Rung-singlet phase of the $S=\frac{1}{2}$ two-leg spin-ladder with four-spin cyclic exchange

K. P. Schmidt,[1] H. Monien,[2] and G. S. Uhrig[1]
[1]*Institut für Theoretische Physik, Universität zu Köln, Zülpicher Straße 77, D-50937 Köln, Germany*
[2]*Physikalisches Institut, Universität Bonn, Nußallee 12, D-53115 Bonn, Germany*
(Received 20 November 2002; published 22 May 2003)

Using continuous unitary transformations (CUTs) we calculate the one-triplet gap for the antiferromagnetic $S=\frac{1}{2}$ two-leg spin ladder with additional four-spin exchange interactions in a high order series expansion about the limit of isolated rungs. By applying an efficient extrapolation technique we calculate the transition line between the rung-singlet phase and a spontaneously dimerized phase with dimers on the legs. Using this extrapolation technique we are able to analyze the crossover from strong rung coupling to weakly coupled chains.

DOI: 10.1103/PhysRevB.67.184413 PACS number(s): 75.10.Jm, 74.25.Ha, 75.50.Ee

After the discovery of high-T_c superconductivity in cuprates in 1986, low-dimensional quantum antiferromagnetism has attracted much attention. Recently it has become clear that the minimum magnetic model for cuprate systems has to include four-spin exchange terms in addition to the usual nearest neighbor Heisenberg exchange interaction.[1–10] One important subclass of such models are the two-leg ladder systems. The nearest-neighbor Heisenberg model on the two-leg ladder without four-spin interaction is a gapped spin liquid. This system is in the rung-singlet phase and the first excitations are triplets.[11–14] In the limit of zero rung coupling there are two isolated gapless spin chains. Including four-spin exchange interactions several quantum phases occur.[15–17] Possible phases include a spontaneously dimerized phase where the dimers are located in a meanderlike structure on the legs, scalar and vector chirality phases, a region of dominant collinear spin, and a ferromagnetic phase.[16] Real two-leg ladder cuprates, however, are always in the rung-singlet phase but relatively close to the quantum phase transition to the spontaneously dimerized phase.[4,9] Therefore, it is in particular important to understand the properties of this transition.

In this paper we will calculate the gap around the limit of isolated rungs. We obtain reliable results in a wide range of parameters belonging to the rung-singlet phase. The transition curve to the spontaneously dimerized phase is computed. In addition, starting from the strong coupling limit of isolated rungs, the limit of isolated spin chains is discussed.

We consider the $S=\frac{1}{2}$ antiferromagnetic two-leg spin ladder plus additional four-spin exchange terms H_{cyc}

$$H=J_{\perp}\sum_{i}\mathbf{S}_{i,1}\cdot\mathbf{S}_{i,2}+J_{\parallel}\sum_{i,\tau}\mathbf{S}_{i,\tau}\cdot\mathbf{S}_{i+1,\tau}+H_{\mathrm{cyc}}, \tag{1a}$$

where i denotes the rungs and $\tau\in\{1,2\}$ the legs and

$$H_{\mathrm{cyc}}=2J_{\mathrm{cyc}}\sum_{\mathrm{plaquettes}}[(\mathbf{S}_{1,i}\cdot\mathbf{S}_{1,i+1})(\mathbf{S}_{2,i}\cdot\mathbf{S}_{2,i+1})+(\mathbf{S}_{1,i}\cdot\mathbf{S}_{2,i}) \times(\mathbf{S}_{1,i+1}\cdot\mathbf{S}_{2,i+1})-(\mathbf{S}_{1,i}\cdot\mathbf{S}_{2,i+1})(\mathbf{S}_{1,i+1}\cdot\mathbf{S}_{2,i})]. \tag{1b}$$

