY-model are obtained for an infinite system without frustration by a continued fraction technique based on Green's functions [19]. Using this method the simpler solvability of the XY-model allows to iterate up to 80 times for an infinite chain with periodicities up to 120. These data are included as an additional check that no spurious effects due to finite size or insufficient iteration are investigated.

The results in Figure 7 for a dispersionless elastic energy comply perfectly with exponentially repulsive solitons (2). There is no sign of a long range interaction $\propto 1/l$ as postulated by Horovitz for finite cutoffs as they occur naturally in discrete lattice models [17,18]. In particular, no attraction for dispersionless elastic energies are found [29].

A dispersionless elastic energy is of course a drastic simplification of the real phononic system. Cross already argued [13] that a pinning in k-space should influence the order of the transitions. We expect that the D $\rightarrow$ I phase transition becomes first order if the elastic energy itself favors the distortion at $k = \pi$. This means that $\hat{K}(\pi)$ is minimum if the elastic energy can be expressed as $E_{elast} = \frac{1}{2}\sum_k \hat{K}(k)|\delta_k|^2$. The argument compares, for a given wave vector q close to π, the elastic energy $\hat{K}(q)$ of a sinusoidal modulation (ii) with the one of an array of domain walls with the same periodicity $2\pi/q$. Since the latter has also contributions of higher harmonics $\pm 3q$, $\pm 5q$,

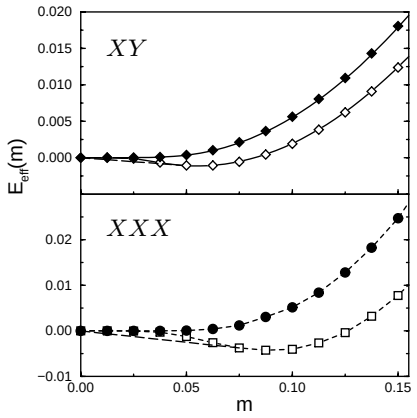

Fig. 7. Affine representation of the ground state energy. The long-dashed lines indicate the convex hulls to the lower curves. XY-model: The upper solid curve shows E_{eff} for a dispersionless elastic energy with $K_0 = 0.625$. The lower solid curve shows E_{eff} for a dispersive elastic energy ($\tilde{K} = 6K_0$) as discussed in the following section. Both curves are obtained *via* the continued fraction technique. The filled and open diamonds depict DMRG results for an 80 site chain. XXX-model: DMRG results in the dispersionless case (filled circles) and for $\tilde{K} = 6K_0$ (open squares) for $K_0 = 1.7$ and $\alpha = 0.35$. The dashed lines are guides to the eye.

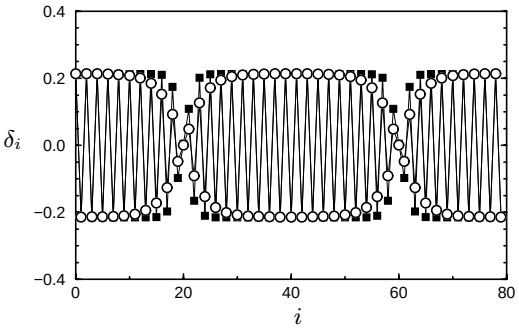

Fig. 8. Modulations for $S_z = 1$ for the same parameters as in Figure 7 for the XXX-model.

$\pm 7q$, ... its elastic energy is $\sum_n |a_{(2n+1)q}|^2 \hat{K}(q)$ where the coefficients $|a_{(2n+1)q}|^2$ are symmetric about π. Thus the elastic energy is higher than the one for the sinusoidal modulation. By this mechanism higher harmonics are suppressed due to the elastic energy leading to a smoother and more sinusoidal modulation. If the convex curve for the adaptive modulation in Figure 3 is influenced in a way to approach the discontinuous curve for sinusoidal modulation one must expect a region of concavity for small m. Hence the convex hull differs from the curve itself and a jump in the magnetization occurs: the transition is first order. Put differently, we expect that a dip in the elastic energy at the zone boundary leads to an *attraction* of the solitons.

