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

(September 25, 2002)

Using continuous unitary transformations (CUT) 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 a novel extrapolation technique we calculate the transition line between the rung-singlet phase and a spontaneously dimerized phase with dimers on the legs. Using this efficient extrapolation technique we are able to analyze the crossover from strong rung coupling to weakly coupled chains.

PACS numbers: 75.10.Jm, 74.25.Ha, 75.50.Ee

After the discovery of high-$T_c$ superconductivity in 1986, low dimensional quantum antiferromagnetism has attracted much attention in condensed matter physics. Recently it has become clear that the minimum magnetic exchange without four-spin interaction is a gapped spin liquid. This system is in the rung-singlet phase and first excitations are triplets. In the limit of zero rung coupling there are two isolated gapless spin chains. Including four-spin exchange interactions several new quantum phases occur. Possible phases include a spontaneously dimerized phase where the dimers are located in a meander-like structure on the legs, scalar and vector chirality phases, a region of dominant collinear spin and a ferromagnetic phase. However, real two-leg ladder cuprate systems are always in the rung-singlet phase but relatively close to the quantum phase transition to the spontaneously dimerized phase. 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 strongly coupling limit of isolated rungs, the limit of isolated rungs chains is discussed.

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

$$H = J_\perp \sum_i S_{i,1} S_{i,2} + J_\parallel \sum_{i,\tau} S_{i,\tau} S_{i+1,\tau} + H_{\text{cyc}}$$

(1a)

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

$$H_{\text{cyc}} = 2J_{\text{cyc}} \sum_{\text{plaquettes}} \left[ (S_{1,i} S_{1,i+1})(S_{2,i} S_{2,i+1}) + (S_{1,i} S_{2,i})(S_{1,i+1} S_{2,i+1}) - (S_{1,i} S_{2,i+1})(S_{1,i+1} S_{2,i}) \right].$$

(1b)

The exchange couplings along the rungs and along the legs are denoted by $J_\perp$ and by $J_{\parallel}$, respectively. $J_{\text{cyc}}$ denotes the strength of the four-spin magnetic exchange term. 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)

$$H^p = J^p_\perp \sum_i S_{i,1} S_{i,2} + J^p_\parallel \sum_{i,\tau} S_{i,\tau} S_{i+1,\tau} + H^p_{\text{cyc}}$$

(2a)

$$H^p_{\text{cyc}} = \frac{J^p_{\text{cyc}}}{2} \sum_{ijkl} \left( P_{ijkl} + P_{ijkl}^{-1} \right).$$

(2b)

Both Hamiltonians are identical except for couplings along the diagonals 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. 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 $H_{\text{eff}}$ which conserves the number of rung-triplets, i.e. $[H_0,H_{\text{eff}}] = 0$ where $H_0 := H|_{J_{\parallel}=0,J_{\text{cyc}}=0}$. The ground state of $H_{\text{eff}}$ is the rung-triplet vacuum. The effective Hamiltonian $H_{\text{eff}}$ is calculated in order 11 in $x := J_{\parallel}/J_{\perp}$ and $x_{\text{cyc}} := J_{\text{cyc}}/J_{\perp}$. Thereby, we obtained the ground-state energy $E_0 = \langle 0 | H_{\text{eff}} | 0 \rangle$ and the one-triplet dispersion $\omega(k) = \langle k | H_{\text{eff}} | k \rangle - E_0$. The one-triplet dispersion $\omega(k)$ has a minimum for $k = \pi$, the one-triplet gap $\Delta(x,x_{\text{cyc}}) := \omega(\pi)$. By such perturbative approaches working on the operator level the spin ladder without cyclic exchange has been investigated previously with great success.

The standard approach to calculate a phase transition line with series expansions is to use dlogPadé approximants on $\Delta(x,x_{\text{cyc}})$. This yields reliable results only in a very small region about the exactly known phase transition point $x = 1/5, x_{\text{cyc}} = 1/5$ (See grey square in Fig. 3 or similarly in Fig. 4). Generally, for $x = x_{\text{cyc}}$ the dispersion and the gap are known exactly.
\[
\omega(k) / J_\perp = 1 + (2 \cos(k) - 3)x
\]
\[
\Delta(x, x / J_\perp) = 1 - 5x
\]
(3)

The results extrapolated in \( x \) are reliable for \( x \in [0, 1, 0.3] \) where the gap closes linearly in \( x \) and \( x_{\text{cyc}} \). For Hamiltonian \( H^p \) (2) the analogous situation is found at and about the exact point \( x^p = x^p_{\text{cyc}} = 1/4 \) as shown in Ref. 21. Note that we use the parameters with superscript \( p \) to distinguish results for the Hamiltonian \( H^p \) (2) clearly from those for the Hamiltonian \( H \) (1).

