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Impurity energy level in the Haldane gap

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An impurity bond J' in a periodic one-dimensional antiferromagnetic spin-1 chain with exchange J is considered. Using the numerical density matrix renormalization-group method, we find an impurity energy level in the Haldane gap, corresponding to a bound state near the impurity bond. When $J'<J$ the level changes gradually from the edge of the Haldane gap to the ground-state energy as the deviation $\mathrm{dev}=(J-J')/J$ changes from 0 to 1. It seems that there is no threshold. Yet, there is a threshold when $J'>J$. The impurity level appears only when the deviation $\mathrm{dev}=(J'-J)/J'$ is greater than B_c, which is close to 0.3 in our calculation.

I. INTRODUCTION

The Heisenberg model of one-dimensional (1D) antiferromagnetic (AF) chains is

$$H=J\sum_i \mathbf{S}_i\cdot\mathbf{S}_{i+1} \tag{1}$$

with $J>0$. Up till now, the exact solution of this Hamiltonian is available only when $s=1/2$. The solution is obtained by the Bethe ansatz,[1] showing no gap in the energy spectrum. Haldane made his famous conjecture[2] that 1D AF chains of integer spin have a gap, while those of half-integer spin have a gapless spectrum. Since then, a lot of work has been done. In particular, a valence-bond-solid (VBS) picture was proposed by Affleck *et al.*,[3,4] to interpret the ground state of the integer spin AF chains. The proposed picture agrees quite well with both experimental[5] and numerical[6] studies.

An important issue of integer spin AF chains is the doping effect which involves some fundamental many-body quantum problems.[7] DiTusa *et al.*[8] have done doping experiments with Zn or Ca in $\mathrm{Y_2BaNiO_5}$, which contains 1D AF chains of Ni-(O)-Ni-(O)-$\cdots$. In the Zn doping case, the nonmagnetic $\mathrm{Zn^{2+}}$ ion substitutes $\mathrm{Ni^{2+}}$ to sever the AF chain giving rise to finite length effect. In the Ca doping case, with $\mathrm{Ca^{2+}}$ substituting the off-chain atom $\mathrm{Y^{3+}}$, holes are introduced in the oxygen orbitals along the Ni-O chain, modifying the superexchange interaction and producing an impurity state inside the Haldane gap, as seen by neutron-scattering experiments. The latter case can be represented by changing J to J' at the impurity bond. We focus on the latter case in this paper. Thus we write down our Hamiltonian as

$$H=J\sum_i \mathbf{S}_i\cdot\mathbf{S}_{i+1}+(J'-J)\mathbf{S}_0\cdot\mathbf{S}_1\,. \tag{2}$$

The impurity bond is put between sites 0 and 1.

Recently a calculation of the dynamic structure factor based on the Schwinger-boson approach was performed for the bond-doping case,[7] which first indicated the existence of a threshold for the bond-coupling deviation. According to this calculation, a bound state is induced by the impurity only when the deviation exceeds this threshold, and the impurity level is located in the middle of the Haldane gap, almost independent of bond coupling when temperature is much lower than the Haldane gap.

The recently developed numerical method of density matrix renormalization group[9,10] (DMRG) has achieved great success in calculating the low-energy spectrum of 1D Heisenberg AF chains,[11] so it is interesting and natural to use this method to study the doping effect on the Haldane gap systems. Such a calculation was carried out by Sorenson and Affleck (SA).[12] They reported the existence of the threshold, but the impurity energy level they obtained changes gradually as the strength of impurity bond changes. The existence of the threshold is in agreement with the Schwinger boson calculation,[7] but the gradual change of the impurity level is in disagreement with the latter. However, these authors have used open boundary conditions and the way they added new sites may affect the bound state itself (see the discussion in

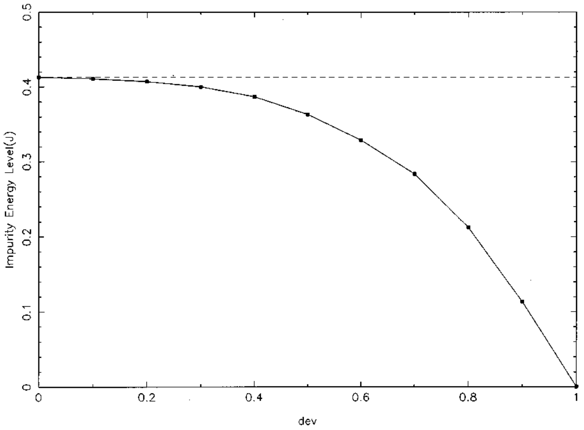
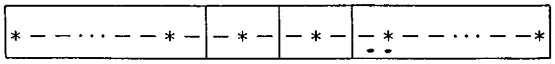


