

Bound states in weakly disordered spin ladders

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Abstract

We study the appearance of bound states in the spin gap of spin- $\frac{1}{2}$ ladders induced by weak bond disorder. Starting from the strong-coupling limit, i.e., the limit of weakly coupled dimers, we perform a projection on the single-triplet subspace and derive the position of bound states for the single impurity problem of one modified coupling as well as for small impurity clusters. The case of a finite concentration of impurities is treated with the coherent-potential approximation (CPA) in the strong-coupling limit and compared with numerical results. Further, we analyze the details in the structure of the density of states and relate their origin to the influence of impurity clusters.

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During the past decade spin ladder systems have attracted large interest among theoretical and experimental physicists (see Ref. [1] for a review) leading to considerable progress in understanding properties of such systems. In this paper we focus on spin ladders with weak bond disorder and we allow couplings along both rungs and legs to be

modified. The Hamiltonian is

$$H = \sum_{l=1}^N [J_{R,l} \vec{S}_{l,1} \cdot \vec{S}_{l,2} + (J_{L,l,1} \vec{S}_{l,1} \cdot \vec{S}_{l+1,1} + 1 \leftrightarrow 2)]. \quad (1)$$

N is the number of sites and $\vec{S}_{l,i}$ denotes a spin- $\frac{1}{2}$ operator acting on site l on leg i ; $i = 1, 2$. As we have shown in Ref. [2] the presence of bond impurities can induce bound states in the spin gap. In extension of our previous work [2] we address two examples and present results for the density of

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states (DOS) of the single-triplet excitation: (i) a random, binary distribution of impurities on rung sites with a large impurity concentration and (ii) binary distributions of modified couplings on legs and rungs. Thus, impurities are distributed according to the probability density

$$P(J_l) = c_{R,L}\delta(J_l - J'_{R,L}) + (1 - c_{R,L})\delta(J_l - J_{R,L}) \quad (2)$$

where $J_{R,L}$ denote the couplings of the pure system and $J'_{R,L}$ are the modified couplings. In both cases, we assume the perturbations to be uncorrelated. Furthermore, the concentrations for rung impurities c_R and for leg impurities c_L are independent.

To treat this problem, we proceed by first mapping the spin- $\frac{1}{2}$ operators onto bond-boson operators s_l^\dagger and $t_{\alpha,l}^\dagger$ [3], where s_l^\dagger creates a singlet on the l th rung and $t_{\alpha,l}^\dagger$ a triplet excitation with orientation $\alpha = x, y, z$, respectively. Next, the singlet is integrated out and we restrict our study to the one-triplet subspace. Thus, triplet interactions and quantum fluctuations are neglected which is equivalent to first-order perturbation theory in J_L/J_R for the pure model.

The resulting effective Hamiltonian reads

$$H_{\text{eff}} = \sum_{l=1}^N \left[J_{R,l} t_l^\dagger t_l + \frac{J_{L,l,1} + J_{L,l,2}}{4} (t_{l+1}^\dagger t_l + \text{h.c.}) \right]; \quad (3)$$

omitting the spin index α but keeping in mind that the spectrum is three-fold degenerate. The dispersion of the homogeneous model is $\varepsilon_k = J_R + J_L \cos(k)$, k being the momentum (see, e.g., Ref. [4]). The spectrum of this effective model in the presence of impurities can be obtained numerically for very large system sizes and has to be sampled over many realizations of impurity distributions (numerical-impurity averaging, NAV). Analytically, the self-energy $\Sigma(E)$ ($E \rightarrow E + i0^+$) of the one triplet Green's function $G(E)$ is accessible via diagrammatic techniques. Here we apply the coherent-potential approximation (CPA) to the case of $c_R > 0$; $c_L = 0$; the self-energy being a self-consistent solution of the

equation (see, e.g., Ref. [5])

$$\Sigma(E) = \frac{c_R \delta J_R}{1 - G(E)[\delta J_R - \Sigma(E)]}. \quad (4)$$

δJ_R is defined as $J'_R - J_R$, compare Eq. (3).

