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Abstract

Using the density matrix renormalization group technique, we calculate numerically the low energy excitation spectrum and magnetization curve of the spin-1 antiferromagnetic chain in a staggered magnetic field, which is expected to describe the physics of $R_2BaNiO_5 (R \neq Y)$ family below the Néel temperature of the magnetic rare-earth (R) sublattice. These results are valid in the entire range of the staggered field, and agree with those given by the non-linear σ model study for small fields, but differ from the latter for large fields. They are consistent with the available experimental data. The correlation functions for this model are also calculated. The transverse correlations display the anticipated exponential decay with shorter correlation length, while the longitudinal correlations show explicitly the induced staggered magnetization.

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The quasi-one-dimensional magnets have been the focus of analytic, numerical and experimental studies since Haldane pointed out the difference between the integer spin Heisenberg antiferromagnetic (AF) chains and the half-integer chains in 1983. [1] By mapping the Heisenberg spin chains onto the $O(3)$ nonlinear σ-model, [2] he conjectured that the low-energy excitation spectrum displays a finite gap for the integer spin systems while it is gapless for half-integer spin chains. This conjecture has been verified by later experiments on quasi-one-dimensional spin-1 materials such as NENP and Y_2BaNiO_5 which show clear evidence of the Haldane gap. [3] Nowadays, the pure one-dimensional Haldane systems are fairly well understood, and a reliable estimate for the Haldane gap $\Delta = 0.41048(2)J$ for spin-1 chains has been obtained by both density matrix renormalization group (DMRG) calculation [4] and finite size exact diagonalization. [5]

More recent developments on the Haldane systems concern various effects of external perturbations: doping with magnetic or non-magnetic impurities [6] and applying external magnetic field. The impurity doping may introduce bound states within the Haldane gap, [7] while applying uniform external magnetic field splits the degenerate Haldane triplet state into transverse and longitudinal modes. [8] The longitudinal mode becomes softened upon increase of the magnetic field, and at a critical field H_c the system enters a new phase with long-range AF order. Of course, a staggered applied magnetic field is even more interesting which would induce non-vanishing staggered magnetization and affect the Haldane gap excitation spectrum, but such a staggered field cannot be materialized by an external source.

Most recently, a series of experiments performed on the family of quasi-one-dimensional materials with a general formula R_2BaNiO_5, [9–16] where R is one of the magnetic rare-earth elements substituting fully or partially Y (for brevity we denote this replacement by $R \neq Y$), have made it possible to study the effect of the staggered magnetic field on the Haldane systems in detail. All members of this family contain spin-1 Ni^{2+} linear chains and the in-chain AF exchange coupling is rather strong. (The detailed structure of this family of compounds is described in Ref. [11]). The reference compound Y_2BaNiO_5 is found to be highly one-dimensional with negligible interchain interactions, [9] and no magnetic order has been observed so far even at very low temperatures. [6] Hence it is believed to be an almost ideal example of the Haldane-gap system. Other members have magnetic R^{3+} ions in addition to the spin-1 Ni^{2+} ions. These ions are positioned between two neighboring Ni chains, weakly coupled to the Ni^{2+} ions and the coupling between themselves is also very weak. Nevertheless, these magnetic ions are AF ordered below certain Néel temperature T_N. These ions do not affect the Ni chains substantially above T_N, keeping their Haldane features untouched, but the 3D AF ordered R^{3+} sublattice below T_N has dramatical effects on these chains, imposing a staggered magnetic field. The neutron scattering experiments on powder samples and small size single-crystals of Nd_2BaNiO_5 and Pr_2BaNiO_5 [13,15,16] show an increase of the energy gap below the Néel temperature.

