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Abstract
In several frustrated systems, incommensurate behaviours are often observed. For the $S = 1$ bilinear–biquadratic model, we show that the main oscillatory behaviour, which is proportional to the free edge spins, is eliminated in the incommensurate subphase, considering the average of triplet and singlet energy spectra under open boundary conditions. In the same way, the π-mode oscillation is also removed in the commensurate subphase. Moreover, we find that higher-order corrections are exponentially decaying from an analysis of small-size data.

1. Introduction

Commensurate–incommensurate (C–IC) transitions are interesting phenomena in frustrated quantum spin systems. In Haldane gap systems, incommensurabilities have often been regarded as troublesome problems and have rarely been discussed in detail until recently. In inelastic neutron scattering experiments, Xu *et al* [1] have revealed that a quasi-one-dimensional oxide, $Y_{2-x}Ca_xBaNiO_5$, has an incommensurate double-peaked structure factor. However, an analytical interpretation for incommensurabilities has not been clear.

The spin-1 bilinear–biquadratic model,

$$\mathcal{H} = \sum_{i=1}^{N} h_i, \qquad h_i = \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \alpha(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2, \tag{1}$$

which plays the role of a prototype of Y_2BaNiO_5, has the C–IC change point which corresponds to the Affleck–Kennedy–Lieb–Tasaki (AKLT) point $\alpha = \alpha_D = 1/3$ [2, 3]. The AKLT point is solvable and has an energy gap above the valence-bond-solid (VBS) ground state [4, 5]. The VBS state has recently been getting more attention with reference to quantum entanglements [6–9].

Analysing the structure factor among the commensurate and incommensurate subphases, and also the C-IC change point, we have deduced two candidates for the *real* structure factor

unifying these two regions and the AKLT point [10, 11]. Following the Sørensen–Affleck prescription [12], we have constructed Green functions from the candidates, and compared them with the energy gap obtained numerically under the open boundary conditions [13]. Thus, we have found that the Green function consists of two elements which have anomalies in the upper-or lower-half plane.

In this paper we will show that incommensurate oscillatory behaviours in the incommensurate subphase can be cancelled, using triplet and singlet energy spectra. In the same way, we can obtain comparable results in the commensurate case. Moreover, we discuss higher-order corrections considering small-size systems.

2. Short review of singlet–triplet energy gap

The gapped Haldane phase has nonvanishing, nonlocal string order [16] and effectively free $S = 1/2$ spins at the ends of open chains [14, 15]. These edge spins bring a low-lying excitation triplet, which is degenerate with the ground state in the thermodynamic limit [14]. While this excitation is clearly a boundary effect, it is linked to the bulk behaviour because of the existence of nonlocal string order [3].

According to Sørensen and Affleck (SA) [12], the effective Hamiltonian can be connected using the Green function:

$$\mathcal{H}_{\text{eff}} = (-1)^N \mathbf{S}'_L \cdot \mathbf{S}'_R \lambda^2 \int \frac{\mathrm{d}q\,\mathrm{d}\kappa}{(2\pi)^2} G(q,\kappa) \exp(\mathrm{i}qN)\delta(\kappa), \tag{2}$$

where $\mathbf{S}'_L$ and $\mathbf{S}'_R$ are spin-1/2 operators at the ends of chain. Considering the Clebsch–Gordan coefficient, we obtain singlet and triplet expectation values for edge spins as

$$\begin{aligned}
\langle S| \mathbf{S}'_L \cdot \mathbf{S}'_R |S\rangle &= -3/4, \\
\langle T| \mathbf{S}'_L \cdot \mathbf{S}'_R |T\rangle &= 1/4,
\end{aligned} \tag{3}$$

where $|T\rangle = |s^T = 1, s_z = \pm 1, 0\rangle$ and $|S\rangle = |s^T = 0, s_z = 0\rangle$.[1] Thus the energy difference between the singlet and triplet states can be described with the Green function:

$$\begin{aligned}
\Delta E_{\text{ST}}(N) &\equiv E_T - E_S \\
&= (-1)^N \lambda^2 \int \frac{\mathrm{d}q}{2\pi} G(q,0) \exp(\mathrm{i}qN),
\end{aligned} \tag{4}$$

where E_T and E_S are the triplet and singlet energies, respectively.

Figure 1 shows the energy gap behaviours of the model (1) with different chain lengths. Increasing the chain length on some fixed α in the commensurate subphase, we see that the energy gap oscillates between even and odd chains and decreases exponentially fast, while this behaviour is not simple in the incommensurate subphase. The even–odd oscillation is modulated by the frustration in the incommensurate subphase.