The exchange couplings along the rungs and along the legs are denoted by $J_{\perp}$ and by $J_{\parallel}$, respectively. J_{cyc} denotes the strength of the four-spin magnetic exchange terms. There is also another way based on cyclic permutations P_{ijkl} to include the leading four-spin exchange term. It differs in certain two-spin terms from Eq. (1)

$$H^{p}=J_{\perp}^{p}\sum_{i}\mathbf{S}_{i,1}\cdot\mathbf{S}_{i,2}+J_{\parallel}^{p}\sum_{i,\tau}\mathbf{S}_{i,\tau}\cdot\mathbf{S}_{i+1,\tau}+H_{\mathrm{cyc}}^{p} \tag{2a}$$

$$H_{\mathrm{cyc}}^{p}=\frac{J_{\mathrm{cyc}}^{p}}{2}\sum_{\langle ijkl\rangle}(P_{ijkl}+P_{ijkl}^{-1}). \tag{2b}$$

Both Hamiltonians are identical except for couplings along the diagonals[3] if $J_{\perp}$ and $J_{\parallel}$ are suitably redefined. First, we use Hamiltonian H (1) since it is established that the four-spin terms are the most significant ones if the magnetic Hamiltonian is seen as effective model for the low-lying modes of a realistic insulating three-band Hubbard model.[8] But results for Hamiltonian H^{p} (2) will also be presented.

We use a continuous unitary transformation (CUT) to map the Hamiltonian H to an effective Hamiltonian H_{eff} which conserves the number of rung-triplets, i.e., $[H_0,H_{\mathrm{eff}}]=0$, where $H_0:=H|_{[J_{\parallel}=0,J_{\mathrm{cyc}}=0]}$.[18] The ground state of H_{eff} is the rung-triplet vacuum. The effective Hamiltonian H_{eff} is calculated in order 11 in $x:=J_{\parallel}/J_{\perp}$ and $x_{\mathrm{cyc}}:=J_{\mathrm{cyc}}/J_{\perp}$. Thereby, we obtained the ground-state energy $E_0=\langle 0|H_{\mathrm{eff}}|0\rangle$ and the one-triplet dispersion $\omega(k)=\langle k|H_{\mathrm{eff}}|k\rangle-E_0$. The one-triplet dispersion $\omega(k)$ has a minimum for $k=\pi$, the one-triplet gap $\Delta(x,x_{\mathrm{cyc}}):=\omega(\pi)$. By such perturbative approaches working on the operator level the spin ladder without cyclic exchange has been investigated previously with great success.[19,20]

The standard approach to calculate a phase transition line with series expansions is to use dlogPadé extrapolations on $\Delta(x,x_{\mathrm{cyc}})$. This yields reliable results only in a very small region about the exactly known phase transition point $[x=1/5,x_{\mathrm{cyc}}=1/5]$ (see gray square in Fig. 3 or similarly in Fig. 4). Generally, for $x=x_{\mathrm{cyc}}$ the dispersion and the gap are known exactly

$$\omega(k)/J_{\perp}=1+[2\cos(k)-3]x, \tag{3a}$$

$$\Delta(x,x)/J_{\perp}=1-5x. \tag{3b}$$

The results extrapolated in x are reliable for $x\in[0.1,0.3]$ where the gap closes linearly in x and x_{cyc}. For Hamiltonian

H^p (2) the analogous situation is found at and about the exact point $x^p = x^p_{\rm cyc} = 1/4$ as shown in Ref. 21. We use the parameters with superscript p to distinguish results for the Hamiltonian H^p (2) clearly from those for the Hamiltonian H (1).

We advance extrapolation techniques[23,22] in order to investigate the rung-singlet phase for larger/lower values of x and $x_{\rm cyc}$. The series expansion is expressed not in external parameters such as x and $x_{\rm cyc}$, but in an internal energy, similar in spirit to work for the Ising model.[23] So high series expansion and renormalization group ideas are combined. Our approach outreaches previous work in two aspects. (i) Our final results are given as functions of the external variables. (ii) In the problem studied, the natural internal variable is the one-triplet gap which we compute including all information on short distances. Previously only three macroscopic moments were addressed to define a correlation length. This caveat induced considerable qualitative differences between the continuum and the lattice model.[23] We define

$$G(x) = 1 - \overline{\Delta}(x) = 1 - \frac{\Delta(x, rx)}{(1+x)J_\perp}, \tag{4}$$