We assume that these chains can be still considered one-dimensional, being put in a staggered field created by 3D ordered R^{3+} ions at low temperatures. The Hamiltonian can be then written as :

$$H = J \sum_i \left[\mathbf{S}_i \cdot \mathbf{S}_{i+1} + h(-1)^i S_i^z \right], \tag{1}$$

where J is the exchange constant (to be taken as energy unit, i.e., J =1). The dimensionless staggered field $h = gS\mu_B H_\pi / J$ with H_π as the physical staggered field, which, in turn, is proportional to the R sublattice magnetization M_R

$$H_\pi = \alpha M_R. \tag{2}$$

g=2 is the theoretically predicted gyromagnetic ratio of the Ni ion. The direction of the staggered field has been chosen as the z axis. This Hamiltonian has been considered using the mean-field theory [17,16] as well as by mapping onto the O(3) nonlinear σ model (NLSM). [20]

In this Communication we use the DMRG technique to calculate the low energy excitation spectrum and magnetization curve of the Hamiltonian Eq.(1). The obtained field dependence of the gap and the staggered magnetization is consistent with the experimental results. These results are valid in the entire range of the staggered field and recover those given by non-linear σ model for small fields but differ from the latter for large fields. Moreover, we calculate the spin-spin correlation functions for this model. The transverse correlations display an exponential decay as anticipated for the spin-1 AF chain, with a shorter correlation length, while the longitudinal correlations show explicitly the induced staggered magnetization.

We follow the standard DMRG algorithm [4,18,19] to calculate the low-energy excitations of the Hamiltonian (1), adopting the periodic boundary conditions (PBC). We use the infinite-chain algorithm up to chain length N=60 and keep as many as 400 optimized states during each sweep. The largest truncation errors are of the order of 10^{-8} for smaller h, while for bigger h, these errors are as small as 10^{-13}, which means our results are even more reliable for bigger h.

The numerical results for the change of the lowest excitation energies (the Haldane gap) of Hamiltonian (1) $\Delta - \Delta_0$ are presented in Fig. 1 as functions of the dimensionless staggered magnetic field h. In the absence of this field the longitudinal (Δ_L) and transverse (Δ_T) modes are degenerate, forming the Haldane triplet. For non-zero h, these modes will split with respect to each other. Both of them will increase with the staggered magnetic field, while the longitudinal gap increases faster than the transverse one. For small staggered fields, the increase of the longitudinal gap will be nearly three times faster then the transverse ones, while for larger staggered fields, this ratio will decrease, and is is approximately two for the largest staggered field we considered.

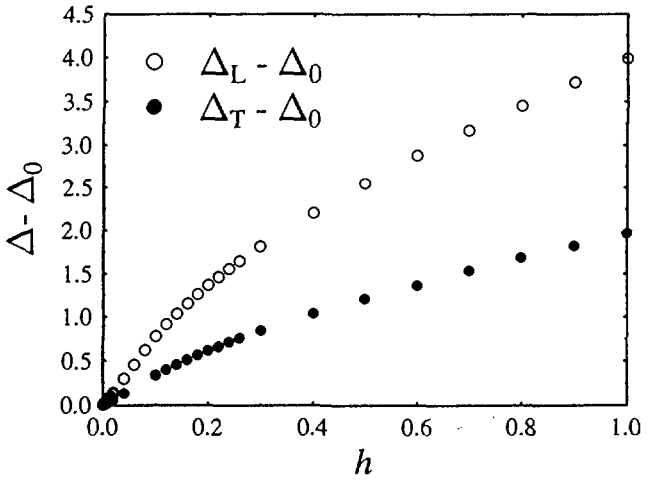

FIG. 1. The DMRG results for the transverse (solid circle) and longitudinal (empty circle) energy gaps as functions of the staggered magnetic field for spin-1 chain.

