On the Incommensurate Phase in Modulated Heisenberg Chains

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Using the density matrix renormalization group method (DMRG) we calculate the magnetization of frustrated $S = \frac{1}{2}$ 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.

I. 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$_3$[5] or NaV$_2$O$_5$[6]), Haldane systems (e.g. Ni(C$_5$H$_{10}$N$_2$)$_2$N$_2$ClO$_4$[4]) and spin ladders (e.g. SrCu$_2$O$_3$[7] or Cu$_2$(C$_5$H$_{12}$N$_2$)$_2$Cl$_4$[8]). 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[3]).

Some of these systems exhibit interesting features in external magnetic fields, for instance, a transition from a commensurate to an incommensurate phase. At this external magnetic fields, for instance, a transition from a commensurate to an incommensurate phase. At this point we take the elastic energy to be dispersionless, i.e. diagonal in real space

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

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

$$\hat{H}_{\text{Zeeman}} = g\mu_{B}HS_{z} \ ,$$

$$E_{\text{elast}} = K_{0} \sum_{i} \delta_{i}^{2} \ ,$$

$$J(i) = J(1 + \delta_{i}) \ ,$$

where $\alpha$ 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.

A. 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.

$$\delta_{i} = (-1)^{i} \delta$$

(i)
The amplitude $\delta$ 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 $m \propto \sqrt{H_c - H}$ [20,22]. The same power law is found for $\alpha > \alpha_c$ [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 $m = 1/4$, see Fig. 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 [13,12]. Thus a more appropriate choice for the modulation is,

$$\delta_i = \delta \cos(qr_i)$$

as it was suggested in [13,12]. 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 (i) yielding only a constant contribution at given amplitude which will be dropped for the following consideration.

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 $E(m) = \langle H_{\text{chain}} \rangle + E_{\text{elast}} \rangle / L$ as a function of the magnetization in Fig. 2. 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 $\delta^2$ at $q = \pi$ and $\delta^2/2$.
otherwise. We see that in the D phase all $\delta_i$ are maximally distorted whereas in the sinusoidally modulated phase there are also large regions with weaker distortion. So neither the elastic energy is not 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 Fig.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 Fig.3 is depicted in Fig.4.

Calculating the corresponding local magnetizations 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.

B. 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 $\delta_i$. 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. who applied exact diagonalization and Monte-Carlo-Simulations to a slightly different model. The dimerization amplitudes $\delta_i$ are calculated self-consistently by minimizing $\langle \hat{H}_{\text{chain}} \rangle + E_{\text{elast}}$ which leads to

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

where the last term ensures that the $\delta_i$ satisfy the constraint $\sum_{i=1}^L \delta_i = 0$. Following this equation is used to improve iteratively the local distortions $\delta_i$. The expectation values are taken with respect to the ground state of the previous iteration. Starting from the sinusoidal modulation 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 Fig.5.
By minimizing this expression for repulsion ($w$) above $H$ portionality constant $e$ and negative for attraction. The typical distance of interacting spinons which are far enough from each other, the spinons is $\propto$ the order of the transitions. We expect that the D→I phase transition becomes first order if the elastic energy $\delta_l$ equals $0$. This in turn leads to the drastic increase of $m$ which increases exponentially slowly just for not too large values of $\alpha$.

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 Fig.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 Fig.3 (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.3) 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

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

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 Fig.3.

FIG. 5. Incommensurate modulation: local distortions $\delta_i$ 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 Fig.3. Open squares: Magnetization with a dispersive elastic energy as discussed at the end of the paragraph. $K = 6K_0$, $K_0$ and $\alpha$ unchanged.

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

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

which would be constant zero if no interaction between the solitons existed. Note that $E_{\text{eff}}(m)$ is convex if and only if $E(m)$ is. In Fig.3 the generic resulting curves are shown with filled symbols (solid line) for the XY—model and the spin isotropic XYZ—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 Fig.3 for a dispersionless elastic energy comply perfectly with exponentially repulsive solitons [3]. 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 [27,18]. 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→I phase transition becomes first order if the elastic energy itself favors the distortion at $k = \pi$. This means that $K(\pi)$ is minimum if the elastic energy can be expressed as $E_{\text{elast}} = \frac{1}{2} \sum_k K(k)|\delta_k|^2$. The argument compares for
elastic energy corresponds in real space to refer to the same amplitudes in the D phase. This cavity for small sinusoidal modulation one must expect a region of concavity to approach the discontinuous curve for a smoother and more sinusoidal modulation. If the monics are suppressed due to the elastic energy leading sinusoidal modulation. By this mechanism higher harmonics thus the elastic energy is higher than the one for the transition is first order. Put differently, we expect that a dip in the elastic energy at the zone boundary leads to a first 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 Fig. 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.