In our previous study [13], which has been performed to explain these behaviours, we found
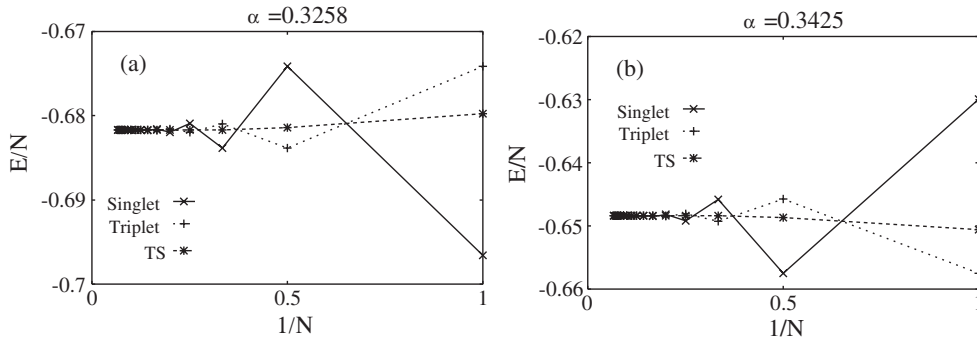
$$\Delta E_{\text{ST}}(N) = \begin{cases}
(-1)^N \widetilde{A} \exp(-\widetilde{m}N) \sin(\sqrt{d}N), & (\alpha > 1/3) \\
0, & (\alpha = 1/3) \\
(-1)^N \widetilde{A} \exp(-\widetilde{m}N) \sinh(\sqrt{d}N), & (\alpha < 1/3).
\end{cases} \tag{5}$$

The parameters, $\widetilde{A}$, $\widetilde{m}$, and d, depend on $\alpha - \alpha_D$ and have been determined with the nonlinear least-squares fitting method, as shown in [13]. We have found that the C–IC change is

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[1] $\mathbf{S}'_i \cdot \mathbf{S}'_j = [(\mathbf{S}'_i + \mathbf{S}'_j)^2 - \mathbf{S}'^2_i - \mathbf{S}'^2_j]/2.$
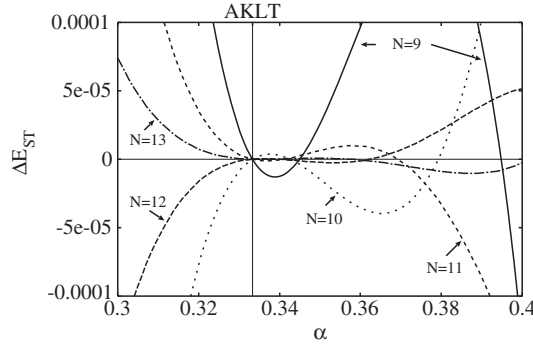
Figure 1. Oscillation of the energy gap of edge states. The energy gaps with different chain lengths ($N = 9, \ldots, 13$) are plotted as a function of α.

Figure 2. Cancellation of triplet–singlet energies. Triplet and singlet energy spectra, and the average of the triplet–singlet energies, are plotted as a function of $1/N$ for $1 \leqslant N \leqslant 15$ when (a) $\alpha = 0.3258$ (commensurate case) and (b) 0.3425 (incommensurate case).

characterized by the following Green function:

$$G(q, 0) \sim \frac{1}{(q - \mathrm{i}\widetilde{m})^2 - d} + \frac{1}{(q + \mathrm{i}\widetilde{m})^2 - d}. \tag{6}$$

3. Average of triplet–singlet energies
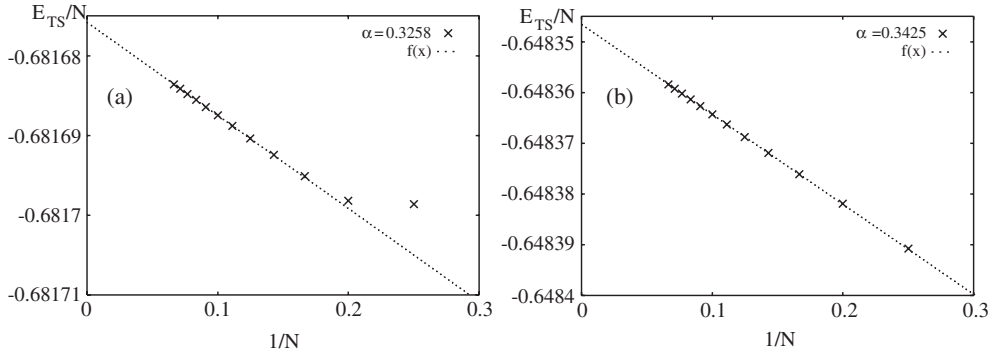
Now we define the average of triplet–singlet energies:

$$\overline{E}_{TS} \equiv (E_S + 3E_T)/4. \tag{7}$$

From equations (2) and (3), we expect that we can eliminate the principal term caused by the anomalies of the Green function using this average.