In the following, we advance a recently introduced extrapolation technique\textsuperscript{22} in order to investigate the rung-singlet phase for larger/lower values of \( x \) and \( x_{\text{cyc}} \). The main idea is to express the series expansion not in external parameters of the system like \( x \) and \( x_{\text{cyc}} \), but in an internal energy. Thereby, we combine high series expansion and renormalization group ideas. The natural internal energy scale of the two-leg ladder is the one-triplet gap. In practice, we define the function
\[
G(x) = 1 - \Delta(x) = 1 - \frac{\Delta(x, x)}{(1 + x) J_\perp}
\]
(4)

where \( r = x_{\text{cyc}} / x = J_{\text{cyc}} / J_\parallel \) will be kept constant for the extrapolation in \( x \). The function \( G(x) \) behaves like \( G \propto x \) 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 \( \Delta = \Delta / [(1 + x) J_\perp] \) measures the gap in units of \( J_\perp + J_\parallel \) to ensure empirically a monotonic behavior of \( \Delta \) as function of \( x \). Then the existence of the inverse \( x(G) \) is assured. Next we consider the derivative of \( \Delta(x) \)

\[
\frac{d\Delta(x)}{dx} = -\frac{dG}{dx}.
\]
(5)

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

\[
-\frac{dG}{dx} = P(G),
\]
(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 \( x \) as discussed in Ref. 22. Because the gap is a monotonic decreasing function for \( r = \text{const} \) we can use dlogPadé approximants for \( P(G) \) since \(-dG/dx \) is non-negative. Integrating Eq. (6) yields

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

Therefore, integrating the left hand side to \( G_0 = 1 \), i.e. \( \Delta = 0 \), provides the phase transition point \( [x_0, r x_0] \) for a given \( r \). For any \( G_0 \in [0, 1] \) the gap is \( \Delta(x_0, r x_0) / J_\perp = (1 + x_0)(1 - G_0) \). In this way, \( \Delta(x, x_{\text{cyc}}) \) 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\textsuperscript{21}. The triplet gap scales as

\[
\Delta = \lambda J_\perp - \lambda' J_{\text{cyc}}
\]
(8)

in leading order in \( J_\perp \) and \( J_{\text{cyc}} \). Here \( \lambda \) and \( \lambda' \) are non-universal constants\textsuperscript{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\textsuperscript{15,23}. Rearranging Eq. (8) we obtain

\[
\frac{\Delta}{J_\parallel} = \frac{\lambda}{x_c} - \frac{x}{x_c}
\]
(9)

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

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

In the case of \( r \to 0 \) we expect \( \Delta = 0 \) and \( \Delta' = -\lambda / x^2 = -\Delta'' / \lambda \) from Eq. (9). Exploiting \( \Delta = \Delta'' / \lambda \) in a biased dlogPadé approximant we find \( \lambda = 0.41 \pm 0.03 \) in very good agreement with Quantum Monte Carlo results \( \lambda_{\text{QMC}} = 0.41 \pm 0.01 \) from Ref. 24.

In Fig. 1 the solid line corresponds to the dlogPadé [7, 2] for \( \Delta'(G = 1, r) \). For \( r < 0.3 \) the asymptotic formula (10) is well reproduced by the approximant. A

![ FIG. 1. For Hamiltonian \( H \) (1); black lines show the dlogPadé approximants for \( d\Delta / dx \) at \( G = 1 \) as a function of \( r = x_{\text{cyc}} / x \). The grey line is a fitted spline which follows the asymptotic behavior Eq. (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 \( r \lesssim 0.5 \).](image)
minute (not discernible) offset at \( r = 0 \) occurs as a natural consequence of the dlogPadé approximation which describes a quantity of a given sign only. Using the value \( \lambda = 0.41 \pm 0.01 \) we deduce for the second non-universal constant \( \lambda' \) the value

\[
\lambda' = 0.85 \pm 0.2 \ .
\]  

(11)

If we perform the same analysis for Hamiltonian (2) we obtain Fig. 2 leading to the same result for \( \lambda' \) given in Eq. (11). This fact corroborates the validity of the analysis and agrees perfectly with the finding by Müller et al.\(^{21}\) stating that the relevant term in the cyclic exchange is the 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 approximants. This works better for Hamiltonian (2) (see Fig. 2) than for Hamiltonian (1) (see Fig. 1). But the interpolating functions are in any case quite similar. The uncertainty in the interpolation leads to the error bars in the subsequent extrapolations shown in Figs. 3 and 4. These extrapolations are done for values \( r \lessgtr 0.5 \) by subtracting the interpolated values depicted in Figs. 3 and 4 from the truncated series for \( \Delta(G) \) 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. This supports our approach to include the properties of the weakly coupled chains in the extrapolations. Finally the subtracted bias is re-added to arrive at the proper result.

