Midgap States in Antiferromagnetic Heisenberg Chains with A Staggered Field

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We study low-energy excitations in antiferromagnetic Heisenberg chains with a staggered field which splits the spectrum into a longitudinal and a transverse branch. Bound states are found to exist inside the field induced gap in both branches. They originate from the edge effects and are inherent to spin-chain materials. The sine-Gordon scaling $h_s^{2/3} \log h_s^{1/6}$ ($h_s$: the staggered field) provides an accurate description for the gap and midgap energies in the transverse branch for $S = 1/2$ and the midgap energies in both branches for $S = 3/2$ over a wide range of magnetic field; however, it can fit other low-energy excitations only at much lower field. Moreover, the integer-spin $S = 1$ chain displays scaling behavior that does not fit this scaling law. These results reveal intriguing features of magnetic excitations in spin-chain materials that deserve further investigation.

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Quantum spin chains have been a source of fascinating developments in physics and many related fields since the early days of quantum theory [1, 2, 3, 4]. They serve as model systems for revealing fundamental physics in many materials. Progress in experimental techniques has led to the synthesis and characterization of many quasi-one-dimensional materials in the last two decades. A very active field of theoretical and experimental research has emerged for the study of novel magnetic properties in low-dimensional spin systems where quantum fluctuations play a crucial role [5, 6].

Intriguing low-energy phenomena like the spin gap induced by magnetic field have been observed in many recently synthesized materials such as Cu(C₂D₅COO)₂3D₂O [3, 4], Yb₄As₃ [3, 10, 11] and CuCl₂( dimethylsulfoxide) [17]. The Dzyaloshinskii-Moriya (DM) interaction is intrinsic to these materials due to an alternating structure of molecular or spin-orbital interactions [12, 13]. Although it is one order of magnitude smaller than the standard Heisenberg exchange interaction in these materials, significant effects of the DM interaction have been unveiled recently when the materials are subjected to external magnetic fields [4, 8, 14]. An energy gap proportional to some power of the magnetic field opens up. These systems can be generally modeled by the following Hamiltonian,

$$\hat{H} = \sum_i \left( J \hat{S}_i \cdot \hat{S}_{i+1} - (-)^i \mathbf{D} \cdot \hat{S}_i \times \hat{S}_{i+1} \right. - \left. \mu_B \mathbf{H} \cdot \left[ \mathbf{g}^s + (-)^i \mathbf{g}^t \right] \cdot \hat{S}_i \right),$$

where the three terms in the summation are the antiferromagnetic Heisenberg, DM and Zeeman splitting interactions, respectively. While the exchange coupling constant $J$ and the uniform (staggered) $\mathbf{g}^s$ ($\mathbf{g}^t$) can be determined from the neutron scattering and electron spin resonance experiments, the $\mathbf{D}$-vector can be obtained only through theoretical analysis of the gap values in comparison with experiment [8, 11, 13].

The DM term can be eliminated by performing a spin rotation about the $\mathbf{D}$ vector by an angle $\alpha = \pm \frac{1}{2} \tan^{-1}(D/J)$ on the alternating sites. After neglecting anisotropic terms in the limit of $D \ll J$, which are only needed to account for the field dependence of the gap in different crystallographic directions [14], the relevant physics is captured by the effective Hamiltonian [4],

$$\hat{H} = J \sum_i [\hat{S}_i \cdot \hat{S}_{i+1} - h_u \hat{S}_i^z - (-)^i h_s \hat{S}_i^z],$$

where $h_u$ and $h_s$ are the effective dimensionless (scaled by $\mu_B/J$, and $J$ is taken as the energy unit hereafter) uniform and staggered field, respectively. This Hamiltonian has been mapped onto the quantum sine-Gordon model using the bosonization technique [4] and the aforementioned novel magnetic properties are described in terms of soliton, antisoliton, and breather excitations [4, 15, 16, 17].

