Novel massless phase of Haldane-gap antiferromagnets in magnetic field

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The behavior of Haldane-gap antiferromagnets in strong magnetic field is not universal. While the low-energy physics of the conventional 1D spin-1 Heisenberg model in its magnetized regime is described by one incommensurate soft mode, other systems with somewhat perturbed coupling constants can possess two characteristic soft modes in a certain range of the field strength. Such a two-component Luttinger liquid phase is realised above the massive Haldane-gap phase, and in general above any massive nonmagnetic phase, when the ground state exhibits short range incommensurate fluctuations already in the absence of the field.

Quantum mechanical systems possessing a spectral gap in their ground state are usually very robust: the gap can persist even if relatively large perturbations are added to the Hamiltonian. This is exactly the case for the one-dimensional spin-1 antiferromagnetic chain where the existence of an energy gap, the Haldane gap, is well documented and understood for the Heisenberg model. In the more general SU(2) symmetric bilinear-biquadratic spin-1 model

\[ H = \sum_{i=1}^{N-1} [S_i S_{i+1} + \beta (S_i S_{i+1})^2] - h \sum_{i=1}^{N} S_i^z, \tag{1} \]

in which \( \beta = 0 \) yields the conventional Heisenberg model, the Haldane gap survives in the whole range \(-1 < \beta < 1\), thus there is a large region in the \( \beta \)-space where the quadratic term has seemingly no effect on the low-energy physics. The Haldane gap disappears in the integrable critical points \( \beta = \pm 1 \) beyond which new phases appear. For \( \beta < -1 \) translation invariance is spontaneously broken and dimerization occurs. In the region \( \beta > 1 \) the bilinear-biquadratic model is believed to remain gapless with soft modes at momenta \( k = 0, \pm 2\pi/3 \). Since the system is one dimensional no long-range order exists in this phase either: the correlation functions decay algebraically.

The emergence of the Haldane gap in the vicinity of the \( \beta = 1 \) point, the so-called Uimin-Lai-Sutherland (ULS) point, has been investigated recently by Itoi and Kato in the absence of magnetic fields \( h = 0 \). The ULS model has an SU(3) symmetry which is broken down to SU(2) when \( \beta \) is tuned away from 1. They identified the critical theory of the ULS point with the \( k = 1 \) SU(3) Wess-Zumino-Witten-Novikov (WZWN) model and concluded that the SU(3) symmetry breaking perturbation, represented by the deviation term with \( (\beta - 1) \) in the Hamiltonian, is irrelevant for \( \beta > 1 \), i.e., the system remains critical there, but it becomes marginally relevant and gives rise to a dynamic mass generation (the Haldane gap) for \( \beta < 1 \). The transition is of the Berezinskii-Kosterlitz-Thouless (BKT) type, i.e., the gap open exponentially slowly away from the ULS point. These findings are supported by earlier numerical results.

When there is a magnetic field present the SU(2) symmetry of the bilinear-biquadratic model breaks down to U(1). At the ULS point, however, where the symmetry is higher, the quantities \( N_+, N_0, \) and \( N_- \), denoting the numbers of +, 0, and – spin states in the wave function, with \( N_+ + N_0 + N_- = N \) the length of the chain, are independently conserved. Thus the remaining continuous symmetry for \( \beta = 1 \), \( h > 0 \) is \( U(1) \times U(1) \). For \( \beta < 1 \) when the strength of the field is higher then the value of the gap, the Haldane gap collapses and the low-energy physics of the magnetized system is governed by gapless excitations. The emerging periodicity is a function of the field strength and in the generic situation incommensurate. Finally, when the field is strong enough all the spins align and the magnetization saturates.

At the ULS point, where the Haldane gap no longer exists, the analysis of the Bethe Ansatz equations showed that the magnetization growth is not smooth. There is a second order phase transition which leads to a cusp in the the magnetization curve \( m = m(h) \) at a critical field \( h_c \approx 0.941 \). When there is a magnetic field present the SU(2) symmetry of the bilinear-biquadratic model breaks down to U(1). At the ULS point, however, where the symmetry is higher, the quantities \( N_+, N_0, \) and \( N_- \), denoting the numbers of +, 0, and – spin states in the wave function, with \( N_+ + N_0 + N_- = N \) the length of the chain, are independently conserved. Thus the remaining continuous symmetry for \( \beta = 1 \), \( h > 0 \) is \( U(1) \times U(1) \). For \( \beta < 1 \) when the strength of the field is higher then the value of the gap, the Haldane gap collapses and the low-energy physics of the magnetized system is governed by gapless excitations. The emerging periodicity is a function of the field strength and in the generic situation incommensurate. Finally, when the field is strong enough all the spins align and the magnetization saturates.