The staggered magnetic moment of the system with chain length N is defined as

$$M_\pi(N) = \frac{1}{N}\sum_i (-1)^i \langle S_i^z \rangle, \tag{3}$$

the longest chain in our calculation being N=60. Then the staggered magnetic moment for infinite long chain M_π can be obtained by extrapolating $M_\pi = \lim_{N\to\infty} M_\pi(N)$. Obviously, this quantity is a function of the staggered field, and our numerical results are shown in Fig. 2. Considering Eq. (2), this figure is nothing but the relation between the magnetization of the Ni sublattice and the R sublattice, and it is qualitatively in agreement with the experimental data in Fig. 2 of Ref. [16]. Our numerical results show that in small staggered fields, the magnetization change linearly with the increase of the field, so we can easily extract the "zero field" staggered magnetic susceptibility $\chi^{(s)}(0)$=18.50/J. This value fully agrees with the results obtained from the transfer-matrix renormalization group [21], Quantum Monte Carlo [22] and the NLSM calculations. [20] We fit our results using the following function:

$$M_\pi = a \ \arctan(b\ h) + (1 - \frac{\pi}{2}a)\tanh(c\ h^d) \tag{4}$$

with a=0.412, b=38.106, c=1.195, d=0.621. The fitting line is also shown in Fig. 2. To compare with the NLSM results [20] in detail, in Fig. 2, we use their analytic relation

$$\chi^{(s)}(0)h = M_\pi(1 + 1.56M_\pi^2 + 2.4M_\pi^4 + 3.27M_\pi^6)$$

with their value $\chi^{(s)}(0) = 18.7/\mathrm{J}$ as a reference. We see clearly that the analytic expression is very good for small staggered fields, while for larger staggered fields it deviates from our numerical results significantly. We have also calculated the magnetic moment for large h which is not shown in Fig. 2. Our result indicates that the moment should saturate in large enough staggered magnetic field for both isotropic and (single-ion) anisotropic cases. The unsaturated moment at zero-temperature observed so far in various experiments tells us that the induced staggered magnetic field on Ni chains is, probably, not large enough yet. This issue was also discussed earlier. [16]

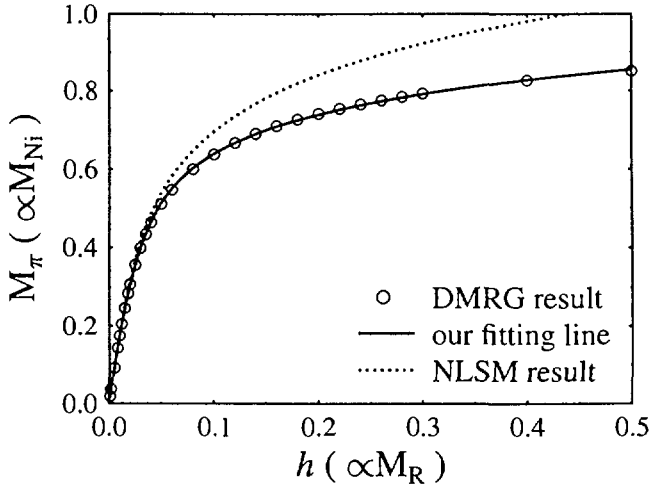

FIG. 2. The staggered magnetization curve for spin-1 chain. The staggered magnetic field is proportional to the magnetization of the R sublattice. The numerical results (solid circle) are fitted by a function with four parameters (solid line) (see Eq. (4)), with a=0.412, b=38.106, c=1.195, d= 0.621, respectively; the analytic results given by non-linear σ model are also presented (dotted line).

From the above results, we obtain the values of the transverse as well as the longitudinal gap as functions of the magnetic moment of the Ni sites, which can be compared directly with the analytic NLSM result

(see Fig. 3). These results are also consistent with the experimental data. [13,20] As for the comparison with the NLSM treatment we see again that in small staggered fields, the analytic and numerical results are in good agreement with each other, while for larger staggered fields, the analytic results deviate significantly from the numerical simulations. Both longitudinal and transverse gaps increase faster in simulations than the NLSM predicts. Since for our DMRG calculations, larger is the staggered field, more reliable are the results, so the disagreement of magnetization moment and the gaps between these two approaches raises a question whether the NLSM mapping is valid or not for large staggered magnetic fields.