Despite intensive investigations, quasi-one-dimensional spin systems with DM interaction continue to display surprising new physics. In this paper we show that the excitation spectra are split into a longitudinal and a transverse branch, while edge effects result in midgap states in both branches for open chains with both integer and half-integer spins in the thermodynamic limit. These midgap states are inherent to real spin-chain materials which always have chain ends. The existing field theory is established in the context of the quantum sine-Gordon model for periodic spin-1/2 chains [4, 17]. It is very important to clarify how soliton, antisoliton, and breather modes in the field theory are related to the gap and midgap states in different branches. Recent electron spin resonance experiment [18] on a spin-1/2 chain
compound [Pyrimidine-Cu(NO$_3$)$_2$(H$_2$O)$_2$]$n$(CuPM) revealed that some excitation modes, including one of the most intensive modes, cannot be fully described in terms of the quantum sine-Gordon model [4]. This raises fundamental issues regarding the nature of these magnetic excitations. Moreover, current discussions focus almost exclusively on the $S = 1/2$ case; it is of great interest to examine the low-energy excitations of higher-spin chains [19, 20] and their possible connections to the spin-1/2 chain and the field theoretical description.

We use the density matrix renormalization group (DMRG) method [21, 22] to study directly the Hamiltonian defined by Eq. (2) for both integer ($S=1$) and half-integer ($S=1/2$ and 3/2) spin chains. We find the same qualitative behavior for the gap and midgap states over a wide range of $h_u$ and, consequently, focus below on the effect of $h_s$ at $h_u=0$. Unless explicitly stated otherwise, we use open boundaries in all calculations. The results are obtained by keeping 400 states, but examined at low fields with 800 states. The truncation errors are on the order of $10^{-7}$ for $S = 3/2$ and much smaller for $S=1/2$ and 1. The gap and midgap energies in the thermodynamic limit were obtained by extrapolating numerical results for up to 200 sites to the long-chain limit.

![FIG. 1: The staggered field dependence of the transverse and longitudinal gaps ($\Delta_T$: solid circles; $\Delta_L$: solid triangles) and the midgap-state energies ($\Delta_m^T$: open circles; $\Delta_m^L$: open squares) for the spin-1/2 chain. The lines are fittings to the $h_s^{2/3} \log |h_s|^{1/6}$ scaling behavior anticipated from the conformal field theory [4]. The slopes of the plots which determine, up to log corrections, the scaling exponents of the leading order term are shown in the inset with the same axis labels, in the logarithmic scale. Data show a common scaling exponent of $\gamma = 2/3$ when the field is not too high.](image)

Figure 1 shows the low-lying energies relative to the non-degenerate ground state for the spin-1/2 chain. At $h_u = 0$ the spectrum splits into a transverse branch with $|S_{tot}^z|=1$ and a longitudinal branch with $S_{tot}^z=0$, with gaps $\Delta_T$ and $\Delta_L$, respectively, determined by scaling analyses that confirm the continuous nature of each spectrum in the large-$L$ limit. Midgap states appear in both branches. The gaps and the midgap-state energies $\Delta_m^T$ and $\Delta_m^L$ are obtained from the extrapolations of the DMRG data as shown in Fig. 2.

![FIG. 2: The excitation energies versus $1/L$ for several lowest states of the spin-1/2 chain labeled by $S_{tot}^x$ (upper panel) and $S_{tot}^x$ (lower panel) ($\alpha = A, B, C$). They all scale to zero as $L \to \infty$ at $h_s = 0$. At finite $h_s$ ($h_s = 0.05$ shown), they split into a longitudinal (lines) and a transverse (symbols) branch with distinct gap and midgap states ($S_{tot}^x(1) \to \Delta_m^T$, $S_{tot}^x(1) \to \Delta_T$, $S_{tot}^x(0) \to \Delta_m^L$, $S_{tot}^x(0) \to \Delta_L$, see the text for details). The conformal field theory for the spin-1/2 chain under a staggered magnetic field predicted [4] the scaling behavior $h_s^{2/3} \log |h_s|^{1/6}$ for the induced gap. We apply this scaling form to our numerical results as shown in Fig. 1. It is interesting to note that the field theory not only provides a good description in the low-field region for the transverse gap, a periodic chain feature, as expected, but also fits well the transverse midgap, a genuine open boundary edge effect (see below). The scaling exponents at the low field limit share the common value of $2/3$ predicted by the field theory. However, the fitting range is different for the two branches: the deviation from the predicted scaling behavior starts at $h_s \approx 0.03$ in the longitudinal branch while a satisfactory fitting persists beyond $h_s=0.1$ for the transverse branch. Moreover, the midgap state appears in the transverse branch as soon as $h_s$ is applied, but it does not become distinguishable in the longitudinal branch while a satisfactory fitting persists beyond $h_s=0.1$ which corresponds to a field of 14 Tesla in copper benzoate [8]. It suggests that the midgap state in the transverse branch should be observable at low fields, while much higher fields are required for its identification in the longitudinal branch. Since the midgap states are due to the chain-end effect,
their intensity is proportional to the impurity/defect concentration. Samples with high level of nonmagnetic impurity doping may be needed for their detection.