Figure 2 shows bare triplet and singlet energies and averages of triplet–singlet energies plotted as a function of $1/N$ for (a) $\alpha = 0.3258$ (commensurate case) and (b) 0.3425 (incommensurate case). We see that the average of triplet–singlet energies on a fixed α varies linearly with $1/N$ not only in the incommensurate subphase but also in the commensurate subphase.

We perform the least-squares fit to the averages of triplet–singlet energies using the following fitting function:

$$f(N) = c_0 + c_1/N. \tag{8}$$

Figure 3. Finite-size effect in the average of the triplet–singlet energies and a least-squares fitting line $(c_0 + c_1/N)$ are plotted when (a) $\alpha = 0.3258$ and (b) 0.3425.
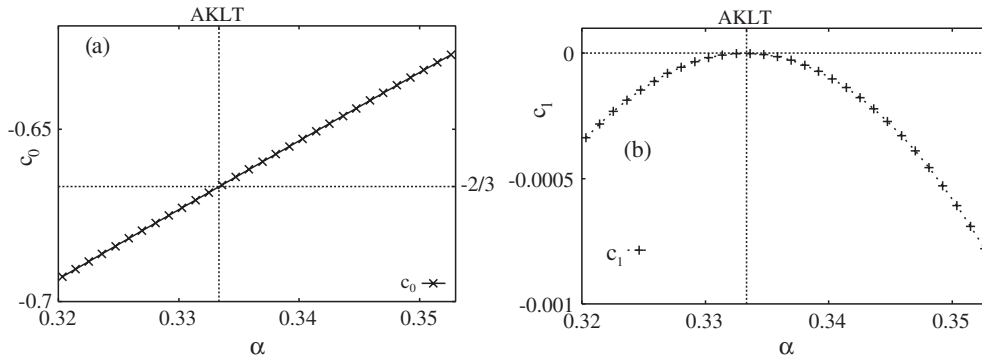
Figure 4. Coefficients (a) c_0 and (b) c_1 in equation (8) are plotted near the AKLT point. It appears that $c_0 \propto \alpha - \alpha_D$ and $c_1 \propto (\alpha - \alpha_D)^2$.

Figure 3 shows the data of triplet–singlet averages and $f(N)$. When (a) $\alpha = 0.3258$, each coefficient is obtained as $c_0 = -0.681\,675\,81 \pm 2 \times 10^{-9}$ and $c_1 = -1.1671 \times 10^{-4} \pm 2 \times 10^{-8}$ for $8 \leqslant N \leqslant 15$. In the same way, $c_0 = -0.648\,346\,5831 \pm 2 \times 10^{-10}$ and $c_1 = -1.772\,95 \times 10^{-4} \pm 2 \times 10^{-9}$ when (b) $\alpha = 0.3425$. The average of the triplet–singlet energies $\overline{E}_{TS}/N$ seems to behave highly linearly in the small-α region. In fact, we observe that coefficients of $O(1/N^2)$ and $O(1/N^3)$ are very small. Hence, we can say that a higher power of $1/N$ does not appear.

Figure 4 shows coefficients c_0 and c_1 in equation (8) obtained with the least-squares fitting. The second term in equation (8) comes from surface effects. Since the surface effects are caused by the one-dimensionality, they are different from the effect of edge spins. Additionally, the surface effects are perfectly zero, namely $c_1 = 0$, at the AKLT point[2]. Moreover, c_1 always shows a negative value except the AKLT point. We see that the fitting parameters c_0 and c_1 behave approximately as $\alpha - \alpha_D$ and $(\alpha - \alpha_D)^2$, respectively.

