Low-energy properties and magnetization plateaus in a 2-leg mixed spin ladder

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Using the density matrix renormalization group technique we investigate the low-energy properties and the magnetization plateau behavior in a 2-leg mixed spin ladder consisting of a spin-1/2 chain coupled with a spin-1 chain. The calculated results show that the system is in the same universality class as the spin-3/2 chain when the interchain coupling is strongly ferromagnetic, but the similarity between the two systems is less clear under other coupling conditions. We have identified two types of magnetization plateau phases. The calculation of the magnetization distribution on the spin-1/2 and the spin-1 chains on the ladder shows that one plateau phase is related to the partially magnetized valence-bond-solid state, and the other plateau state contains strongly coupled S=1 and s=1/2 spins on the rung.

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I. INTRODUCTION

The field of low dimensional quantum spin systems has been a focus in condensed matter physics for about two decades since Haldane pointed out the difference between the integer spin Heisenberg antiferromagnetic (HAF) chains and the half-integer spin chains. This conjecture has been verified by later analytic, numerical and experimental studies.

In recent years, the physics of spin ladders consisting of different number of coupled HAF spin-1/2 chains has attracted much attention. The spin ladders of even number coupled chains have a finite gap in low-energy spectrum and those of odd number coupled chains are gapless. The comparison of the quantum spin chains with the spin ladders suggests that there may be some relations between the two systems. For the 2-leg ladders, White showed numerically that its ground state has a finite gap between the ground state and the low-lying excitation states for Heisenberg chains with integer spin, while it is gapless for half-integer spin chains. This conjecture has been verified by later analytic, numerical and experimental studies.

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The effect of the magnetic field on the spin chains and the spin ladders has been a topic of great interest. In the presence of a magnetic field, a spin-1/2 chain will not open a gap until the applied magnetic field is greater than the saturate field. While for a spin-1 chain, because of the existence of the Haldane gap, there is a critical field where the gap is closed and the system remains gapless from the critical field to the saturate field. Below the critical field, there is a plateau at magnetization per site m=0. For those chains with higher spins, bond-alternating or other additional interactions, and the spin ladders, the magnetization process may also display plateaus at non-zero m. It is shown that for a spin chain with periodic structures, in a uniform magnetic field the magnetization plateaus may exist at the magnetization per site m when the condition

\[ n(S - m) = \text{integer} \]  

is satisfied. Here n is the period of the ground state and S is the site spin. For ladder systems, the condition needs some slight modification. The simplest case where a non-zero m magnetization plateau may exist is the traditional translationally invariant S=3/2 spin chain, with n=1, and m=1/2 satisfying Eq. (1). But detailed analyses have shown that there is no plateau in this case except when single-ion anisotropy D is present and D > 0.93.

Considerable attention has been given to mixed spin chains in recent years. Materials with mixed (S_1, S_2) chain structures have been synthesized. Both types of excitations, gaped and gapless, in the low-energy spectrum of the ferrimagnetic quantum alternating spin (1,1/2) chain have been obtained. Magnetization plateau behavior in such systems, and in coupled alternating spin chains also has been studied.

In this paper, we present the results of the low-energy properties and the magnetization plateau behavior of a mixed spin ladder consisting of a spin-1/2 chain coupled with a spin-1 chain

\[ H = \sum_{i=1}^{N} (J_1 \mathbf{s}_i \cdot \mathbf{s}_{i+1} + J_2 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J' \mathbf{S}_i \cdot \mathbf{s}_i) \]  

using the density matrix renormalization group (DMRG)
Here $\mathbf{S}$ and $\mathbf{s}$ denote the spin operators on the spin-1 and spin-1/2 chains. $N$ is the number of translational invariant cell $(\mathbf{S}, \mathbf{s})=(1,1/2)$. The number of total lattice sites is $L = 2N$. We consider the case of antiferromagnetic intrachain coupling $J_1, J_2 > 0$ in this work. To simplify the discussion, we fix $J_1 + J_2=2$ and make $J_1$ change its value from 0 to 2. The interchain coupling $J'$ can be ferromagnetic or antiferromagnetic. It is of considerable interest to examine the effect of the nature of the interchain coupling on the properties of the mixed spin ladder, especially the possibility of introducing new phases as in the case of the spin-1/2 isotropic ladder.