To examine the origin of the midgap states, we consider a bond impurity model [22]. A coupling $J'$ is added between the two end spins and varied from 0 (open boundary) to $J$ (periodic boundary). The midgap states develop in each branch when $J'$ deviates from $J$, indicating that these states appear as a consequence of the edge effect. The same effect is also observed in all higher-spin chains discussed below. Alternatively, we show in Fig. 2 for the spin-1/2 case that the midgap states can be traced back to the three lowest excitation states with $S_{\text{tot}} = 1$ at $h_s = 0$, labeled as $S_A^1$, $S_B^1$, and $S_C^1$, respectively. A comparison of the $h_s = 0$ and 0.05 data shows that state $S_A^1$ splits into midgap states $S_A^1(1)$ and $S_A^1(0)$, state $S_B^1$ splits into $S_B^1(1)$ that becomes the bottom of the transverse continuum and $S_B^1(0)$ that is a midgap state degenerate with $S_A^1(0)$, and state $S_C^1$ splits into $S_C^1(1)$ degenerate with $S_B^1(1)$ and $S_C^1(0)$ which is the bottom of the longitudinal continuum. The lowest excitation state $S_A^1$ with $S_{\text{tot}} = 0$ moves higher in energy and enters the longitudinal continuum at $h_s > 0$, which mixes two states $S_A^1(0)$ and $S_B^1(0)$ at about $L = 36$.

We now turn to the spin-1 case where the spectrum is gapful at $h_s = 0$. In the thermodynamic limit, the ground state of the open chain is four-fold degenerate owing to the topological edge effect as interpreted in the valence-bond-solid (VBS) picture [24]. The staggered field splits the four-fold degenerate ground state into three mixed states: a $S_B^1 = 0$ ground state, a doubly degenerate $|S_{\text{tot}}^1\rangle = 1$ transverse midgap state and a $S_C^1 = 0$ longitudinal state. The dependence of the gap and midgap-state energies on $h_s$ is shown in Fig. 3. In addition to the midgap states originating from a mixture of the $|S_{\text{tot}}^1\rangle = 0$, 1 states in the ground-state manifold, there are also midgap states with $S_{\text{tot}}^1 = 0$ and $|S_{\text{tot}}^1\rangle = 2$ below but close to the bottom of the longitudinal continuum. We have tried fitting the results to the field theoretical formula, but found that the $h_s^{2/5}|\log h_s|^{1/6}$ scaling is unsuitable for $S = 1$ in any field range. While this is not surprising for the gaps at low field since they have finite values at $h_s = 0$, the fact that it does not apply to the midgap energies that do scale to zero at $h_s = 0$ strongly suggests different intrinsic behavior for integer and half-integer spin cases [3].

Figure 4 shows the scaling behavior of the gap and midgap-state energies of the spin-3/2 chain. The low-field sine-Gordon scaling derived for the spin-1/2 chain also fits these results. In particular, the two lowest midgap states are well described beyond $h_s = 0.1$. It highlights common central charge [25] and topological features [26] intrinsic to all half-integer-spin chains. However, subtle yet important differences exist between the $S = 1/2$ and $S = 3/2$ cases. Unlike the spin-1/2 case where bound midgap state develops at low field explicitly in the transverse branch only, midgap states appear in both branches at very low fields for $S = 3/2$. Moreover, in the spin-3/2 case the $h_s^{2/3}|\log h_s|^{1/6}$ scaling fits the gaps only in the low field limit ($h_s < 0.02$), while the fitting works very well for the two lower midgap states in both branches over a much larger field range. Meanwhile, similar to the $S=1$ case, additional midgap states fall off from the bottom of the longitudinal continuum (not shown in Fig. 4 for clarity since a few of them are very close to the bottom at low fields). These similarities and distinctions between different half-integer spin chains deserve further studies.

