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1991 J. Phys.: Condens. Matter 3 1359

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J. Phys.: Condens. Matter 3 (1991) 1359–1362. Printed in the UK

LETTER TO THE EDITOR

On the excitations in a $S = 1$ linear chain Heisenberg antiferromagnet with $S = \frac{1}{2}$ impurities

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Received 4 January 1991

Abstract. It is argued that a $S = 1$ linear chain Heisenberg antiferromagnet containing some amount of $S = \frac{1}{2}$ impurities has integer-spin excitations, induced by doped spins. These excitations results from the breaking of a single valence bond on a site neighbouring the impurity.

A study of one-dimensional integer-S antiferromagnets (1D AFM) became a subject of considerable interest after Haldane first showed [1] that they are described at low energies by the O(3)σ-model (with a coupling $g = 2/S$ for large S) and that the quantum fluctuations not only wash out sublattice magnetization (which is peculiar for any one-dimensional system with a continuous symmetry), but also produce a finite internal scale, i.e. a correlation length $\xi \sim e^{\pi S}$. This drives the system out of criticality into a paramagnetic state. In addition to theoretical investigations and numerical experiments favouring this conjecture [2], an idea of a paramagnetic ground state for $S = 1$ antiferromagnets was also confirmed experimentally by the neutron scattering [3] and susceptibility measurements [4] in a strongly one-dimensional and rather isotropic $S = 1$ antiferromagnet $Ni(C_2H_8N_2)_2NO_2(ClO_4)$ (NENP) and similar substances.

As a way of describing a disordered but unique state of the $S = 1$ antiferromagnet, Affleck *et al* [5] extended the idea of Anderson about valence bonds [6] and proposed a model in which each $S = 1$ site spin is represented as a symmetrized combination of two $S = \frac{1}{2}$ spins. The ground-state wavefunction is given as a product of singlet configurations (valence bonds) of neighbouring pairs of $S = \frac{1}{2}$ spins, so that two $S = \frac{1}{2}$ spins from the same site form singlets with two nearest neighbours. Graphically this ground state is represented as a product of valence bonds between all pairs of neighbouring spins (see figure 1(a)). This state, called a valence bond solid (VBS), does not break symmetry and is thus a good candidate for a $T = 0$ paramagnetic ground state. For a special ratio of coefficients in bilinear and biquadratic couplings of neighbouring spins, i.e. when the Hamiltonian can be rewritten as a sum of projection operators on the $S = 2$ state for each pair, this ground state was proved to be an exact one [5] that allowed a true correlation length and the gap for excitations to be found.

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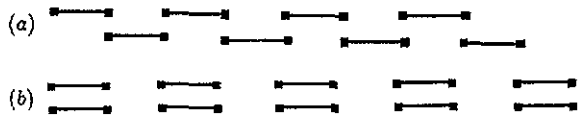

Figure 1. (*a*) A valence bond solid (VBS) state for the $S = 1$ 1D AFM is given by representing each $S = 1$ spin as a symmetrized product of two $S = \frac{1}{2}$ spins. They form singlet configurations (valence bonds) with both neighbours. (*b*) Dimerized phase for $S = 1$. Both $S = \frac{1}{2}$ spins from a given site couple to one and the same neighbour. This results in the doubling of a period and in breaking of a symmetry of translations by one site.

In a recent article Hagiwara *et al* [7] proposed a new method to study the ground-state properties of 1D AFM. It was pointed out that in case of doping by $S = \frac{1}{2}$ impurities (Cu^{2+} for NENP) the two valence bonds terminating on the site, occupied by the impurity, will be broken [8]. As a result, the system will have a finite number of separate clusters with three $S = \frac{1}{2}$ weakly interacting spins. This will result in $S = \frac{1}{2}$ and $S = \frac{3}{2}$ low-energy excitations (see figure 2(*a*)). These excitations were apparently observed in the ESR measurements of NENP doped with Cu^{2+} (see [7]).

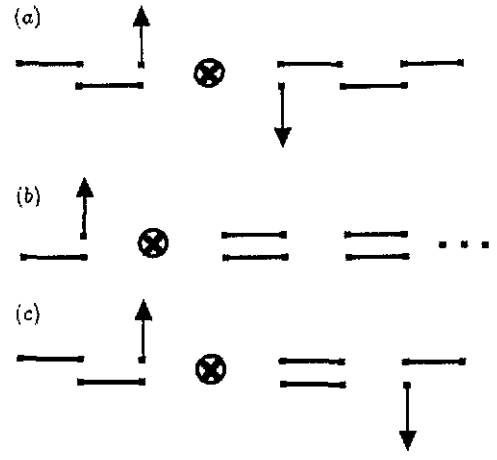

Figure 2. (*a*) A configuration with two broken valence bonds near the impurity site (⊗). The impurity spin couples to the host spins much more weakly than do the host spins between themselves and thus it causes only local perturbations in the VBS state, producing $S = \frac{3}{2}$ and $S = \frac{1}{2}$ configurations with neighbouring $S = \frac{1}{2}$. (*b*) A configuration where the VBS phase between two adjacent impurity states is substituted by a dimerized phase. This results in local states with integer S. (*c*) A configuration resulting from the hopping of a single valence bond near the impurity site. This is enough to decouple the half-integer states of (*a*) into a free $S = \frac{1}{2}$ state and integer-S states formed by impurity and host spins.