Fig. 1 contains our results for the DOS. First, we discuss the comparison of our numerical data and analytical computations for case (i), i.e., a binary distribution of rung impurities with $J_R = 1$, $J_L = 0.2$, and $\delta J_R = -0.2$ as shown in Fig. 1(a). The concentration of impurities is $c_R = 0.5$. Note that leg couplings are not perturbed. Both curves (solid: NAV, dashed: CPA) are symmetric with respect to $E = 0.9$ while the original band for $c_R = 0$ was centered around $E = 1$. In the limit of $c_R = 1$ the band will be centered around $E = 0.8$ possessing a bandwidth of 0.2. The CPA gives a qualitatively good description of the overall structure of the DOS. As the effective Hamiltonian (3) is that of a one-dimensional non-interacting disordered system, one expects a smooth DOS in the thermo-dynamic limit. However, the NAV shows additional structures [see, e.g., the peaks a, ..., h in Fig. 1(b)] which are stable against variation of N for the system sizes investigated. These peaks can be attributed to the presence of

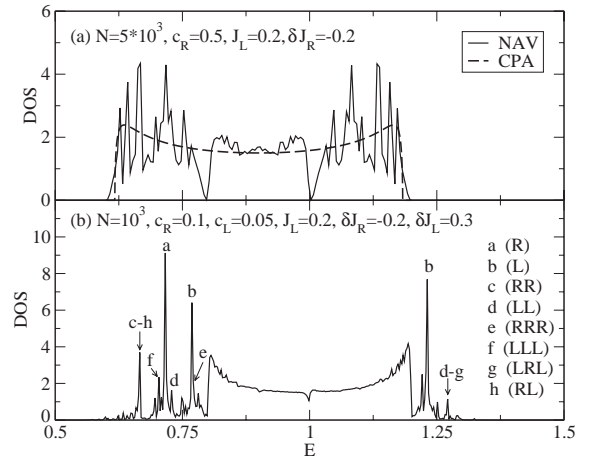


Fig. 1. Panel (a): Comparison of CPA and NAV for a large concentration of rung impurities ($c_R = 0.5$, $c_L = 0$). Panel (b): NAV for bond-impurities on both rungs and legs. The letters label peaks originating from certain impurity clusters as indicated in the legend. See text for more details. In both cases, NAV was performed over typically 5000 random samples.

impurity clusters (see below). Small impurity clusters like, e.g., (RR) (two modified couplings on neighboring rungs) or (R0R) (two modified couplings on rungs separated by one non-perturbed rung) appear as soon as the concentration is finite and lead to discrete peaks in the DOS. The corresponding eigenenergies can be computed exactly by solving Schrödinger's equation (see Ref. [2]).

The influence of small impurity clusters will be further elucidated in the discussion of the second example (ii) where we have numerically computed spectra in the presence of finite concentrations of both rung and leg impurities. Fig. 1(b) shows the resulting DOS for $J_R = 1, J_L = 0.2, \delta J_R = -0.2, \delta J_L = J'_L - J_L = 0.3$ and $c_R = 0.1, c_L = 0.05$. Note that $c_L = 1$ corresponds to all leg couplings on both legs being modified.

In Fig. 1(b), the shape of the original band is still visible for $0.8 < E < 1.2$ as the impurity concentrations are fairly small. Both below and above the band, bound and anti-bound states appear. Their positions can be related to certain impurity clusters in the following way. We consider a single impurity or a single cluster in an otherwise clean system and compute the eigenenergies of the corresponding states outside the original band, if such states are present (see

Ref. [2] for a detailed discussion). Then, the main peaks visible in Fig. 1(b) can easily be identified as being caused by small clusters or single impurities such as (R), (RR), or (RL). Here, (RL) denotes a modified rung coupling and one of the neighboring leg-coupling modified.

Thus, at low concentrations, the structure of the DOS can basically be explained in terms of non-interfering, isolated impurity clusters. The physical reason is that the wave functions of bound-states are less extended in real space, if ratio $\delta J_R/J_R$ or $\delta J_L/J_L$, are large (see Ref. [2] for more details on the single-impurity wave function).

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