Finally, we remark on the nature of the midgap states that share some common topological origin for all spin magnitudes. Although the gap at $h_s = 0$ is considered a fundamental criterion to distinguish the integer and half-integer spin cases [1], [3], it has been shown that an extra Berry phase contribution reflecting the topological feature leads to edge states in all open spin chains with $S > 1/2$ [27]. Most recently, it was also shown [28] that a topological string order originally derived [28, 29] for integer-spin chains exists in half-integer-spin chains as well. Nonetheless, the topological edge effect has been experimentally identified so far only in integer-spin chain materials where the excitation spectrum is gapful and topological excitations unstable against external disturbances (such as doping), can be measured. For the $S = 1$ case, this effect was observed in $Y_1-x\text{BaCa}_x\text{NiO}_5$ [30] and $Y_2\text{BaNi}_{1-x}\text{Mg}_x\text{O}_5$ [31]. The present results unveil the topological edge effects driven by the staggered magnetic field. The midgap states split off from the degenerate ground state of $S = 1$ chain (and all other integer-spin chains) represent a secondary (field induced) topological edge effect since bound midgap states are al-

![Figure 3: The staggered field dependence of the transverse and longitudinal gaps (ΔT: solid circles; ΔL: solid squares) and the midgaps (Δs: open circles, |S_{\text{tot}}^1| = 1; ΔL^s: open squares, S_{\text{tot}}^1 = 0; down-triangles: S_{\text{tot}}^1 = 0, diamonds: S_{\text{tot}}^1 = 0, and up-triangles: |S_{\text{tot}}^1| = 2) in the spin-1 chain. The lines are guide to the eyes only. The midgap states falling off from the longitudinal continuum are not connected by lines for clarity.](image-url)
ready observable at \( h_s = 0 \). Meanwhile, additional bound states fall inside the field induced gap from the continuum spectrum of all spin chains with \( S \geq 1 \) at \( h_s > 0 \).

![Graph](image)

**FIG. 4:** The staggered field dependence of the transverse and longitudinal gaps (\( \Delta_s \): solid circles; \( \Delta_L \): solid squares) and the corresponding lower midgap-state energies (\( \Delta^0_L \): open circles; \( \Delta^0_s \): open triangles) in the spin-3/2 chain. The lines are fittings to \( h_s^{2/3} \log |h_s|^{1/6} \) for these low-energy excitations.

It should be noted that the staggered field \( h_s \) arises from a nonzero uniform field \( h_u \) in real materials. The latter does not change the qualitative scaling behavior when the field is not too strong \([1, 14]\). We have examined the gap and midgap states at nonzero \( h_u \) and found the same qualitative results at realistic \( h_s/h_u \) ratios although the classification of the longitudinal and transverse branches no longer holds strictly because of the breaking of the axial symmetry by \( h_u \).

In summary, we have shown that bound midgap states generally exist in open boundary antiferromagnetic Heisenberg chains with a staggered magnetic field. Some of the gap and midgap energies for the half-integer spin chains fit well to a scaling function derived from the quantum sine-Gordon model. However, it is revealed that (i) other low-energy excitations of the half-integer spin chains do not fit equally well and (ii) the scaling behavior of the integer spin chain is qualitatively different. Further experimental and theoretical investigations are called for to fully identify low energy excitations, especially the midgap states as a general phenomenon in open spin chains.