where $r = x_{\rm cyc}/x = J_{\rm cyc}/J_\parallel$ will be kept constant for the extrapolation in x. The function $G(x)$ behaves as $G \propto x$ for $x \to 0$ so that any expansion in x can be converted in an expansion in G. Using the expansion for $\Delta(x)$ we calculated the inverse function $x = x(G)$ as a series in G up to order 11 from Eq. (4). The quantity $\overline{\Delta} = \Delta/[(1+x)J_\perp]$ measures the gap in units of $J_\perp + J_\parallel$ to ensure empirically a monotonic behavior of $\overline{\Delta}$ as function of x. Then the existence of the inverse $x(G)$ is assured. Next we consider the derivative of $\overline{\Delta}(x)$

$$\frac{d\overline{\Delta}(x)}{dx} = -\frac{dG}{dx}. \tag{5}$$

Substituting $x = x(G)$ in Eq. (5) we obtain

$$-\frac{dG}{dx} = P(G), \tag{6}$$

where $P(G)$ is the truncated series of order 10 in G. Note that even the convergence of the truncated series $P(G)$ is significantly better than the convergence of the truncated series $\Delta'(x)$ in x.[22] Because the gap is a monotonic decreasing function for $r = {\rm const}$ we can use dlogPadé extrapolations for $P(G)$ since $-dG/dx$ is non-negative. Integrating Eq. (6) yields

$$-\int_0^{G_0} \frac{dG}{P(G)} = \int_0^{x_0} dx = x_0. \tag{7}$$

Therefore, integrating the left hand side to $G_0 = 1$, i.e., $\Delta = 0$, provides the phase transition point $[x_0, rx_0]$ for a given r. For any $G_0 \in [0,1[$ the gap is $\Delta(x_0, rx_0)/J_\perp = (1+x_0)(1-G_0)$. In this way, $\Delta(x, x_{\rm cyc})$ is obtained.

First, we examine the behavior of the gap in the limit of small r and $G = 1$. This corresponds to the situation of two spin chains which are weakly coupled by the four-spin interactions. Bosonization results show that the only relevant operator is the four-spin leg-leg interaction.[21] The triplet gap scales as

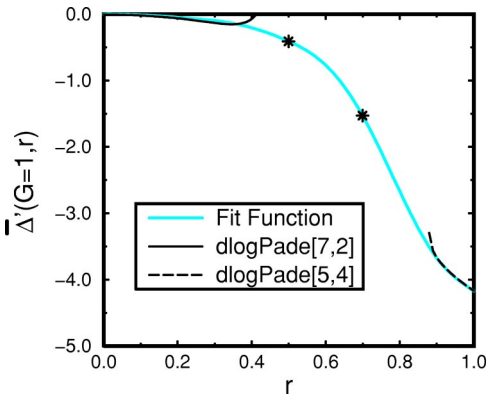

FIG. 1. For Hamiltonian H (1); black lines show the dlogPadé approximants for $d\overline{\Delta}/dx$ at $G = 1$ as a function of $r = x_{\rm cyc}/x$. The gray line is a fitted spline which follows the asymptotic behavior (10) with $\lambda = 0.41$ and $\lambda' = 0.85$ at small values of r and approximates the available dlogPadé results. The points marked by stars are set by hand to guide the spline smoothly in the intermediate region. The extrapolations in Figs. 3 and 4 require actually only the values $r \approx 0.5$.

$$\Delta = \lambda J_\perp - \lambda' J_{\rm cyc} \tag{8}$$

in leading order in $J_\perp$ and $J_{\rm cyc}$. Here λ and λ' are nonuniversal constants.[15] In our case we have a critical theory with central charge $c = \frac{3}{2}$ and SU(2) symmetry which is described as the $k = 2$ Wess-Zumino-Witten model.[15,24] Rearranging Eq. (8) we obtain

$$\frac{\Delta}{J_\parallel} = \frac{\lambda}{x_c}\frac{x_c - x}{x}, \tag{9}$$

where $x_c = \lambda/(\lambda' r)$ is the value of x where the gap vanishes for given r. Therefore, the derivative of $\overline{\Delta}$ for small r at $G = 1$, i.e., $x = x_c$, is given by

$$\overline{\Delta}'(G=1, r) = -\frac{(\lambda' r)^2}{\lambda + \lambda' r}. \tag{10}$$