The mixed spin ladder is illustrated in Fig. 1. From intuitive point of view, when the interchain coupling is strongly ferromagnetic this mixed spin ladder is expected to be equivalent to the spin-3/2 Heisenberg chain, which is gapless in the low-energy spectrum with a spin wave velocity $\nu =3.87$ and belongs to the same universality Haldane class as the $S=1/2$ Heisenberg chain. Our calculated low-energy properties provide strong support for this view. When the interchain coupling is antiferromagnetic, the calculated low-energy spectrum does not show clear evidence for the equivalence.

\begin{figure}[h]
\centering
\includegraphics[width=0.4\textwidth]{fig1.png}
\caption{The illustration of the 2-leg mixed spin ladder. Large (small) circles denote $S=1$ ($s=1/2$) spin. Intrachain coupling $J_1, J_2 > 0$.}
\end{figure}

The magnetic plateau study shows that the $J' >0$ and $J' <0$ phases behave differently. In the presence of a uniform magnetic field $H$, an additional term

$$H' = -H \sum_i \left( S_i^z s_i^z \right)$$

needs to be added to Hamiltonian (2). When $J_1$ and $J'$ equal zero, there is a $m=1/2$ magnetization plateau from magnetic field $H=0$ to the critical field of the spin-1 chain, which is related to the partially magnetized valence-bond-solid (VBS) state of the $S=3/2$ spin chain. In our calculation, besides this magnetization plateau phase, we also have identified another magnetization plateau phase when the interchain coupling is strongly antiferromagnetic. We have calculated the magnetization distribution on the two chains at $m = 1/2$. In the first plateau phase, the magnetization is mainly from the spin-1/2 chain as expected. But in the second plateau phase, the magnetization comes mainly from the spin-1 chain, while the spins are antiparallel to the applied field in the spin-1/2 chain.

We will show the calculated low-energy properties of the 2-leg mixed spin ladder in Sec. III. The magnetization plateau behavior and the phase diagram are discussed in Sec. III. Finally, in Sec. IV we present the conclusion of the calculated results and some discussion on the 2-leg mixed spin ladders with general mixed spin cell $(\mathbf{S}, \mathbf{s})$.

\section{II. LOW ENERGY PROPERTIES}

The ground state and low-energy excitation states of Hamiltonian (2) are calculated using DMRG by keeping 400 states. We use the open boundary condition (OBC) and calculate up to the cell length $N=60$. The largest truncation error is of the order of $10^{-7}$.

We calculated the energies and correlation functions of the lowest state in $S^z_{tot}=0, 1, 2, 3$ sectors for different $J_1, J_2$ and $J'$. For all the parameters we calculated, the low-energy spectrum is gapless at the thermodynamic limit and except for those very small $J'$, it is similar for different $J_1$ and $J_2$. In the following we present the calculated results of the excitation energy of low-lying states, the spin excitation in the system, and the spin-spin correlation functions for the 2-leg mixed spin ladder with $J_1 = J_2 = 1$.

\begin{figure}[h]
\centering
\includegraphics[width=0.4\textwidth]{fig2.png}
\caption{Excitation energy times the number of cells $N(E_n - E_0)$ for $n=1$ (filled circle), $n=2$ (open circle) and $n=3$ (open square) are plotted versus $1/\ln N$ for $J_1=1.0$ and $J'=0$. (a) $J'=-4$, (b) $J'=4$.}
\end{figure}

The excitation energy of several lowest states times cell length $N(E_n - E_0)$ as a function of $1/\ln N$ for $J'= -4$ and 4 are shown in Fig. 2(a) and (b) respectively. Here the energy of the lowest state for $S^z_{tot} = k$ sector is denoted as $E_k$. For $J' = -4$, the results are nearly identical to that of the spin-3/2 chain. Because we use OBC
in the calculation, there is a s=1/2 free end spin which can be understood by valence bond solid picture. The $S_{\text{tot}}^z=0$ and $S_{\text{tot}}^z=1$ state will be degenerate in the thermodynamic limit. The energy spacing of the two quasi-degenerate ground states scales as $1/(N \ln N)$, exactly same as that for a pure spin-3/2 chain. For $J'=4$, there is no end spin. Here the $S_{\text{tot}}^z=0$ state is the only ground state in the thermodynamic limit, and the first excitation state at finite chain length is a true excitation state. The energy spacing between this state and the ground state no longer scales as $1/(N \ln N)$.