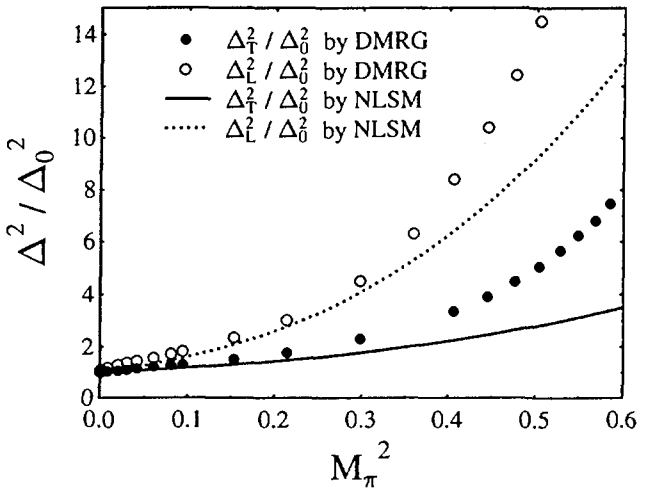

FIG. 3. The numerical results for the transverse gaps (solid circle) and the longitudinal gaps (empty circle) *versus* the magnetic moment on Ni sites; the NLSM results are shown (solid line for transverse gaps and dotted line for longitudinal gaps) in the same figure.

Besides calculating the low-energy spectrum of the one-dimensional systems, the DMRG method also provides a direct and simple way to calculate the spin-spin correlation functions which can shed some further light on the nature of the system under study. For a pure Haldane system, the correlation decays exponentially, following

$$\langle S_0^{x(z)} S_l^{x(z)} \rangle = (-1)^l A \frac{e^{-\frac{l}{\xi}}}{\sqrt{l}}, \tag{5}$$

where ξ=6.03 is the correlation length obtained by the numerical study, [4] and A is a constant. When a staggered field is applied, the AF long-range order will be induced along the z-direction, so $\langle S_0^z S_l^z \rangle$ will not decay any more. However, $\langle S_0^z S_l^z \rangle - \langle S_0^z \rangle \langle S_l^z \rangle$ will still decay exponentially. Of course, the transverse correlations $\langle S_0^x S_l^x \rangle$ decay exponentially as before, but with modified exponents. In Fig. 4(a) and Fig. 4(b), the functions $C_{xx}(l) = \ln(\sqrt{l}|\langle S_0^x S_l^x \rangle|)$ and $C_{zz}(l) = \ln(\sqrt{l}|\langle S_0^z S_l^z \rangle - \langle S_0^z \rangle \langle S_l^z \rangle|)$ are shown for different staggered fields. We see that both functions decay exponentially following Eq. (5) and the correlation lengths ξ_{xx} and ξ_{zz} decrease with increasing staggered field. As h increases, the reduced longitudinal correlations decay much faster. We have extracted the correlation lengths and extrapolated them to infinite chain length by considering the chain length dependence of ξ_{xx} and ξ_{zz}. We find that $\xi_{xx}^{-1} \sim \Delta_T$ and $\xi_{zz}^{-1} \sim \Delta_L$, and both results can be fitted by $\xi^{-1} = 0.402 * \Delta$ (Fig. 5), which coincides exactly with $\xi = 6.03$ obtained for the isotropic spin chain ($h = 0$, $\Delta_0 = 0.41$). [4] This is an independent check of the self-consistency in our calculations.