In this letter we wish to point out that doping may also produce another type of impurity induced excitation, namely, $S = 1$ excitations in the case of $S = \frac{1}{2}$ impurities. The idea is very simple and based on the fact that the VBS state is not the only state for the $S = 1$ antiferromagnet. The other possibility is a dimer state with a spontaneously broken symmetry of translations by one site. In terms of valence

bonds this state corresponds to the case where both $S = \frac{1}{2}$ spins of a given site form a singlet configuration with the left (or right) neighbour (see figure 1(*b*)). The transition between a VBS and dimer state is known to occur at the SU(2) integrable point for $S = 1$ [9, 10]. The critical theory at that point is given by the $k = 2$ WZW model [9].

Suppose first that we are very close to the transition point. Then the hopping of a valence bond will cost only a small amount of energy. Correspondingly, it will be energetically favourable not to break valence bonds in order to get clusters of three $S = \frac{1}{2}$ spins, but, instead, to substitute all valence bonds between two adjacent impurity sites by a region of dimerized phase. The loss of energy, $\Delta E_1 \sim LE_{\mathrm{VD}}$, where L is the distance between impurities and E_{VD} is the energy difference between the VBS and dimer states, will be compensated by the energy gain, $\Delta E_2 \sim J$, of leaving the valence bond unbroken. Clearly, the distances from a given impurity to its adjacent ones on the left and the right are not necessarily the same. As a result, the insertion of a dimer configuration may become favourable only, say, to the left of a given impurity, while to the right a neighbouring valence bond will be broken resulting in a $S = \frac{1}{2}$ state at the host spin neighbouring the impurity. In this case an impurity spin will have only one $S = \frac{1}{2}$ neighbour as opposed to two neighbouring $S = \frac{1}{2}$ in the model of Hagiwara *et al* [7] (see figure 2(*b*)). A weak coupling $(J_{\parallel} S_1^z \; S_2^z + J_{\perp} S_1^{\perp} \; S_2^{\perp})$ between host and impurity $S = \frac{1}{2}$ spins will then produce local states with $S = 0$ and $S = 1$, that is in a magnetic field one will obtain low-energy branches with

$$\omega_{1,2} = \frac{J_{\parallel}}{2} \pm \mu_{\mathrm{b}} H \left(\frac{g_1 + g_2}{2} \right)$$

$$\omega_{3,4} = -\frac{J_{\parallel}}{4} \pm \sqrt{\left(\frac{J_{\perp}}{2} \right)^2 + (\mu_{\mathrm{b}} H)^2 \left(\frac{g_1 + g_2}{2} \right)^2}$$

where g_1 and g_2 are g-factors for the host and impurity spins, respectively. Note that as in [7], no single ion anisotropy term is possible, since both spins have $S = \frac{1}{2}$. This field dispersion is clearly different from that calculated for the clusters with half-integer spin. It is also worth mentioning that for $g_1 \neq g_2$, the $S = 0$ state couples with the magnetic field.

Of course, for small doping, impurity excitations with integer S can become favourable only very close to the transition point between the VBS and dimer phases. In NENP the correlation length is only about seven lattice spacings. In this case, we expect that instead of large clusters of a dimerized phase, only a small number of $S = 1$ singlet states (dimers) terminating on a site with a free $S = \frac{1}{2}$ state can be inserted near each impurity (figure 2(*c*)). However, the interaction between host and impurity spins is short-ranged and thus the hopping of even a single valence bond will lead to a decoupling between integer-S states formed by impurity and host spins and a state of a separate $S = \frac{1}{2}$. There is no gain in energy in the last case since the number of broken valence bonds is the same as that where the impurity is surrounded by two $S = \frac{1}{2}$ states. The configuration on figure 2(c) thus corresponds to an excited state with the energy E_{VD}. However, these energies are quite acceptable in neutron scattering experiments with NENP. The impurity induced excitations with integer S do not depend on the direction of the applied magnetic field and thus could be observed as isotropic contributions to the field dispersions of the excitation energies.

AB is grateful to F D M Haldane for useful discussion on the VBS phase in antiferromagnets. This work was supported by NSF Grants DMR 88-17613 (AB) and DMR 88-09854 through the Science and Technology Center for Superconductivity (AC) at the University of Illinois at Urbana-Champaign.

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