The difference of the expectation value of the $z$ component of each spin site in the excitation states to the ground state is shown in Fig. 3. For $J'=4$, due to the reflection symmetry of the system, the expectation value $\langle S_i^z \rangle$ for $S_{\text{tot}}^z=0$ state is zero for all $i$, we show $\langle S_i^z \rangle$ directly. For $J'=-4$, considering the existence of the end state, we show $\langle S_i^z \rangle_{n} - \langle S_i^z \rangle_{1}$. These differences exhibit spin-wave-like feature of the excitations. It is noticed that the excitation of the spin-1 part and that of the spin-1/2 part are in phase for $J'=-4$ but out of phase for $J'=4$. There is also clear difference between the two cases near the chain end.

In Fig. 3 we show the correlation between neighboring site spins as a function of $J$'. The trends of these results are easy to understand by considering the proper limiting cases. When $J' \to -\infty$, $\langle S_i^z S_{i+1}^z \rangle$ approaches 1/6, showing that the cell composed by the nearest-neighbor (1, 1/2) spin pair behaves like a $S=3/2$ spin; when $J' \to \infty$, it approaches $-1/3$, the (1, 1/2) spin pair is coupled as a spin singlet. The correlation $\langle S_i^z S_{i+1}^z \rangle$ decreases monotonically to a constant when $J' \to -\infty$, whereas when $J'$ is positive, it first increases and reaches its maxima at $J' \sim 1$ and then it decreases to zero for very large $J' \to \infty$. The two intrachain correlation functions $\langle S_i^z S_{i+1}^z \rangle$ and $\langle S_i^z S_{i+1}^z \rangle$ reduce their magnitude when $J'$ move away from zero. For $J' \to -\infty$, they will decrease to non-zero constants while for $J' \to \infty$, they will decrease to zero.

We believe there is a phase transition between the strongly ferromagnetic rung coupling region and the strongly antiferromagnetic rung coupling region. The existence of the end free spin reveals the VBS topological order in the ferromagnetic rung coupling region. Such a topological order is absent in antiferromagnetic rung coupling region. Therefore a quantum phase transition should occur. We will further explore this phase transition in a future study.

### III. Magnetization Plateau

For a gapless system, the conformal field theory shows that the upper and lower critical magnetic field $H^+$ and $H^-$ where the ground state of the system under magnetic field has magnetization $m = M/N$ is

$$H_m^+ = \lim_{N \to \infty} \frac{E(N, M+1) - E(N, M)}{N}$$

$$H_m^- = \lim_{N \to \infty} \frac{E(N, M) - E(N, M-1)}{N}.$$  

Here $E(N, I)$ is the lowest energy in the subspace of an $N$-cell system with the $z$ component of the total spin $\sum_i S_i^z = I$. If $H_m^+ = H_m^-$, there is no plateau at magnetization $m$ in the thermodynamic limit and when the applied magnetic field is $H_m$, the system has magnetization $m$. If $H_m^+$ and $H_m^-$ are not equal, there will be a magnetization plateau at $m$ with a width $D_m = H_m^+ - H_m^-$. By calculating the width of a length-$N$ system

$$D_m(N) = E(N, M+1) + E(N, M-1) - 2E(N, M),$$

$$D_m$$, the plateau width at magnetization $m$ can be obtained by considering the infinite length limit.
\[ D_m = \lim_{N \to \infty} D_m(N). \] (6)

According to Eq. (6), Hamiltonian (2) may have a plateau at magnetization per cell \( m = 1/2 \). Using DMRG, we have calculated \( D_m(N) \) of this system and obtained two different plateau phases.

### A. \( J' = 0 \) limit

Before presenting the DMRG results, we examine the limiting case of \( J' = 0 \). In this case, the mixed spin ladder described by Hamiltonian (2) decouples into individual spin-1/2 and spin-1 chains. When a magnetic field is applied to the decoupled system, the spin-1 chain will not be magnetized until the field is larger than the critical field \( H_{c1}^j = J_2 \Delta S_{s=1} \), where \( \Delta S_{s=1} \) is the Haldane gap of the pure spin-1 chain; while the gapless spin-1/2 chain will begin magnetization as soon as the magnetic field is nonzero and reach its saturate magnetization at \( H_{c2}^j = 2J_1 \). If \( H_{c2}^j < H_{c1}^j \), when the spin-1/2 chain has been saturated, the spin-1 chain has not been magnetized. Consequently, there will be a magnetization plateau between \( H_{c2}^j \) and \( H_{c1}^j \), with a magnetization per cell \( (S, s) \) of \( m = 1/2 \). This plateau will happen when \( J_1 \) is small and \( J_2 \) is large. Since we fix \( J_1 + J_2 = 2 \), we can obtain a critical point for \( J_1 \) where this plateau is diminished by taking

\[ J_2 \Delta S_{s=1} = H_{c1}^j = H_{c2}^j = 2J_1. \] (7)

We have \( J_1^j = \frac{2 \Delta S_{s=1}}{2 + \Delta S_{s=1}} \). The Haldane gap of the spin-1 chain \( \Delta S_{s=1} \) has been calculated with high accuracy. \( J_1^j \sim 0.41 \), so \( J_1^j \approx 0.34 \). When \( J_1 < J_1^j \), there is a plateau at \( m = 1/2 \) with a width of \( D_{1/2} = 2 \Delta S_{s=1} = (2 + \Delta S_{s=1})J_1 \).