![Diagram](https://example.com/diagram.png)

**FIG. 8.** Modulations for $S_z = 1$ for the same parameters as in Fig. 7 for the $XYZ$-model.

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 $\tilde{K}$.

**C. Adiabatic Gaps**

So far we aimed at the average magnetization as a function of the applied magnetic field. Another interesting

with diagonal elements $K$ and off-diagonal elements $\tilde{K}$. Generic results for the energies $E(m)$ in affine representation are depicted with open symbols (solid line) in Fig. 6. We find indeed a concavity for small values of $m$. This implies soliton attraction and a first order transition.

Furthermore, we show in Fig. 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 $\tilde{K} > 0$.

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 \( S^z(k) \) or \( S^{-}(k) \) 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 \( \Delta_\pm \) are finite or not. Uhrig et al. [12] were only able to compute \( \Delta_+ + \Delta_- \), since this quantity did not require the knowledge of the corresponding magnetic field.

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

\[
E_{\pm}(m,H) := \frac{1}{L} (\hat{H}_{\text{chain}})_{S_x = m L \pm 1} + \frac{K_0}{2L} \sum_i \delta_i^2 - \left( m \pm \frac{1}{L} \right) g \mu_B H
\]  

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 \( S^z(k) \) or \( S^{-}(k) \) without reaction of the lattice part. Then the gaps are defined by

\[
\Delta_{\pm}(m) = E_{\pm}(m,H) - E(m,H).
\]

The gaps \( \Delta_+ \) and \( \Delta_- \) for a 100 site ring are displayed in Fig. 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].

![FIG. 9. The energy gaps \( \Delta_+ \) (filled squares) and \( \Delta_- \) (open squares) as a function of the magnetization for \( L = 100 \), \( \alpha = 0.35 \) and \( K_0 = 2.38 \) Most importantly, we can show by Fig. 9 that both gaps are indeed finite and of equal order of magnitude. It is interesting that apparently \( \Delta_+ \) is smaller at small magnetization and \( \Delta_- \) is smaller at larger magnetization. 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.

III. 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 [18] 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. Hav-
ing calculated the ground state in the corresponding $S_z$-
subsector we use equation (1) to deduce the improved set of $\{s_i\}$. This step is repeated (typically 6 to 10 times)
until the change of the ground state energy becomes suffi-
ciently 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 those of the contin-
ued fraction technique [13] 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.

IV. SUMMARY AND DISCUSSION

In this work we considered modulated $S = \frac{1}{2}$ Heisen-
berg 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 in-
crease 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 tran-
sition is found. This finding could be explained by com-
puting 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 mod-
ulation which minimizes the total energy including a
quadratic elastic energy. Again we find a periodicity cor-
responding 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 do-
main 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 disper-
sion 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 adia-
batic gaps $\Delta_{+/-}$ corresponding to the increment (decre-
ment) of the magnetization by unity. The independent
determination of these gaps requires the complete knowl-
edge of $E(m)$. The calculation was also done for scenario
(iii). It was shown that these gaps are finite in the adia-
batic treatment.

The second order phase transition in the com-
mensurate case is in agreement with the fact that
measurements under applied field for instance on
Cu$_2$(C$_5$H$_2$N$_2$)$_2$Cl$_4$ show no hysteresis effects [3]. This
substance is found to be an antiferromagnetic Heisen-
berg ladder which is equivalent to a strongly dimerized
quasi-one-dimensional Heisenberg chain. The magneti-
zation 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]. Re-
cently 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 dist-
tortion 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 $\alpha = 0.35$, $K \approx 18$ (\(\delta = 0.014\)
in the D phase) - 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 indica-
tion for such a feature in the phonon spectra [36]. The
spring constant $\tilde{K}(k)$, however, in the adiabatic treat-
ment 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 be-
havior 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 incommensu-
rate phase should encourage experimental work to verify
or to falsify this feature, for instance, in CuGeO$_3$.

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