Dynamics of alternating spin chains and two-leg spin ladders with impurities

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Abstract

We study the topological effects of dimer configuration on the high energy dynamics of aligned dimers: alternating spin chains and two-leg spin ladders, with impurites. The well-defined modes at high temperatures obtained by the continued fraction formalism beyond the conventional perturbational approaches are $\omega = 1$ and $\omega = 2$ for alternating spin chains and $\omega = 2$ for two-leg spin ladders. The frequency unit is an antiferromagnetic exchange integral between the spins in a dimer. These characteristic modes strongly localized in clean systems survive the random disturbance in systems with impurities of 10 % concentration or less.

Key words: topological effect; alternating spin chain; two-leg spin ladder; impurity

1. Model and formulation

We investigate the dynamical properties at $T = \infty$ in the aligned dimers described by the Hamiltonian,

$$H = \sum_i (\boldsymbol{S}_{2i} \cdot \boldsymbol{S}_{2i+1} - \alpha \boldsymbol{S}_{2i-1} \cdot \boldsymbol{S}_{2i} - \lambda \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2}), \quad (1)$$

where a vector $\boldsymbol{S}$ on a site denotes a $S = 1/2$ operator and we set the antiferromagnetic exchange integral in a dimer as $J_{\rm AF} \equiv 1$. We study the weakly interacting dimers, where each spin in a dimer weakly interacts with the nearest neighbor spin(s) in an adjacent dimer: the alternating spin chains are given by $\alpha^2 \ll 1$ and $\lambda = 0$; the two-leg spin ladders by $\lambda^2 \ll 1$ and $\alpha = 0$.

We choose the dynamical variable, A, a sum of the spin z-component in a certain dimer as

$$A = S^z_{2j} + S^z_{2j+1}, \quad (2)$$

and evaluate the canonical correlation function defined by $(A(t), A) \equiv \beta^{-1} \int_0^\beta \langle A(t - {\rm i}\hbar\lambda) A^\dagger \rangle d\lambda - \langle A(t) \rangle \langle A^\dagger \rangle$ with $\langle O \rangle = {\rm Tr}[O {\rm e}^{-\beta H}]/{\rm Tr}[{\rm e}^{-\beta H}]$ and $\beta = 1/k_{\rm B}T$. The Laplace transform of $a_0(t) = (A(t), A)(A, A)^{-1} = (1/2\pi{\rm i}) \oint {\rm d}z {\rm e}^{zt} \overline{a}_0(z)$ is written in a continued fraction [1] with a recurrence relation [2]:

$$\overline{a}_0(z) = \cfrac{1}{z + \cfrac{\Delta_1}{z + \cfrac{\Delta_2}{z + \cdots}}}, \quad (3)$$

$$\Delta_n = (f_n,\ f_n^\dagger)\ (f_{n-1},\ f_{n-1}^\dagger)^{-1}, \quad (4)$$

$$f_{n+1} = {\rm i}L f_n + \Delta_n\ f_{n-1}, \quad (5)$$

where the Liouville operator ${\rm i}L$ is defined as ${\rm i}LO = ({\rm i}/\hbar)\ [H, O]_-$. We choose Eq. (2) as f_0, i.e., $f_0 = A$. The boundary conditions are $\Delta_0 = 1$ and $f_{-1} = 0$. Equation (4) of the static quantities determines the dynamical behaviors of a system. Equation (5) helps classify the excitation modes and leads to the expansion of $A(t)$ as $A(t) = {\rm e}^{{\rm i}Ht/\hbar} A {\rm e}^{-{\rm i}Ht/\hbar} = \sum_{n=0} a_n(t) f_n$. The orthogonality of the basis vectors $\{f_n\}$ implies that $(f_\mu, f_\nu) \propto \delta_{\mu\nu}$. We evaluate the scalar product at $T = \infty$, i.e., $\beta \to 0$, by neglecting fluctuations and taking the trace of operator products owing to ${\rm e}^{-\beta H} = 1$. Thus we have, for instance, $(f_0, f_0) = \langle A^2 \rangle = 2a$ with $a = S(S+1)\hbar^2/3 = 1/4$ to set $\hbar \equiv 1$.

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2. Alternating spin chains: $\alpha^2 \ll 1$ and $\lambda = 0$

The dynamics for $\alpha^2 \ll 1$ and $\lambda = 0$ has been studied for the Heisenberg model with $\boldsymbol{S} = (S^x, S^y, S^z)$ [3,4]. Equation (4) is $\{\Delta_1, \Delta_2, \Delta_3, \Delta_4, \Delta_5, \Delta_6\} \simeq \{2a\alpha^2, 4a, 6a, 6a, 4a, O(\alpha^2)\}$ and $\Delta_{n\geq 7} = O(a)$. We assume that the dip keeps at $n = 6$ in the infinite $\{\Delta_n\}$ and then approximate $\Delta_{n\geq 8} = \Delta_7$ in Eq. (3) to have

$$\overline{a}_0(z) = \frac{z(z^4 + 5z^2 + 4)}{z^2(z^4 + 5z^2 + 4) + g(z, \alpha)}. \tag{6}$$

The factor of $g(z, \alpha) \propto \alpha^2$ produces well-defined peaks, no shoulders, over the Lorentzian-like tail at

$$|\omega| = 1,\ 2 \tag{7}$$

owing to $z^4+5z^2+4 = (z-2\mathrm{i})(z-\mathrm{i})(z+\mathrm{i})(z+2\mathrm{i})$. The result is beyond that obtained by the conventional perturbational approach. Equation (6) with $\alpha = 0$ leads to $\overline{a}_0(z) = z^{-1}$ and $\mathrm{Re}\ \overline{a}_0(-\mathrm{i}\omega^+) = \pi\delta(\omega)$, which means that Eq. (2) is a constant of motion.