The behavior of Haldane-gap antiferromagnets in strong magnetic field is not universal. While the low-energy physics of the conventional 1D spin-1 Heisenberg model in its magnetized regime is described by one incommensurate soft mode, other systems with somewhat perturbed coupling constants can possess two characteristic soft modes in a certain range of the field strength. Such a two-component Luttinger liquid phase is realised above the massive Haldane-gap phase, and in general above any massive nonmagnetic phase, when the ground state exhibits short range incommensurate fluctuations already in the absence of the field.
Early speculations\[6\] that the S2-S1 phase transition of the ULS model may also take place in the Heisenberg chain at $\beta = 0$ was finally refuted by Takahashi and Sakai\[7\] who found that in the whole range $0 < m < 1$ the low-energy physics is described by a $c = 1$ U(1) conformal field theory (CFT) which is equivalent to the one-component Luttinger liquid, thus only an S1 phase appears. The Luttinger liquid parameters vary smoothly as a function of the magnetization. Naturally arises the question whether the appearance of the Haldane gap in the ground state only allows the S1 behavior seen for the pure Heisenberg model, or there is a certain domain in parameter space where multi-component Luttinger liquids such as an S2 phase can occur above the S0 Haldane phase. To clarify this question is the principal aim of this Letter.

The first indication that the Haldane gap of the bilinear-biquadratic model may collapse into an S2 phase comes from the numerical observation that at $h = 0$ the VBS point $\beta_{\text{VBS}} = 1/3$, where the ground state can be constructed exactly using nearest-neighbor valence bonds, is in fact a disorder point, beyond which short range fluctuations in the ground state become incommensurate\[8\]. However, due to the finite correlation length, the peak at $\pi$ in the static structure factor will be dominated by the most slowly decaying terms, and the other is the finite difference of the two split gap minimum rapidly shifts from the antiferromagnetic to the ULS value $2/\pi$. Of course, any linear combinations of these two, where the emerging incommensurability makes the incommensurate.

One can define a third special point $\beta_{\text{Disp}}$, which is \textit{a priori} distinct from (but close to) the above two, where the emerging incommensurability make the subprocess amplitude. Two may also show up in the correlation functions, which

\[\delta E = E_\alpha - E_\beta = \frac{2\pi}{N} \left[ v_1 (\Delta_1^+ + \Delta_1^-) + v_2 (\Delta_2^+ + \Delta_2^-) \right] \]  

with

\[\Delta_1^+ = \frac{1}{2} \left[ Z_{11}d_1 + Z_{21}d_2 \pm \frac{Z_{22}d_1 - Z_{12}d_2}{2 \det Z} \right]^2 + n_1^+ \]

\[\Delta_2^+ = \frac{1}{2} \left[ Z_{12}d_1 + Z_{22}d_2 \pm \frac{Z_{11}d_1 - Z_{12}d_2}{2 \det Z} \right]^2 + n_2^+ \]

where $E_\beta$ is the energy of the ground state, the index $\alpha = \{d_1, d_2; l_1, l_2; n_1^+, n_1^-, n_2^+, n_2^-\}$ is a shorthand for eight integer (half-integer) quantum numbers specifying the eigenstate, and the matrix $Z_{\alpha\beta}$, $\alpha, \beta = 1, 2$ is the "dressed charge matrix" responsible for the interaction of the two BA components. The relative momentum of the state $\alpha$ reads

\[\delta P = P_\alpha - P_\beta = Q + \frac{2\pi}{N} (\Delta_1^+ - \Delta_1^- + \Delta_2^+ - \Delta_2^-) \]

where $Q = Q_\alpha$ is an $O(1)$ term

\[Q = 2\pi (1 - P_\gamma) d_1 + 2 \pi P_\gamma d_2 + \pi l_1.\]

The physical interpretation of the quantum numbers is as follows: $l_\alpha$ ($d_\alpha$) represents the number of particles added to (transferred from the left Fermi point to the right in) component $\alpha$. $n_\alpha^\pm$ is the number of small momenta particle-hole pairs created in component $\alpha$ around the left (−) and the right (+) Fermi points. While $l_\alpha$ and $n_\alpha^\pm \geq 0$ are always integers, $d_\alpha$ is integer or half integer with $d_{1,2} \equiv l_{2,1}/(2 \text{ mod } 1)$. This structure is analogous to the one found in the 1D Hubbard model where the two components are called "charge" and "spin", resp. In the present case $l_1 = \Delta N_0 + \Delta N_-$, $l_2 = \Delta N_+$ for which there are selection rules when a given type of correlation functions is considered.