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[1] H. Bethe, Z. Phys. 71, 205 (1931).
[2] L.D. Faddeev and L.A. Takhtajan, Phys. Lett. A 85, 375 (1981).
[3] F.D. Haldane, Phys. Rev. Lett. 50, 1153 (1983).
[4] M. Oshikawa and I. Affleck, Phys. Rev. Lett. 79, 2883 (1997); Phys. Rev. B 60, 1038 (1999).
[5] S. Sachdev, Quantum Phase transitions, Cambridge University Press (2000).
[6] C. Broholm, et al., in High Magnetic Fields: Applications in condensed matter physics and spectroscopy, C. Berthier et al., Eds. Springer-Verlag (2003).
[7] D.C. Dender, D. Davidovic, D.H. Reich and C. Broholm and G. Aeppli, Phys. Rev. B 53, 2583 (1996).
[8] D.C. Dender, P.R. Hammar, D.H. Reich and C. Broholm, Phys. Rev. Lett. 79, 1750 (1997).
[9] M. Kohgi, K. Iwasa, J. Mignot, B. Fak, P. Gegenwart, M. Lang, A. Ochiai, H. Aoki, and T. Suzuki, Phys. Rev. Lett. 86, 2439 (2001).
[10] P. Fulde, B. Schmidt, and P. Thalmeier, Europhys. Lett. 31, 323 (1993).
[11] M. Oshikawa, K. Ueda, H. Aoki, A. Ochiai and M. Kohgi, J. Phys. Soc. Jpn. 68, 3181 (1999); H. Shiba, K. Ueda, and O. Sakai, J. Phys. Soc. Jpn. 69, 1493 (2000)
[12] I. Dzyaloshinskii, J. Phys. Chem. Solids 4, 241 (1958)
[13] T. Moriya, Phys. Rev. 120, 91 (1966)
[14] J.Z. Zhao, X.Q. Wang, T. Xiang, Z.B. Su, and L. Yu, Phys. Rev. Lett. 90, 207204 (2003).
[15] F.H.L. Essler, Phys. Rev. B 59, 14376 (1999).
[16] F.H.L. Essler and A.M. Tsvelik, Phys. Rev. B 57, 10592 (1998).
[17] M. Kenzelmann, Y. Chen, C. Broholm, D. H. Reich, and Y. Qiu, Phys. Rev. Lett. 93, 017204 (2004).
[18] S.A. Zvyagin, A.K. Kolezhuk, J. Krzystek, and R. Feyrermer, Phys. Rev. Lett. 93, 027201 (2004).
[19] A. Zheludev, E. Ressouche, S. Maslov, T. Yokoo, S. Raymond and J. Akimitsu, Phys. Rev. Lett. 80, 3630 (1998).
[20] J.Z. Lou, X. Dai, S.J. Qin, Z.B. Su and L. Yu, Phys. Rev. B 60, 52 (1999)
[21] S.R. White, Phys. Rev. Lett. 69, 2863 (1992).
[22] I. Peschel, X. Wang, M. Kaulke and K. Hallberg, Density Matrix Renormalization, LNP, 528, Springer-Verlag (1999).
[23] X. Wang and S. Mallwitz, Phys. Rev. B 53, R492 (1996).
[24] I. Affleck, T. Kennedy, E.H. Lieb, and H. Tasaki, Phys. Rev. Lett. 59, 799 (1987).
[25] K. Hallberg, X. Wang, P. Horsch and A. Moreo Phys. Rev. Lett. 76, 4955 (1996).
[26] J.Z. Lou, S.J. Qin, and C.F. Chen, Phys. Rev. Lett. 91, 087204 (2003); C. F. Chen, Phys. Rev. B 70, 092404 (2004).
[27] T.K. Ng, Phys. Rev. B 50, 555 (1994).
[28] M.P.M. den Nijs and K. Rommelse, Phys. Rev. B 40, 4709 (1989).
[29] S.R. White and D.A. Huse, Phys. Rev. B 48, 3844 (1993).
[30] J.F. DiTusa, S.W. Cheong, J.H. Park, G. Aeppli, C. Broholm, and C.T. Chen, Phys. Rev. Lett. 73, 1857 (1994).
[31] M. Kenzelmann, G. Xu, I.A. Zaliznyak, C. Broholm, J.F. DiTusa, G. Aeppli, T. Ito, K. Oka, and H. Takagi, Phys. Rev. Lett. 90, 087202 (2003).