We pay attention to Eq. (5), the basis vectors $\{f_n\}$ of alternating spin chains to characterize the high energy excitations at Eq. (7). The largest elements in $\{f_{n\leq 5}\}$ are written by the 6-spin alignments with 3 dimers:

$$\begin{aligned}
&(S_{2j-4}S_{2j-3}S_{2j-2}S_{2j-1}S_{2j}S_{2j+1}),\\
&(S_{2j-2}S_{2j-1}S_{2j}S_{2j+1}S_{2j+2}S_{2j+3}),\\
&(S_{2j}S_{2j+1}S_{2j+2}S_{2j+3}S_{2j+4}S_{2j+5}).
\end{aligned} \tag{8}$$

The delocalization energy would correspond to the single singlet-to-triplet local excitation, $1 = 1/4-(-3/4)$, in a dimer within a 6-spin alignment in (8), and twice to the double one in 2 dimers within it. Each spin fluctuates not freely at all, but with very short-ranged and very weak correlations still existing at $T = \infty$.

3. Two-leg spin ladders: $\lambda^2 \ll 1$ and $\alpha = 0$

The dynamics for $\lambda^2 \ll 1$ and $\alpha = 0$ has also been clarified for the Heisenberg model [5]. Equation (4) is $\{\Delta_1, \Delta_2, \Delta_3, \Delta_4,\} \simeq \{8a\lambda^2, 4a, 12a, O(\lambda^2)\}$ and $\Delta_{n\geq 5} = O(a)$. We assume that the dip keeps at $n = 4$ in the infinite $\{\Delta_n\}$ and then approximate $\Delta_{n\geq 6} = \Delta_5$ in Eq. (3) to have

$$\overline{a}_0(z) = \frac{z(z^2 + 4)}{z^2(z^2 + 4) + h(z, \lambda)} \tag{9}$$

with $h(z, \lambda) \propto \lambda^2$, which produces well-defined peak at

$$|\omega| = 2. \tag{10}$$

To see the high energy excitation at Eq. (10), we again return to Eq. (5), the basis vectors $\{f_{n\leq 3}\}$ for the two-leg spin ladders. The largest elements in $\{f_{n\leq 3}\}$ are the 4-spin alignments with 2 dimers:

$$\begin{aligned}
&(S_{2j-2}S_{2j-1}S_{2j}S_{2j+1}),\\
&(S_{2j}S_{2j+1}S_{2j+2}S_{2j+3}).
\end{aligned} \tag{11}$$

The delocalization energy would be $\omega = 1$; however, it is not this but $\omega = 2$, Eq. (10), corresponding to the double singlet-to-triplet local excitation within 4-spin alignments in (11)

4. Aligned dimers with impurities

The previous sections are devoted to the topological effects of dimer configuration on the high energy dynamics of aligned dimers: how geometrically we put dimers in line affects the dynamics of such system.

When a small amount of energy is accidentally turned on in a dimer, $\boldsymbol{S}_{2j} + \boldsymbol{S}_{2j+1}$, written by site j shown in Eq. (2) out of $\sum_i$ in Eq. (1), how does this energy delocalize in aligned dimers? For the alternating spin chains, the well-defined excitation modes described by Eq. (7) produced in 10 spins of (8) carry the energy to spread out away from the dimer via the spins $\boldsymbol{S}_{2j-5}$ and $\boldsymbol{S}_{2j+6}$. Similarly, for the two-leg spin ladders, the well-defined excitation modes described by Eq. (10) produced in 6 spins of (11) carry the energy to spread out away from the dimer via the spins $\boldsymbol{S}_{2j-3}$ and $\boldsymbol{S}_{2j+4}$.

If an impurity sits on a site away from $2j - 5$ and $2j + 6$ for the alternating chains and from $2j - 3$ and $2j + 4$ for the two-leg spin ladders, then the strongly-localized modes produced in spins of (8) and (11) may not be affected by that impurity, respectively. The critical value of impurity concentration is, respectively, about $1/(10 + 2) \simeq 0.08$ and $1/(6 + 2) \simeq 0.12$. Therefore, when impurities are randomly distributed in a system, we expect that the characteristic modes strongly localized in clean systems survive the random disturbance in systems with impurities of 10 % concentration or less.

This site dependent dynamical study is relevant to experiments such as neutron scattering, Raman scattering and ESR.

References

[1] H. Mori, Prog. Theor. Phys. **33** (1965) 423.

[2] M. H. Lee, Phys. Rev. B **26** (1982) 2547.

[3] I. Sawada, Phys. Rev. Lett. **83** (1999) 1668.

[4] I. Sawada, Physica B **284-288** (2000) 1541.

[5] I. Sawada, J. Phys. Chem. Solids **62** (2001) 373.