In the case of $r \to 0$ we expect $\overline{\Delta}' = 0$ and $\overline{\Delta}' = -\lambda/x^2 = -\overline{\Delta}^2/\lambda$ from Eq. (9). Exploiting $\overline{\Delta}' = -\overline{\Delta}^2/\lambda$ in a biased dlogPadé extrapolation we find $\lambda = 0.4 \pm 0.03$ in very good agreement with quantum Monte Carlo results $\lambda_{\rm QMC} = 0.41 \pm 0.01$ from Ref. 25.

In Fig. 1 the solid line corresponds to the dlogPadé [7,2] for $\overline{\Delta}'(G=1,r)$. For $r < 0.3$ the asymptotic formula (10) is well reproduced by the extrapolation. A minute (not discernible) offset at $r = 0$ occurs as a natural consequence of the dlogPadé extrapolation which describes a quantity of a given sign only. Using the value $\lambda = 0.41 \pm 0.01$ we deduce for the second nonuniversal constant λ' the value

$$\lambda' = 0.85 \pm 0.2. \tag{11}$$

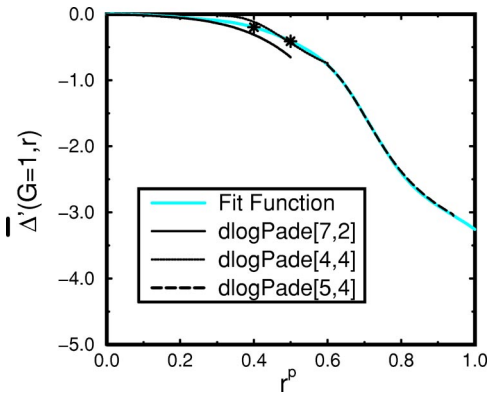

FIG. 2. Same as in Fig. 1 for Hamiltonian H^p (2).

If we perform the same analysis for Hamiltonian (2) we obtain Fig. 2 leading to the same result for λ' given in Eq. (11). This supports the validity of the analysis and agrees perfectly with Ref. 21 in that the relevant term in the cyclic exchange is the leg-leg coupling so that both Hamiltonians (1),(2) lead to the same result for large leg couplings and small cyclic exchange couplings.

For larger values of r or r^p we interpolate between various extrapolations. This works better for Hamiltonian (2) (see Fig. 2) than for Hamiltonian (1) (see Fig. 1). But the interpolating functions are quite similar. The uncertainty in the interpolation leads to the error bars in the subsequent extrapolations shown in Figs. 3 and 4. The extrapolations are done for values $r \lesssim 0.5$ by subtracting the interpolated values depicted in Figs. 3 and 4 from the truncated series for $\bar{\Delta}'(G)$ so that we obtain the series of a function that vanishes at $G=1$. We find that many in this way biased dlogPadé approximants yield reliable results which supports our approach to include the properties of the weakly coupled chains in the extrapolations. Finally the subtracted bias is readded to arrive at the proper result.

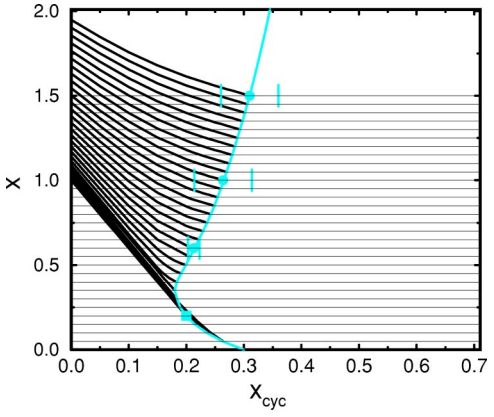

FIG. 3. Extrapolated spin gaps for Hamiltonian H (1) in the $[x,x_{cyc}]$ plane (see main text). The gray line is the obtained phase transition line $\Delta=0$ and the gray square is the exactly known transition point $[x=1/5,x_{cyc}=1/5]$. The points marked by gray circles and error bars indicate the estimated accuracy of the extrapolations. On the left side of the transition line the system is in the rung-singlet phase and on the right side in the spontaneously dimerized phase.