FIG. 1. Impurity energy level vs impurity dev$=(J-J')/J$, when $0<J'<J$. The chain is periodic, and the dashed line indicates the Haldane gap.

the next section). To clarify this issue we have decided to devise a more elaborate scheme to carry out the DMRG calculations.

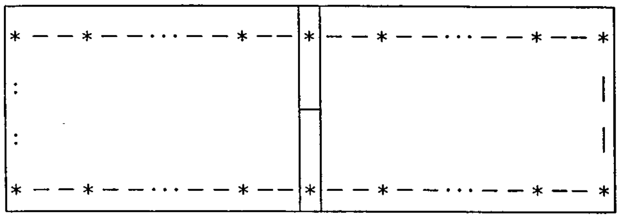
II. DMRG METHOD

The DMRG method has been developed by White and co-workers[9,10] in recent years. Generally, the standard pattern looks like this



Here $*$'s represent sites, while two short bars represent bonds. During each iteration, the chain (superblock) is divided into four blocks, where the left-most and the right-most ones are the same by symmetry consideration. The two middle, newly added blocks contain only two sites. After each run, the left and right halves of the superblock are optimized to form new blocks which are used for the next iteration. This is, however, not good in the presence of an impurity bond. At first glance, it seems right to put the impurity bond in the middle of the chain (this is what SA have done,[12]) but this configuration may introduce some artificial effects. For example, the two middle sites which were optimized with the impurity bond between them, are used in later calculations without impurity bond close to them. When the chain is very long, the impurity bond effect should go to zero during iterations (since there is only one impurity bond), but using this pattern, the effect does not vanish fast enough as iterations go on.

To calculate the impurity level of the periodic chain, we do our numerical work using the following pattern:



Here the impurity bond (denoted by two double dots) is placed on the left-hand side vertically, whereas the bond on the right-hand side vertical is unperturbed. In each iteration we add two sites to the above periodic chain, one at or near the center of the upper part and one at or near the center of the lower part. Using this pattern, we can avoid the difficulties mentioned above. We preserve $m=100$ states in each run and discard the rest. Since S_z is a good quantum number, we use it to reduce the dimension of our Hamiltonian matrix.

Shank transformation has been demonstrated as a powerful extrapolation method to get the Haldane gap precisely.[13] We use it to extrapolate our results to the infinite length limit. To verify the credibility of this method, we also use Aitkens' transformation[14] to extrapolate our finite chain data. They both give very similar values (usually the difference is less than 10^{-3}). As compared with the previous conclusion in special cases, our results show a reasonable precision. So we believe that our value is correct at least up to 10^{-2}.

III. NUMERICAL RESULT

We use the VBS picture[3,4] to give some intuitive explanation of our calculation results, though this picture is not quite precise. According to this picture, when considering the low excitation energy spectrum, the spin 1 of each site can be regarded as two spin 1/2's combined together to form a triplet $S=1$ state, yet the two 1/2 spins of the nearest-neighbor sites form a valence bond, or, a singlet state. Therefore, the ground state of an open chain can be labeled by the sum of the two edge 1/2 spins. The ground state of the 1D AF chain is fourfold degenerate, with one state of $\mathbf{S}_{\text{total}}=0$, where the two 1/2 spins of each edge form a singlet, and three states of $\mathbf{S}_{\text{total}}=1$, where the two 1/2 spins form a triplet. The first excited states are the quintet states with $\mathbf{S}_{\text{total}}=2$, which lie above the ground state by the famous Haldane gap. Above them, the continuous spectrum starts. For a periodic chain, the VBS picture also holds, but the triplet states rise up to the edge of the continuous energy spectrum, leaving the ground-state nondegenerate.