To investigate our hypothesis numerically we use $\hat{K}(k) = K + 2\tilde{K}\cos(k)$ with $K_0 = K - 2\tilde{K}$ kept fixed to refer to the same amplitudes in the D phase. This elastic energy corresponds in real space to

$$E_{elast} = \frac{1}{2}\sum_i \left(K\delta_i^2 + 2\tilde{K}\delta_i\delta_{i+1}\right) = \frac{1}{2}\boldsymbol{\delta}^+ \mathbf{K}\,\boldsymbol{\delta}\ , \tag{4}$$

where $\boldsymbol{\delta}$ is a vector with components δ_i and $\mathbf{K}$ is a cyclic tridiagonal $L \times L$ symmetric matrix of coupling constants with diagonal elements K and off-diagonal elements $\tilde{K}$. Generic results for the energies $\tilde{E}(m)$ in affine representation are depicted with open symbols (solid line) in Figure 7. We find indeed a concavity for small values of m. This implies soliton attraction and a first order transition.

Furthermore, we show in Figure 6 the resulting magnetization curves with and without dispersion of the elastic energy. The difference between the second order transition for the elastic energy without dispersion and the first order transition with dispersion is clearly visible. Additionally, the critical field H_c at which the transition occurs rises on inclusion of the dispersion. This complies also with the above consideration since the energy of a single soliton rises due to $K + 2\tilde{K}\cos(k) > K_0$ except at $k = \pi$ for $\tilde{K} > 0$.

Finally, in Figure 8 the modulation patterns with and without dispersion are compared. Indeed, the inclusion of $\tilde{K} > 0$ makes the modulation softer and more sinusoidal. In conclusion our numerical results convincingly corroborate our expectations for the effect of a dispersive elastic energy.

Numerically, we are not able to decide whether an arbitrarily small $\tilde{K}$ already yields a soliton attraction. For smaller values of $\tilde{K}$ the minima in the affine representation occur for smaller and smaller magnetization and they are more and more shallow. We expect that the soliton attraction exists down to arbitrarily small values of $\tilde{K}$ but it may become irrelevant in practice due to the exponential smallness of the corresponding energies.

We also investigated negative values of $\tilde{K}$. No qualitative change of the soliton interaction was found in comparison to the dispersionless case. The iterative procedure, however, becomes quite unstable already for small negative values of $\tilde{K}$.

2.3 Adiabatic gaps

So far we aimed at the average magnetization as a function of the applied magnetic field. Another interesting quantity which is accessible once $E(m)$ can be computed are the adiabatic gaps. It is a so far unsettled question whether spin-Peierls systems have or have not gaps in the incommensurate phase.

On the one hand, it seems clear that the incommensurate modulation pattern can be shifted along the chains without energy cost. This is certainly true in the continuum description and thus most probable also for not too

small correlation lengths. This quasi-continuous symmetry gives rise to quasi-Goldstone bosons called phasons which are gapless [14]. They do not change the spin sector and thus have $\Delta S_z = 0$. The physics of phasons is beyond an adiabatic treatment of the lattice distortion since within an adiabatic treatment the distortion is assumed to be fixed.

A different issue is the question whether the gaps $\Delta_\pm$ corresponding to $\Delta S_z = \pm 1$ are finite or not. Note that these gaps do not need to be equal since the spin rotation symmetry is broken for finite magnetization. From a non-adiabatic viewpoint one can still infer from the smoothness of the $E(m)$ curves that there are no such gaps in the I phase since the modulation adapts always to the average magnetization. Applying, however, an operator like $S^+(k)$ or $S^-(k)$ [19,25] and asking for the accessible excitation spectrum may lead to a different answer. These operators act only on the spin part of the ground state and leave the modulation unchanged. Thus it is not unreasonable to expect that the gapless excitations are not accessible if their access required a re-arrangement of the whole, in reality three-dimensional, modulation. The underlying question is whether the states $S^\pm(k)|S_z\rangle$ are orthogonal to $|S_z \pm 1\rangle$ or not, if we denote by $|S_z\rangle$ the ground state for the magnetization S_z.

Here we will investigate the simpler question whether in the strictly adiabatic framework the gaps Δ_+ are finite or not. Uhrig *et al.* [19] were only able to compute $\Delta_+ + \Delta_-$ since this quantity did not require the knowledge of the corresponding magnetic field.