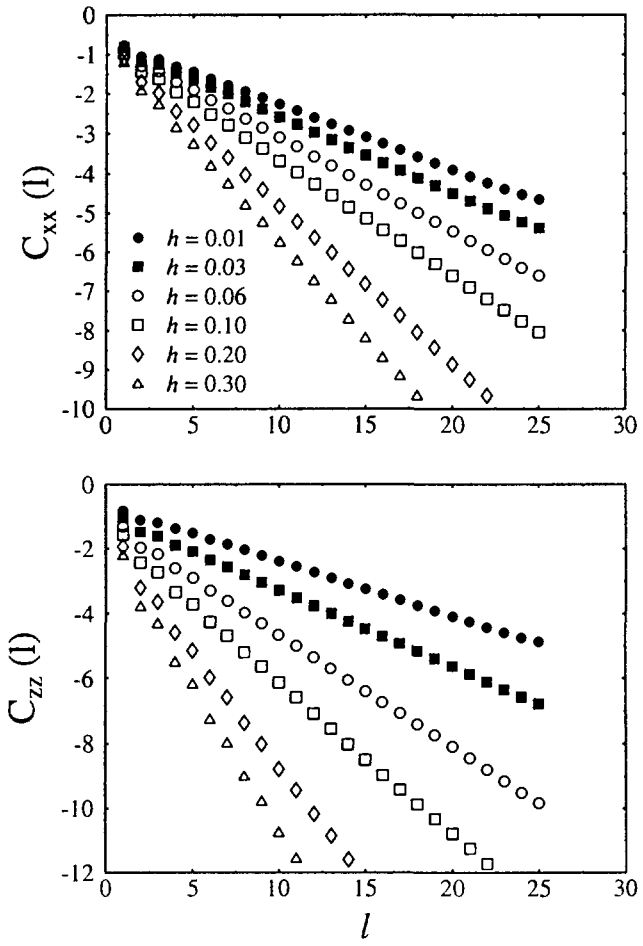

FIG. 4. Spin-spin correlation functions for different values of staggered magnetic field, where l is the distance between the two spins. Both correlations $\langle S_0^x S_l^x \rangle$ and $\langle S_0^z S_l^z \rangle - \langle S_0^z \rangle \langle S_l^z \rangle$ decay exponentially, but the latter decays faster.

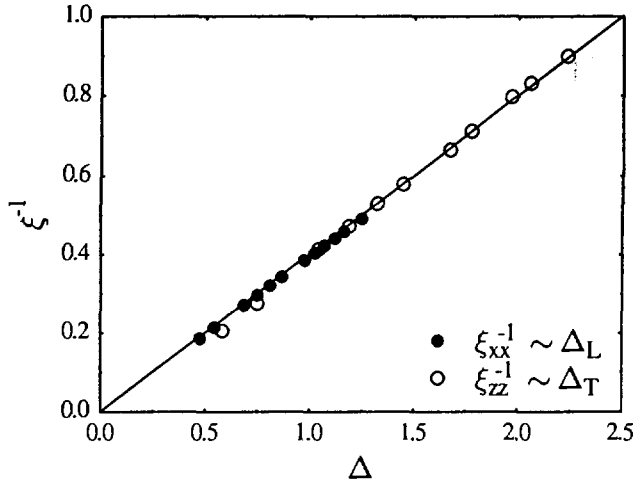

FIG. 5. The inverse correlation lengths ξ_{xx}^{-1} and ξ_{zz}^{-1} for infinite chain length vs. the transverse and longitudinal gaps, respectively. The solid line is the fitting $\xi^{-1} = 0.402 * \Delta$.

In conclusion, by considering a model hamiltonian which describes the physics of a family of mixed-spin materials in the temperature range below T_N of the magnetic rare-earth sublattice, we have calculated numerically the energy gap and the staggered magnetic moment as functions of the staggered magnetic field created by the AF long range order. The obtained results are consistent with the experimental data qualitatively. Our numerical results are also compared with the analytic considerations based on the non-linear σ model. The comparison shows that the NLSM results are good for small staggered fields, while they deviate from the numerical simulations for larger staggered fields. After submitting this paper we saw a new report on polarized neutron study of longitudinal Haldane-gap excitations in Nd_2BaNiO_5. [23] which show somewhat different behavior than expected from the theory. The reason of this discrepancy has to be understood.