The impurity state of the periodic chain is just the $\mathbf{S}_{\text{total}}=1$ triplet state. When $J'/J=0$, the periodic chain becomes an open chain, and this triplet will merge in the $\mathbf{S}_{\text{total}}=0$ ground state in the infinite chain length limit. Thus

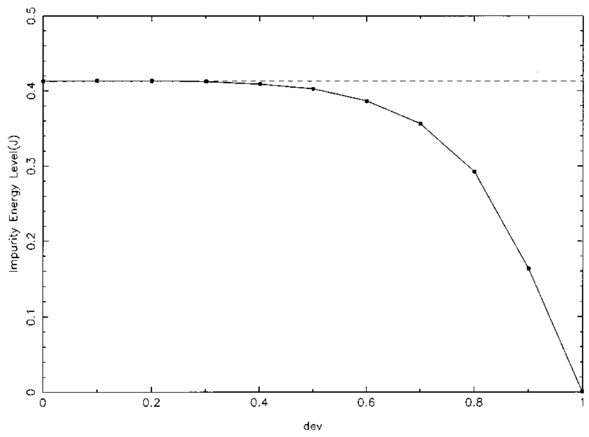


FIG. 2. Impurity energy level vs impurity dev$=(J'-J)/J'$, when $J'>J$. The chain is periodic, and the dashed line indicates the Haldane gap.

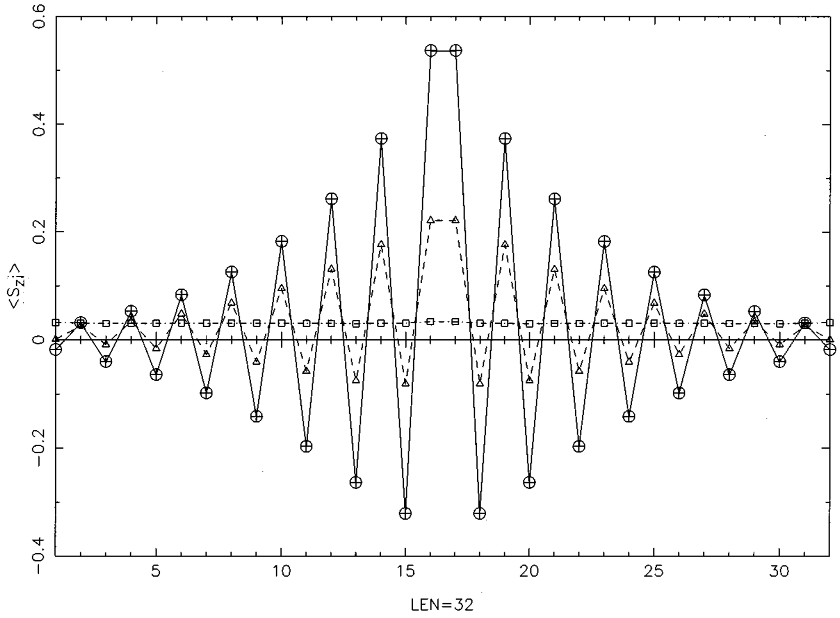


FIG. 3. $\langle S_{zi}\rangle$ of the impurity state as function of chain index i when $J'<J$. The star is for the case of dev=1, while the triangle is for dev=0.6, and the square for dev=0 [dev=$(J-J')/J$]. The impurity bond is placed between sites 15 and 16.

the impurity energy level is at 0. On the contrary, when $J'/J=1$, the periodicity recovers, so the "impurity" level will rise up to the upper edge of the Haldane gap.

Because of the $SO(3)$ symmetry of the Heisenberg Hamiltonian, the $\mathbf{S}_{\text{total}}=1$ triplets are degenerate, so we choose the state $S_z=1$ as a representative of them. Also, we set the ground-state energy as the zero of the energy spectrum.

First we consider the case $0<J'<J$, which means the superexchange is smaller due to doping. The calculated result is presented in Fig. 1, where we see that the impurity level increases linearly near dev=1[dev=$(J-J')/J$], which is in accordance with SA's perturbation argument.[12] However, compared with SA's work,[12] our numerical result favors the conclusion that there is no threshold. As seen from the figure, the impurity energy appears as soon as dev≠0, and shows a quadratic behavior near dev=0. Kaburagi *et al.*[15] have investigated the impurity bond effect in terms of domain-wall exitations. Their variational results show a linear behavior near dev=1 and a quadratic behavior near dev=0. They have also performed diagonalizations by Lanczos method for $N=12$ and 13 chains with results supporting their variational work.