The low-energy excitations of the ULS model in its S2 phase can be interpreted by assuming that they arise from the direct sum of two $c = 1$ conformal field theories (CFTs) each having a different sound velocity $v_1$ and $v_2$, resp. As is indicated by Eq. (3) local physical operators necessarily couple to both CFTs. Conformal invariance then requires that the 2-point functions behave as

\[\langle \phi(x,t)\phi(0,0) \rangle = A_\delta e^{-iQx} \prod_{\alpha, \pm} (x - iv_\alpha t)^{-\Delta_\alpha^\pm} \]  

showing the analog of ”spin-charge separation” for the present spin-1 situation. Let us consider the operator content of the theory: each operator $\phi_\alpha$ (primary or secondary) is labeled by the eight quantum numbers $\alpha$, and has the anomalous dimension $x_\alpha = \Delta_1^+ + \Delta_1^- + \Delta_2^+ + \Delta_2^-$ and conformal spin $s_\alpha = \Delta_1^+ - \Delta_1^- + \Delta_2^+ - \Delta_2^- = 2d_1 + d_2 + n_1^+ - n_1^- + n_2^+ - n_2^-$. Note that the total momentum associated to these operators is $\delta P$ in Eq. (4), involving the $Q$ term as well. There are four marginal operators $M_{1,2,3,4}$ which can be formed using only the $n_{1,2}^\pm$
quantum numbers and setting \( l_\alpha, d_\alpha = 0 \). Their dimension, spin and total momentum \((x = 2, s = 0, \delta P = 0)\) do not depend on the \( Z_{\alpha\beta} \) matrix. The presence of these operators causes the existence of an extended critical domain in the parameter space. The other relevant or marginal operators are all primary, i.e., \( n_\alpha^\pm = 0 \) and all depend on the \( Z_{\alpha\beta} \) matrix. This latter can be calculated numerically for the ULS model by solving a set of coupled integral equations. The results are shown in Fig. 1(a). When \( h = 0 \), \( Z_{11} = Z_{22} = \sqrt{1/3 + 1/2\sqrt{3}} \), \( Z_{12} = Z_{21} = \sqrt{1/3 - 1/2\sqrt{3}} \), and there is an additional marginal operator \( \phi_{1/2,1/2,1,-1} \) (and its equivalents under SU(3) and parity transformations, e.g., \( \phi_{1,1} \)) as can be checked using Eq. (3). (From now on in the index a we omit \( l_\alpha \) and/or \( n_\alpha^\pm \) when they are zero.) The operator \( \phi_{1/2,1/2,1,-1} \) has anomalous dimension \( x = 2 \) and total momentum \( \delta P = 0 \) when \( h = 0 \). This is the principal operator responsible for the SU(3)→SU(2) symmetry breaking processes \( 00 \leftrightarrow +-, -+ \). As was shown in Ref. 4 the interplay of \( \phi_{1/2,1/2,1,-1} \) and the \( \mathcal{M} \) operators (which constitute the SU(3) current interaction in the WZW theory) gives rise to the Haldane gap for \( \beta < 1 \) but maintains criticality for \( \beta > 1 \).

![FIG. 1. Bethe Ansatz results for the ULS model vs the magnetization \( m \). (a) The dressed charge matrix, (b) anomalous dimension and (c) momentum \( Q \) of some selected operators. Some other operators marginal at \( h = 0 \) are not shown. (d) DMRG results for the Fourier transform of the one-point function \( \langle S_0^+ \rangle \). The peak at the Lieb-Schultz-Mattis value \( q = 2\pi m, 2\pi(1 - m) \) only develops for \( m > m_c \).](image)

When \( 0 < h < h_c \) the anomalous dimensions and momenta of the operators present in the ULS model vary as shown in Fig. 1(b). Since the perturbation part of the Hamiltonian, represented by the deviation \((1 - \beta) \) term, transforms under translations with momentum zero, in its decomposition into the operators present in the ULS model at \( h > 0 \) only operators with \( \delta P = 0 \) can appear. This is a serious limitation, since as shown in Fig. 1(c), the two characteristic momenta \( Q_{1,0} = 2\pi(1 - P_z) \) and \( Q_{0,1} = 2\pi P_z \), associated to the large momentum transfer processes of the two components in Eq. (2) become generically incommensurate. \( \phi_{1/2,1/2,1,-1} \) has no longer \( \delta P = 0 \) so it does not contribute. It is in fact an Umklapp operator which appears in the low-energy description only at \( h = 0 \). What contribute are the operators \( \phi_{d_1,d_2,1,-1,n_1^\pm,n_2^\mp} \) with \( d_1, d_2 \) half-integer, and \( n_1^\pm > 0 \) chosen in a way to reinstall \( \delta P = 0 \). However, due to the appearance of the necessary small momentum particle-hole excitations such operators are highly irrelevant. The marginal operators \( \mathcal{M} \) are not able alone to drive the two Luttinger liquid components away from criticality, although they make the universality class change continuously. We conclude that when \( 0 < m < m_c \) the bilinear-biquadratic model must remain in its S2 phase in an extended domain on both sides of the ULS line \( \beta = 1 \).