Acknowledgments

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References

[1] F. D. M. Haldane, Phys. Lett. **93A**, 464 (1983); Phys. Rev. Lett. **50**, 1153 (1983).

[2] For a review see Ian Affleck, in "*Fields, Strings and Critical Phenomena*", edited by E. Brézin and J. Zinn-Justin, North-Holland, Amsterdam, 1989, p. 511.

[3] J. P. Renard *et al.*, Europhys. Lett. **3**, 945 (1987); J. Darriet and L. P. Regnault, Solid State Commun. **86**, 409 (1993); J. F. DiTusa *et al.* , Physica B **194-196**, 181. (1994).

[4] S. R. White and D. A. Huse, Phys. Rev. B**48**, 3844 (1993).

[5] O. Golinelli, Th. Jolicœur, and R. Lacaze, Phys. Rev. B50, 3037 (1994).

[6] J. F. DiTusa *et al.*, Phys. Rev. Lett. **73**, 1857 (1994); K. Kojima *et al.*, Phys. Rev. Lett. **74**, 3471 (1995).
[7] E. S. Sørensen and I. Affleck, Phys. Rev. B**51**, 16115 (1995); Wei Wang, Shaojin Qin, Zhong-Yi Lu, Zhao-Bin Su and Lu Yu, Phys. Rev. B**53**, 40 (1996); Xiaoqun Wang and Steffen Mallwitz, Phys. Rev. B**53**, 492 (1996); Jizhong Lou, Shaojin Qin, Zhaobin Su and Lu Yu, Phys. Rev. B**58**, 12672 (1998).
[8] E. S. Sørensen and I. Affleck, Phys. Rev. Lett. **71**, 1633 (1993).
Lett. **72**,
[9] Guangyong Xu *et al.*, Phys. Rev. B**54**, R6827 (1996).
[10] V. Sachan, D. J. Buttrey, J. M. Tranquada and G. Shirane, Phys. Rev. B**49**, 9658 (1994).
[11] A. Zheludev, J.M. Tranquada, T. Vogt and D. J. Buttrey, Europhys. Lett. **35**, 385 (1996); Phys. Rev. B**54**, 6437 (1996).
[12] A. Zheludev, J. M. Tranquada, T. Vogt and D. J. Buttrey, Phys. Rev. B**54**, 7210 (1996).
[13] A. Zheludev, J. P. Hill and D. J. Buttrey, Phys. Rev. B**54**, 7216 (1996).
[14] T. Yokoo, A. Zheludev, M. Nakamura and J. Akimitsu, Phys. Rev. B**55**, 11516 (1997).
[15] T. Yokoo, S. Raymond, A. Zheludev, S. Maslov, I. Zaliznyak, J. Akimitsu and R. Erwin, preprint: cond-mat/9710015.
[16] A. Zheludev, E. Ressouche, S. Maslov, T. Yokoo, S. Raymond and J. Akimitsu, Phys. Rev. Lett. **80**, 3630 (1998).
[17] S. Maslov and A. Zheludev, Phys. Rev. B**57**, 68 (1998).
[18] S. R. White and R. M. Noack, Phys. Rev. Lett. **68**, 3487 (1992); S. R. White, Phys. Rev. Lett. **69**, 2863 (1992); S. R. White, Phys. Rev. B**48**, 10345 (1993).
[19] Shaojin Qin, Xiaoqun Wang and Lu Yu, Phys. Rev. **56**, R14251 (1997).
[20] S. Maslov and A. Zheludev, Phys. Rev. Lett. **80**, 5786 (1998).
[21] Tao Xiang, Phys. Rev. B **58**, 9142 (1998).
[22] Y. J. Kim, M. Greven, U.-J. Wiese and R. J. Birgeneau, Eur. Phys. J. B **4**, 291 (1998).
[23] S. Raymond *et al.*, Preprint cond-mat/ 9811040.