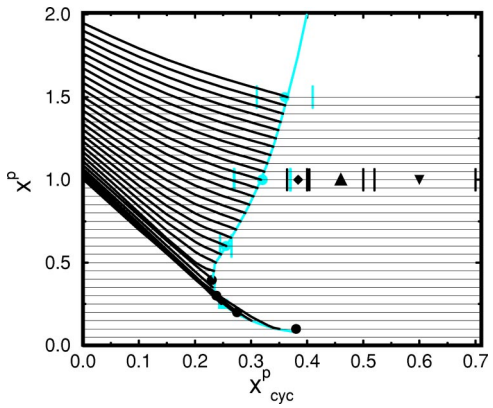

FIG. 4. Same as in Fig. 3 in the $[x^p,x^p_{cyc}]$ plane for Hamiltonian H^p (2). The gray square is the exactly known transition point $[x^p=1/4,x^p_{cyc}=1/4]$. The black circles are points taken from the curves in Ref. 21. The triangles are DMRG results (downward from Ref. 26; upward from Ref. 16). The diamond is determined from the maximization of the central charge by exact diagonalization (Ref. 24).

In the limit $x\to\infty$, we conclude from Eq. (9) that the transition line converges against the asymptotic line

$$x_{cyc}^{asympt}=\lambda/\lambda' \approx 0.52\pm 0.14 \tag{12}$$

using the values for λ and λ' obtained above. This result holds again for both Hamiltonians (1),(2). We cannot confirm the value of $x_{cyc}^{asympt}=0.22$ advocated in Ref. 21.

In Fig. 3 the extrapolated values of the spin gap of the Hamiltonian (1) in the $[x,x_{cyc}]$ plane are presented. The black solid lines denote $\Delta(x_0,x_{cyc})$ for a fixed x_0 as a function of x_{cyc}. These lines are shifted by x_0 in the x direction producing a quasi-three-dimensional plot. The end point of a black line corresponds to $\Delta(x,x_{cyc})=0$ yielding the gray solid line which is the transition line between the rung-singlet phase and the spontaneously dimerized phase. We use biased extrapolations in the range $x\in[0.3,\infty]$ for the transition line. In the range $x\in[0.1,0.3]$ the unbiased extrapolations are safe due to the good convergence of the series near the exactly known transition point (gray square). In the limit $x\to 0$ even the truncated series gives quantitative results. Using Eq. (7) one finds in addition strong evidence for

$$\frac{d\bar{\Delta}}{dx}\propto(1-G)^{\eta} \tag{13}$$

at $x=0$ where $\eta=0.3\pm0.02$. The transition point, i.e., $\Delta=0$, for $x=0$ is found to be $[0,0.3\pm0.002]$. The smooth connection between the different extrapolations corroborates the reliability of our results in a wide region in the $[x,x_{cyc}]$ plane.

In Fig. 4 the corresponding results for the spin gap of the Hamiltonian (2) in the $[x^p,x^p_{cyc}]$ plane are depicted. The biased extrapolation is used for $x^p\gtrsim 0.4$. In addition to quantitative differences there occurs one qualitative difference at low values of x^p. For Hamiltonian (2) no closing of the gap on increasing x^p_{cyc} occurs for $x^p\lesssim 0.1$ as in Ref. 21. Thus the

gray line is not prolonged below $x^p = 0.1$. Apart from this point, the shape of the transition line is similar for both Hamiltonians.

Quantitatively, it is interesting to compare to results obtained by other approaches (Fig. 4). References 26,16 use density matrix renormalization. Reference 24 analyzes the finite size scaling to determine the maximum central charge c. The cyclic exchange where c is maximum yields the critical x^p_{cyc}. The spread and the error bars of the various results allow one to assess the accuracy of the data. We conclude that it is at present not yet settled where precisely the transition between gapped rung-singlet and dimerized phase occurs for the isotropic ladder. We propose to carry out careful finite-size scaling on data for *periodic* systems to clarify this issue. The symmetry change between the rung-singlet and the dimerized phase cannot be represented properly in a *single open* system.