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

\[
x_{\text{cyc}}^{\text{asympt}} = \lambda / \lambda' \approx 0.52 \pm 0.14 \quad (12)
\]

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

In Fig. 3 the extrapolated values of the spin gap of the Hamiltonian (1) in the \( [x, x_{\text{cyc}}] \)-plane are presented. The black solid lines denote \( \Delta(x_0, x_{\text{cyc}}) \) for a fixed \( x_0 \) as a function of \( x_{\text{cyc}} \). These lines are shifted by \( x_0 \) in \( x \)-direction producing a quasi three-dimensional plot. The end-point of a black line corresponds to \( \Delta(x, x_{\text{cyc}}) = 0 \). These points yield the grey solid line which is the transition line between the rung-singlet phase and the spontaneously dimerized phase. As discussed above, we use biased approximants 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 obtained near the exactly known transition point (grey square). In the limit \( x \to 0 \) even the truncated series gives quantitative results. Using Eq. (7) one finds in addition strong evidence for

\[
\frac{d\Delta}{dx} \propto (1 - G)^\eta \quad (13)
\]

at \( x = 0 \) where \( \eta = 0.3 \pm 0.02 \). The transition point, i.e. \( \Delta = 0 \), for \( x = 0 \) is found to be \([0, 0.3 \pm 0.002]\).

The smooth connection between the different extrapolations corroborates the reliability of our results in a wide region in the \([x, x_{\text{cyc}}]\)-plane.

In Fig. 4 the corresponding results for spin gap of the Hamiltonian 2 in the \([x^p, x_{\text{cyc}}]\)-plane are depicted. The biased extrapolation is used for \( x^p \gtrsim 0.4 \). Besides quantitative differences there occurs one qualitative difference at low values of \( x^p \). For Hamiltonian (2) no closing of the gap on increasing \( x_{\text{cyc}}^p \) for \( x^p \gtrsim 0.1 \) was found in agreement with the results in Ref. 21. This is the reason why
the grey 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, see Fig. 4. Refs. 25, 16 use density matrix renormalization. Another work analyzes the finite size scaling to determine the maximum central charge by exact diagonalization. We have given an estimate of the non-universal constants $\lambda$ and $\lambda'$ which appear in these bosonization treatments. The value for $\lambda$ is in very good agreement with quantum Monte Carlo results. 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.

FIG. 4. Same as in Fig. 3 in the $[x^p, x^p_{\text{cyc}}]$-plane for Hamiltonian $H^p$ (2). The grey square is the exactly known transition point $[x^p = 1/4, x^p_{\text{cyc}} = 1/4]$. The black circles are points taken from the curves in Ref. 21. The triangles are DMRG results (downward from Ref. 25; upward from Ref. 16). The diamond is determined from the maximization of the central charge by exact diagonalization.

1. Y. Honda, Y. Kuramoto, and T. Watanabe, Phys. Rev. B 47, 11329 (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); ibid. Phys. Rev. B 62, 8903 (2000).
5. R. Coldea, D. A. Tennant, A. M. Tsvelik, and Z. Tylczynski, Phys. Rev. Lett. 86, 1335 (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., cond-mat/0203472.
10. K. P. Schmidt, C. Knetter, M. Grüninger, and G. S. Uhrig, Phys. Rev. Lett. (2002).
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); ibid. Physica 200-209, 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, cond-mat/0206153 (2002).
17. T. Hikihara, T. Momoi, and X. Hu, cond-mat/0206102 (2002).
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, cond-mat/0206081 (2002).
22. K. P. Schmidt, C. Knetter, and G. S. Uhrig, Acta Polonica Physica, cond-mat/0208358.
23. K. Hijii and K. Nomura, Phys. Rev. B 65, 104413 (2002).
24. M. Greven, R. J. Birgeneau, and U.-J. Wiese, Phys. Rev. Lett. 77, 1865 (1996).
25. Y. Honda and T. Horiguchi, cond-mat/0106426.