We define by $E(m,H) := E(m) - mg\mu_B H$ the ground state energy with self-consistently optimized modulation $\{\delta_i\}$. By

$$E_\pm(m,H) := \frac{1}{L}\langle \hat{H}_{chain}\rangle\Big|_{S_z = mL \pm 1} + \frac{K_0}{2L}\sum_i \delta_i^2 - \left(m \pm \frac{1}{L}\right) g\mu_B H \quad (5)$$

we denote the ground state energy with one additional spin flipped upward (+) or downward (−), respectively, *but* with the modulation $\{\delta_i\}$ belonging to $S_z = mL$, not to $S_z = mL \pm 1$. This means that for $E_\pm(m,H)$ the modulation is not optimized for the given magnetization. This corresponds to the situation accessible by application of $S^+(k)$ or $S^-(k)$ without reaction of the lattice part. Then the gaps are defined by

$$\Delta_\pm(m) = E_\pm(m,H) - E(m,H)\,. \quad (6)$$

The gaps Δ_+ and Δ_- for a 100 site ring are displayed in Figure 9 for $\alpha = 0.35$ and $K_0 = 2.38$ corresponding to $\delta \approx 0.14$ in the D phase. Finite size effects are not yet completely negligible, but the qualitative behavior is the one shown and is in agreement with previous self-consistent renormalized Hartree-Fock results [19].

Most importantly, we can show by Figure 9 that both gaps are indeed finite and of equal order of magnitude. It is interesting that apparently Δ_+ is smaller at small magnetization and Δ_- is smaller at larger magnetization.

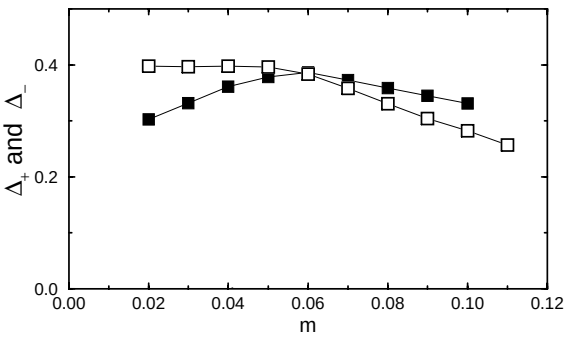

Fig. 9. The energy gaps Δ_+ (filled squares) and Δ_-(open squares) as a function of the magnetization for $L = 100$, $\alpha = 0.35$ and $K_0 = 2.38$

At least in the adiabatic approach, we can show that even the I phase has gaps. It would be interesting if any experimental evidence in favor of the existence of these gaps was found.

3 Computational details

In our DMRG calculation [30,31] we apply periodic boundary conditions to minimize finite size effects. We keep 128 (64) states in the truncation procedure. To account for the incommensurate structure we use the finite size algorithm [30,31]. In the first steps where the system is iteratively increased we use the reflection of the left hand block to build up the superblock although the reflection symmetry is not given at this stage. This initial error is reduced either by supplementary sweeps through the system of the desired length or by intermediate sweeps through the system the length of which is commensurable with the lattice modulation. We tested the accuracy of the DMRG results by comparing the lowest energies of the XY-model with sinusoidal modulation in different S_z-subsectors with exact results for a 60-site ring. Keeping 128 (64) states we find the typical error to be smaller than 10^{-6} (10^{-5}) for $S_z = 0$ and 10^{-5} (10^{-4}) in higher S_z-subsectors. For the selfconsistent calculations in the case of adaptive modulations we used the sinusoidal modulation (ii) as a starting configuration for the curves presented. For larger dimerizations, however, it is more convenient to start with a step-like modulation since the correlation lengths become very small. Having calculated the ground state in the corresponding S_z-subsector we use equation (iii) to deduce the improved set of $\{\delta_i\}$. This step is repeated (typically 6 to 10 times) until the change of the ground state energy becomes sufficiently small, *i.e.* of the order of the truncation error.

For the XY-model we can compare the selfconsistent DMRG results for finite chains with these of the continued fraction technique [19] in the thermodynamic limit. We find that the error due to finite size effects and due to the truncation of the Hilbert space is at most of the order of 10^{-4} (see upper part of Fig. 7). This accuracy is by far

sufficient for the presented qualitatively analysis of the phase transition.