When $J'>J$, the result is shown in Fig. 2, where the impurity level vs dev=$(J'-J)/J'$ is plotted. Again, the level rises linearly near dev=1, in agreement with the argument of SA.[12] A significant feature is the appearance of a threshold B_c, i.e., only when dev$>B_c$ can an impurity-localized state appear. Our B_c is very close to 0.3, and it is different from that of SA (their B_c is 0.5). The case when $J'/J\rightarrow\infty$ (dev→1) can be easily understood as follows: The two spins of the impurity bond form a singlet state because

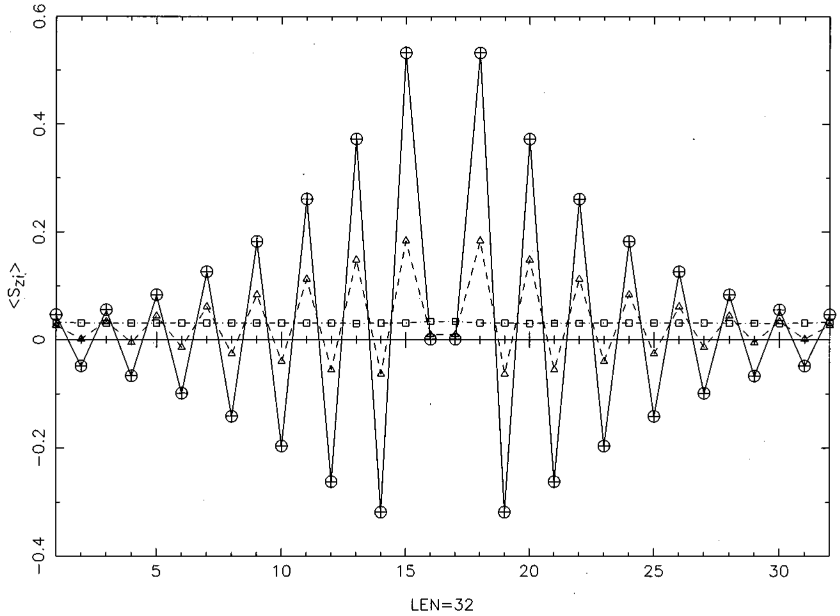


FIG. 4. $\langle S_{zi}\rangle$ of the impurity state as function of chain index i when $J'>J$. The star is for the case of dev=0.999, while the triangle is for dev=0.7, and the square for dev=0 [dev=$(J'-J)/J'$]. The impurity bond is placed between sites 16 and 17.

of the strong coupling, breaking the periodic chain of length L to make an open chain of length L-2. So, as follows from our calculation, the difference between the impurity level and the ground state will go to zero in this limit.

We notice an unusual feature from the finite chain calculations: When $J'>J$, $E(0<\mathrm{dev}<B_L)>E(\mathrm{dev}=0)$, where E is the impurity energy, and B_L is some value depending on the chain length L. Since with the increase of chain length, the difference between $E(0<\mathrm{dev}<B_L)$ and $E(\mathrm{dev}=0)$ goes to zero and B_L to B_c, we believe there is a threshold instead of any other behavior in this range.

Moreover, to ensure that the impurity level means a local state near the impurity bond, we plot $\langle S_{zi}\rangle$ of the periodic chain in Fig. 3 ($J'<J$) and 4 ($J'>J$). In Fig. 3, when $J'/J=0(\mathrm{dev}=1)$, the "boundary 1/2 spin" of open chain appears, just as the VBS picture assumes.[3] When dev goes from 1 to 0, the state becomes more and more delocalized. Figure 4 shows the case of $J'>J$, where the two sites at the middle form a singlet state, while the sites near them show the boundary 1/2 spin, too, when dev→1.

IV. CONCLUSION

Using an elaborate numerical DMRG method, we have investigated the bond doping effect on a 1D AF chain. A threshold B_c exists only when $J'>J$. When $J'>J$ and dev$<B_c$, no impurity state is induced. When $J'>J$ and dev$>B_c$, or $J'<J$, the impurity level in the Haldane gap corresponds to a local state near the impurity bond, and the level changes gradually when dev runs from B_c to 1. The discrepancy of the present study with the Schwinger boson calculation[7] is not fully understood at present. One possiblity is that the Schwinger boson representation introduces an additional symmetry (which sets the impurity level at the middle of the Haldane gap), not inherent to the original quantum spin systems.

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