So far we have excluded data smaller than $N = 8$, since these data differ from equaton (8). Then we proceed to study small-size corrections from equation (8). For a rough estimate, we consider the difference

$$\Delta y(N) = \overline{E}_{TS}(N)/N - (c_0' + c_1'/N) \tag{9}$$

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[2] Of course, $c_0 = -2/3$ at the AKLT point.
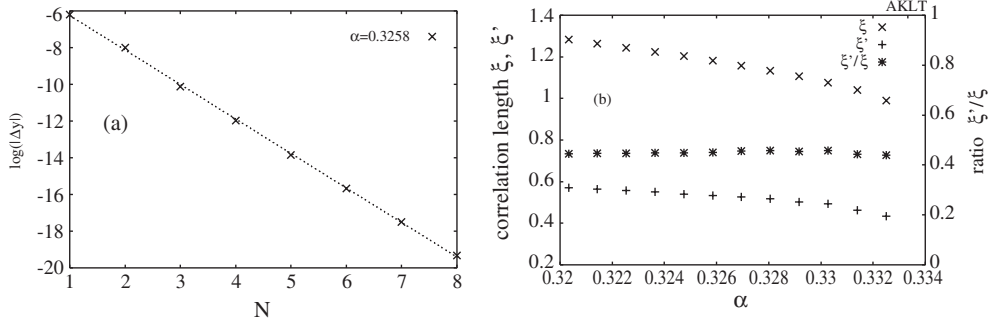
Figure 5. (a) The logarithm of $|\Delta y|$ (equation (9)) is plotted against N. The dotted line is drawn for a guide to the eye. (b) Two different correlation lengths and the ratio ξ'/ξ are plotted in the commensurate region.

for small N, although we use c_0' and c_1', which are determined from the data of $N = 14, 15$. Figure 5(a) shows $\log(|\Delta y|)$ for $1 \leqslant N \leqslant 8$ at $\alpha = 0.3258$ in the commensurate region. Since the logarithm of Δy decreases linearly with N, the difference Δy results in $\Delta y \sim \exp(-N/\xi')$. We estimate ξ' as shown in figure 5(b), and then we find $\xi' \sim \xi/2$ (the correlation length ξ is obtained in the previous study [13]).[3]

In the incommensurate region, we see the oscillatory behaviour again. We roughly estimate the wavenumber of this oscillation, and then we find $q_{IC}' \sim 2(q_{IC}+\pi)$.[4] We will show a detailed calculation in another paper.

4. Summary

We have shown that the principal oscillatory behaviours, which are proportional to $\mathbf{S}_L' \cdot \mathbf{S}_R'$, among the triplet and singlet energy spectra under open boundary conditions cancel out in the commensurate and incommensurate subphases.

We have found that the energy spectra of singlet and triplet states under open boundary conditions consist of the bulk, surface, and edge spin energies:

$$E_C/N = B + S/N + \langle C|\mathcal{H}_{eff}|C\rangle, \qquad (C = \{S, T\}) \tag{10}$$

where B and S are the bulk and surface energies, respectively.

Considering small N, we have found an exponentially decaying correction term, the correlation length and the incommensurate wavenumber of which differ by a factor of two from those obtained by the energy gap of edge states. One possibility is that the correction will be $O((\mathbf{S}_L' \cdot \mathbf{S}_R')^2)$. Therefore, we will need to improve the SA theory so as to contain such higher terms.

We observe similar results for the $S = 1$ next-nearest-neighbour model. Thus the cancellation of triplet–singlet energies can be found in general spin gap systems.

Acknowledgments

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[3] $\xi^{-1} = \widetilde{m} - \sqrt{-d}$ with the parameters of equation (5) in the commensurate region [13].
[4] $q_{IC} = \sqrt{d}$ [13].

References

[1] Xu G *et al* 2000 *Science* **289** 419
[2] Bursill R J *et al* 1995 *J. Phys. A: Math. Gen.* **28** 2109
[3] Schollwöck U *et al* 1996 *Phys. Rev.* B **53** 3304
[4] Affleck I *et al* 1987 *Phys. Rev. Lett.* **59** 799
[5] Affleck I *et al* 1988 *Commun. Math. Phys.* **115** 477
[6] Verstraete F *et al* 2004 *Phys. Rev. Lett.* **92** 087201
[7] Fan H *et al* 2004 *Phys. Rev. Lett.* **93** 227203
[8] Verstraete F and Cirac J I 2004 *Phys. Rev.* A **70** 060302
[9] Fan H *et al* 2006 *Preprint* quant-ph/0605133
[10] Fáth G and Sütö A 2000 *Phys. Rev.* B **62** 3778
[11] Nomura K 2003 *J. Phys. Soc. Japan* **72** 476
[12] Sørensen E S and Affleck I 1994 *Phys. Rev.* B **49** 15771
[13] Murashima T and Nomura K 2006 *Phys. Rev.* B **73** 214431
[14] Kennedy T 1990 *J. Phys.: Condens. Matter* **2** 5737
[15] Hagiwara M *et al* 1990 *Phys. Rev. Lett.* **65** 3181
[16] den Nijs M and Rommelse K 1989 *Phys. Rev.* B **40** 4709