In summary, we have investigated the rung-singlet phase of the $S=\frac{1}{2}$ two-leg spin ladder with additional four-spin interactions. We used a continuous unitary transformation to calculate the one-triplet gap in a high order series expansion about the limit of isolated rungs. The use of an internal energy scale as the new expansion variable enabled us to calculate the transition line between the rung-singlet phase and the spontaneously dimerized phase reliably in a wide region of parameter space. Our results are consistent with the bosonization results in the limit of weakly coupled chains where we reproduce their properties. In addition, we give an estimate of the nonuniversal constants λ and λ' which appear in the bosonization treatment. The value for λ is in very good agreement with quantum Monte Carlo results.[25] We have given an example that the combination of high order series expansion and renormalization group ideas can be a powerful tool.

We thank A. Bühler, C. Knetter, U. Löw, and E. Müller-Hartmann for helpful discussions and the DFG for financial support in SP 1073 and in SFB 608.

[1] Y. Honda, Y. Kuramoto, and T. Watanabe, Phys. Rev. B **47**, 11 329 (1993).
[2] J. Lorenzana, J. Eroles, and S. Sorella, Phys. Rev. Lett. **83**, 5122 (1999).
[3] S. Brehmer *et al.*, Phys. Rev. B **60**, 329 (1999).
[4] M. Matsuda *et al.*, J. Appl. Phys. **87**, 6271 (2000); Phys. Rev. B **62**, 8903 (2000).
[5] R. Coldea *et al.*, Phys. Rev. Lett. **86**, 5377 (2001).
[6] T. Senthil and M. P. A. Fisher, Phys. Rev. Lett. **86**, 292 (2001).
[7] L. Balents, M. P. A. Fisher, and S. M. Girvin, Phys. Rev. B **65**, 224412 (2002).
[8] E. Müller-Hartmann and A. Reischl, Eur. Phys. J. B **28**, 173 (2002).
[9] T. Nunner *et al.*, Phys. Rev. B **66**, 180404 (2002).
[10] K. P. Schmidt, C. Knetter, M. Grüninger, and G. S. Uhrig, Phys. Rev. Lett. **90**, 167201 (2003).
[11] D. G. Shelton, A. A. Nersesyan, and A. M. Tsvelik, Phys. Rev. B **53**, 8521 (1996).
[12] E. Dagotto, J. Riera, and D. Scalapino, Phys. Rev. B **45**, 5744 (1992).
[13] T. M. Rice, S. Gopalan, and M. Sigrist, Europhys. Lett. **23**, 445 (1993); Physica **199-200**, 378 (1994).
[14] T. Barnes, E. Dagotto, J. Riera, and E. S. Swanson, Phys. Rev. B **47**, 3196 (1993).
[15] A. A. Nersesyan and A. M. Tsvelik, Phys. Rev. Lett. **78**, 3939 (1997).
[16] A. Läuchli, G. Schmid, and M. Troyer, Phys. Rev. B **67**, 100409 (2003).
[17] T. Hikihara, T. Momoi, and X. Hu, Phys. Rev. Lett. **90**, 087204 (2003).
[18] C. Knetter and G. S. Uhrig, Eur. Phys. J. B **13**, 209 (2000).
[19] S. Trebst *et al.*, Phys. Rev. Lett. **85**, 4373 (2000).
[20] C. Knetter, K. P. Schmidt, M. Grüninger, and G. S. Uhrig, Phys. Rev. Lett. **87**, 167204 (2001).
[21] M. Müller, T. Vekua, and H.-J. Mikeska, Phys. Rev. B **66**, 134423 (2002).
[22] K. P. Schmidt, C. Knetter, and G. S. Uhrig, Acta Phys. Pol. B **34**, 1481 (2003).
[23] B. G. Nickel and B. Sharpe, J. Phys. A **12**, 1835 (1979).
[24] K. Hijii and K. Nomura, Phys. Rev. B **65**, 104413 (2002).
[25] M. Greven, R. J. Birgeneau, and U.-J. Wiese, Phys. Rev. Lett. **77**, 1865 (1996).
[26] Y. Honda and T. Horiguchi, cond-mat/0106426 (unpublished).