### B. DMRG results

The energy levels \( E(N, N/2) \), \( E(N, N/2 + 1) \) and \( E(N, N/2 - 1) \) of Hamiltonian (2) are calculated using DMRG for different parameters \( J_1 \) and \( J' \). Because of the open boundary condition we use in calculation, for \( J_1 < J_1^j \) and small \( J' \) the edge states also exist even at magnetization \( m = 1/2 \). As a result, the lowest state in the \( N/2 + 1 \) sector may be the edge state. Considering this, we target at least two states for the \( E(N, N/2 + 1) \) sectors, and the plateau behavior corresponds to the second state of this sector \( E_2(N, N/2 + 1) \).

We check the accuracy of our results by examining the case of \( J_1 = 0 \) and \( J' = 0 \), where the largest numerical error is expected for the DMRG calculation. In this case, the decoupled spin-1/2 sites are free spins. The \( m = 1/2 \) plateau begins at zero and lasts to the Haldane gap of the spin-1 chain, \( J_2 \Delta S_{s=1} \sim 0.82 \). Our DMRG calculation gives \( E_2(N, N/2 + 1) = E(N, N/2) \sim 0.832 \).

When \( J' \) deviates from zero while \( J_1 \) still is zero, the width of the plateau will decrease. We show

\[
\begin{align*}
H_{c1}^+ & = E(N, N/2 + 1) - E(N, N/2), \\
H_{c1}^- & = E(N, N/2 + 1) - E(N, N/2 - 1), \\
H_{c2}^+ & = E(N, N/2 + 1) - E(N, N/2 - 1), \\
H_{c2}^- & = E(N, N/2) - E(N, N/2 - 1)
\end{align*}
\] (8)

at \( J_1 = 0 \) and \( J' = 0.6 \) in Fig. 5(a). Clearly \( H_{c1}^+ \) and \( H_{c2}^- \) converge to the same value in the thermodynamic limit. The plateau width is the difference of \( H_{c1}^+ \) and \( H_{c2}^- \) which is about 0.42, smaller than that of the \( J' = 0 \) case. For \( J' < 0 \), the width decreases faster than in the \( J' > 0 \) case. At critical points \( J_{c1}^-(J_1 = 0) \sim 0.85 \) and \( J_{c1}^+(J_1 = 0) \sim 2.2 \), the width decreases to zero and the plateau vanishes. In these cases, the width of the plateau can also be obtained from the difference of the \( E(N, N/2 + 1) \) and \( E_2(N, N/2 + 1) \). \( D_m = \lim_{N \to \infty} [E_2(N, N/2 + 1) - E(N, N/2 + 1)] \). This definition gives \( D_m \) with higher accuracy. The dependence of the width of the plateau on \( J' \) for \( J_1 = 0 \) is shown in Fig. 5(b).

![FIG. 5. Energy difference (a) and (c) \( H_{c1}^+ \) (filled circle), \( H_{c2}^- \) (open circle), \( H_{c1}^- \) (filled square) at \( m = 1/2 \) and the plateau width ((b) and (d)) in the two plateau phases.](image)

For larger \( J' > J_{c1}^+ \), we find another plateau phase. The values of \( H_{c1}^+ \), \( H_{c1}^- \), and \( H_{c2}^- \) at \( J_1 = 0 \) and \( J' = 4.0 \) are shown in Fig. 5(c). For this larger \( J' \), \( E_2(N, N/2 + 1) \) is not an edge state. The non-zero magnetization plateau is obvious. The width of the magnetization plateau for \( J_1 = 0 \) and \( J' > J_{c1}^+ (J_1 = 0) \sim 2.8 \) is shown in Fig. 5(d).