4 Summary and discussion

In this work we considered modulated $S = \frac{1}{2}$ Heisenberg chains with finite magnetization. Three classes of modulation were investigated: (i) fixed dimerization, (ii) fixed incommensurate sinusoidal modulation and (iii) adaptive incommensurate modulation. Our main interest was to investigate the dependence of the magnetization m on the applied magnetic field H.

For scenario (i) we found a second order transition to finite magnetization by means of the finite size DMRG method in agreement with previous calculations. The increase of m just above the critical field H_c is characterized by a square root behavior $m \propto \sqrt{H - H_c}$.

For scenario (ii) we showed that the system favors an incommensurability corresponding to the magnetization $q = 2k_F = 2\pi(1/2+m)$. A prominent first order transition is found. This finding could be explained by computing the discontinuous dependence of the ground state energy $E(m)$ on m at $m = 0$. The discontinuity is linked to the discontinuous jump of the root-mean-square of the local distortions on passing from dimerization ($q = \pi$) to a long-wave length modulated dimerization ($q \approx \pi$).

In scenario (iii) we determined iteratively the modulation which minimizes the total energy including a quadratic elastic energy. Again we find a periodicity corresponding to the magnetization $q = 2\pi(1/2 + m)$. The modulation, however, corresponds for low magnetization rather to a soliton lattice. This means one has differently dimerized regions separated by domain walls. Each domain walls carries one $S = 1/2$. We find a crossover from the solitonic picture at low magnetization to a sinusoidal modulation at higher magnetizations. The transition to finite magnetization is second order although the increase is exponentially steep. The inclusion of a positive dispersion of the elastic energy alters the order of the transition. It is first order then. An exponential attraction of the solitons was identified.

As another interesting quantity we calculated the adiabatic gaps $\Delta_{+/-}$ corresponding to the increment (decrement) of the magnetization by unity. The independent determination of these gaps requires the complete knowledge of $E(m)$. The calculation was also done for scenario (iii). It was shown that these gaps are finite in the adiabatic treatment.

The second order phase transition in the commensurate case (i) is in agreement with the fact that measurements under applied field for instance on $Cu_2(C_5H_{12}N_2)_2Cl_4$ show no hysteresis effects [6]. This substance is found to be an antiferromagnetic Heisenberg ladder which is equivalent to a strongly dimerized quasi-one-dimensional Heisenberg chain. The magnetization increases continuously. The expected square root behavior near H_c, however, was not observed.

We do not know of a substance which can be described by pure sinusoidally modulated exchange couplings. The modulation in the incommensurate phase of $CuGeO_3$ is in fact very close to a sinusoidal modulation [10, 11]. Recently Lorenz *et al.* [32] measured the magnetic field dependence of the spontaneous strain $\epsilon(H)$ in $CuGeO_3$ which is in first approximation proportional to the elastic energy associated to the lattice distortion. It decreases very fast near H_c and saturates approximately at 1/4 of the value in the dimerized phase for $H \approx 22$ T. One can conclude that there is a crossover from a solitonic distortion pattern for small magnetizations to a sinusoidal one for larger magnetizations. Our model allows – for parameter values reasonable for $CuGeO_3$ within a one-dimensional approach $\alpha = 0.35$, $K \approx 18$ ($\Rightarrow \delta = 0.014$ in the D phase [33–35]) – to describe the above crossover quantitatively [32].

The feature so far not understood in $CuGeO_3$ is the first order phase transition D $\rightarrow$ I. From our findings it is tempting to attribute this weak first order property to a positive dispersive elastic energy, *i.e.* a dip in $\omega(k)$ at $k = \pi$. Unfortunately, there is no experimental indication for such a feature in the phonon spectra [36]. The spring constant $\hat{K}(k)$, however, in the adiabatic treatment is proportional to $\omega(k)/g^2(k)$ where $\omega(k)$ is the phonon energy measured by Braden *et al.* [36]. The momentum-dependent spin-phonon coupling $g^2(k)$ is not known presently and may account for the dispersive behavior needed to explain the first order transition D $\rightarrow$ I observed in $CuGeO_3$. At the present stage, we may also speculate that the neglected interchain couplings [37] are decisive for the order of the transition. From our present results we understand that the order of the transition is influenced by the microscopic details of the model.

The finding of finite adiabatic gaps in the incommensurate phase should encourage experimental work to verify or to falsify this feature, for instance, in $CuGeO_3$.

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