![FIG. 2. Phase diagram of the bilinear-biquadratic spin-1 chain in a magnetic field. The one- and two-component Luttinger liquid phases are denoted by S1 and S2, resp. The S1-S2 phase boundary is determined by the DMRG (○ points). The dotted line indicates some uncertainties near the disorder points.](image)

When the magnetic field reaches the critical value \( h_c \) in the ULS model the sound velocity \( v_2 \to 0 \), and the corresponding critical degree of freedom becomes massive. The emerging S1 phase can be described by a single \( c = 1 \) CFT, and the universality class is determined by a scalar dressed charge \( Z \). Once again we do not expect any drastic changes in the low-energy physics as \( \beta \) is perturbed away from 1. The predicted phase diagram is shown in Fig. 2.

In order to find the exact phase boundaries we carried out a detailed numerical analysis using the DMRG technique. Unfortunately the DMRG does not work in momentum space thus a direct search for tracking soft modes by calculating energy gaps is not feasible. Instead, we calculated the decay of the one-point function \( \langle S_0^+ \rangle \) from the edge of an open chain for different values of \( \beta \) and magnetization \( m = S_0^+/N \). The one-point function contain the same information as the equal time two-point correlation function in Eq. (3) (note that the
exponent of the one-point function is half of that of the two-point function), and the appearing soft modes can be identified in the Fourier transforms by making a suitable multi-parameter fit in real space.\cite{12}

Once again exact results can be obtained for the ULS model. Considering \( \langle S^z_j \rangle \) in the S2 phase only operators with \( \delta S^z_{\text{tot}} = 0 \), i.e., \( l_1 = l_2 = 0 \) and \( l_1 = -l_2 = \pm 1 \) can contribute. The most relevant operators are \( \phi_{1,0}, \phi_{0,1}, \phi_{1,-1}, \phi_{1/2,1/2,1,-1} \), and \( \phi_{1/2,-1/2,1,-1} \) (and their equivalents under symmetries). The associated momenta \( Q \) (position of the peak in the structure factor) and the occurring critical exponents can be read off from Fig. 3(b) and (c). The example presented in Fig. 3(d) illustrates that in the S2 phase of the ULS model the only three interactions already at \( \beta = 1 \) contribute when \( \beta \neq 1 \). It is remarkable that in the S2 phase the operator \( \phi_{1,1} \), which has an anomalous dimension over 2 and momentum \( Q_{1,1} = 2\pi(1 - m) \), does not contribute to the correlation function. In the high-field S1 phase, however, the only peak discernible in the structure factor, as shown in Fig. 3(d), is the one with \( Q_1 = 2\pi(1 - m) \), in agreement with the Lieb-Schultz-Mattis theorem.\cite{11}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{fig3}
\caption{The phase diagram, as determined by the DMRG calculation, is shown in Fig. 2. Details of the numerical investigation will be published elsewhere.\cite{12}}
\end{figure}

Our analysis is valid in the strict sense close to the ULS line only. Here the S2–S1 phase transition is clearly associated to the depletion of one of the two “bands” as suggested by the BA. Note that in Fig. 3 the phase boundary does not change very much until about \( \beta \sim 0.5 \) where it seems to decline rather rapidly. A priori we cannot exclude the possibility that some operators become relevant here and open a gap in one of the critical components. This question needs further clarification.

In the bilinear-biquadratic model in Eq. (1) the S2 phase terminates near \( \beta \approx 0.4 \). This is still far in the parameter space from the currently known spin-1 Haldane gap materials for which the biquadratic term is small, and the pure Heisenberg model, although with some anisotropies, is a good description. For these systems only S1 type massless phases (and eventually, for some special values of \( m \), additional S0 type phases, i.e., magnetization plateaus) are expected to appear. However, even here, due to the closeness of the S2 phase somewhat further in the phase diagram, massive but relatively low energy excitations are predicted to show up in the weakly magnetized regime. They are expected to contribute in experiments probing higher lying excitations such as in inelastic neutron scattering, or in situations when short distance physics is important as, e.g., in nonmagnetically doped materials. Although there is no sharp phase transition in this case, the low-field and high-field regimes may look rather different, separated by a more or less narrow crossover region as observed, e.g., in Ref. 7.

In general, a two-component Luttinger liquid phase (S2), and then an eventual phase transition S2→S1 during the magnetization process, is expected to occur whenever the ground state develops incommensurate fluctuations already at \( h = 0 \). It must not necessarily be above a Haldane gap; the spin-1/2 zig-zag ladder, for example, which is expected to describe adequately the quasi-1D antiferromagnet Cs\(_2\)CuCl\(_4\), where the gap is due to dimerization and fluctuations are also predicted to be incommensurate already without a magnetic field\cite{14} is another possible candidate.

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