We have carried out systematic DMRG calculations to determine the magnetization plateau phase diagram shown in Fig. 5. An examination of the calculated results indicate that there are two types of plateau phases corresponding to different magnetic structures in the ladder. In phase I, the magnetization is due to the partially polarized \( s = 1/2 \) spins. In phase II, the spin-1/2 sites
and spin-1 sites are strongly coupled. In phase III, where no plateau is found, the system is in a phase similar to that of a pure spin-3/2 chain. The magnetic features of the two plateau phases in Fig. 6 can be clearly seen in Fig. 7, which shows the magnetization distribution on the spin-1/2 chain defined as

\[ m_\pm = \frac{1}{N} \sum_i \langle s_i^z \rangle \]  

(9)

The magnetization distribution on the spin-1 chain can be derived from \( m_1 = m - m_\pm \), where \( m \) is the total magnetization of the ladder.

When \( J' \to \infty \), \( m_\pm \to -1/6 \), that is, the orientation of the spin-1/2 partition will be antiparallel to the applied magnetic field. Here each \((1,1/2)\) cell is in \( |1/2, 1/2\rangle = \frac{1}{\sqrt{3}}(|1, 1/2, -1/2\rangle - \sqrt{2}|1, 0; 1/2, 1/2\rangle) \) state when \( m=1/2 \).

We also have studied the magnetization process by examining short chains. We show the typical plateau and no-plateau process in Fig. 8(a) and Fig. 8(b) with \( J_1=1.0 \), \( J'= -1.0 \) and \( 3.0 \) respectively. For \( J'= 3.0 \) (phase III in Fig. 6), the existence of the magnetization plateau at \( m=1/2 \) is clear. When the chain length grows, \( h_{1/2}^- \) becomes larger and \( h_{1/2}^- \) becomes smaller, but they converge to different values for the infinite chain. For \( J'= -1.0 \) (phase III in Fig. 6), both \( h_{1/2}^- \) and \( h_{1/2}^+ \) increase with chain length, but \( h_{1/2}^+ \) increase faster. They eventually converge to the same value \( h_{1/2} \), yielding no plateau in this case.

To understand the trends shown in Fig. 8, it is instructive to examine the two limiting cases. When \( J' \to -\infty \), \( m_\pm \to 1/6 \) and \( m_1 = m - m_\pm \to 1/3 \), and the magnetizations on the two chains are half of their saturate values. In this limit, each cell \((1,1/2)\) is in \( |3/2, 1/2\rangle = \frac{1}{\sqrt{3}}(\sqrt{2}|1, 1/2, -1/2\rangle + |1, 0; 1/2, 1/2\rangle) \) state when \( m=1/2 \), and the 1/2-spin and the corresponding 1-spin bond together to form a 3/2-spin.
We find that there is only one quantum phase transition at which the spin gap appears when we increase the rung coupling $J'$ from a negative magnitude to a big and positive one. Beside this quantum phase transition between plateau phase II and plateauless phase III, the phase transition between plateau phase I and plateauless phase III is also a continuum phase transition due to spin gap closing. A more precise understanding of the gap generation and magnetization plateaus in the phase diagram found in this section can be given by bosonization discussions. We expect that further bosonization studies will provide an interpretation of the plateau phase II beyond the obvious origin of its plateau.

IV. CONCLUSION AND DISCUSSION

We have calculated the low-energy properties and magnetization plateau behavior of a 2-leg mixed spin $(S,s)=(1,1/2)$ ladder. From the low-energy properties, we conclude that for strong ferromagnetic interchain coupling, the 2-leg mixed spin ladder is in the same phase as the spin-3/2 chain. There is a magnetization plateau for large enough positive $J'$ but no plateau is found for large negative $J'$. This suggests that at large $J' > 0$, the ladder would behave differently from the spin-3/2 chain.

We have obtained the magnetization plateau phase diagram of Hamiltonian [3] and identified two types of plateau phases. In the partially polarized spin-1/2 phase, because of the anti-ferromagnetic interchain coupling, the orientation of the spin-1/2 chain is antiparallel to the magnetic field, and the spin-1/2 chain and the spin-1 chain are coupled together.

Finally, we discuss some qualitative trends for general mixed spin $(S,s)$ ladders. The basic structure of the phase diagram shown in Fig. [3] is expected to remain valid. For higher spins $(S,s)$, the non-plateau region phase III for $(1,1/2)$ may also become a plateau phase. If $S$ and $s$ are both half-integers, there will be no partially polarized plateau phase. If $S$ and $s$ are one integer and one half-integer, then the low energy spectrum is gapless and there is no plateau at $m=0$. In other cases, the low-energy spectrum is gaped, with a $m=0$ plateau.

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