Low-energy properties of antiferromagnetic spin-1/2 Heisenberg ladders with an odd number of legs

Beat Frischmuth, Stephan Haas, German Sierra, and T. M. Rice
Institute of Theoretical Physics, ETH Hönggerberg, CH-8093 Zürich, Switzerland
(Received 19 November 1996)

An effective low-energy description for multileg spin-$\frac{1}{2}$ Heisenberg ladders with an odd number of legs is proposed. Using a recently developed Monte Carlo loop algorithm and exact-diagonalization techniques, the uniform and staggered magnetic susceptibility and the entropy are calculated for ladders with one, three, and five legs. These systems show a low-temperature scaling behavior similar to spin-$\frac{1}{2}$ chains with longer ranged unfrustrated exchange interactions. The spinon velocity does not change as the number of legs increases, but the energy scale parameter decreases markedly. [S0163-1829(97)50806-X]

Recently, antiferromagnetic Heisenberg spin-$\frac{1}{2}$ ladders attracted much interest, following the discovery of a spin gap in the 2-leg ladder.[1] Also, the crossover from the single chain to the two-dimensional (2D) square lattice, obtained by assembling chains to form ''ladders'' of increasing width, is far from smooth.[2] Heisenberg ladders with an even number of legs, n_l, have a spin gap and short-range correlations, while odd-leg ladders have no gap and power-law correlations. These theoretical predictions have been verified experimentally, in materials such as $(VO)_2P_2O_7$ (Ref. 3) and the homologous series of cuprates $Sr_{n-1}Cu_{n+1}O_{2n}$,[4] which contain weakly coupled arrays of ladders.

Here, we concentrate on odd-leg ladders. Our goal is to derive a low-energy description in terms of $S=\frac{1}{2}$ chains with longer range effective interactions, and examine the evolution with increasing number of legs, n_l. The Heisenberg Hamiltonian for ladders is

$$H=J_{\parallel}\sum_{\leftrightarrow}\vec{S}_{i,\tau}\cdot\vec{S}_{j,\tau}+J_{\perp}\sum_{\updownarrow}\vec{S}_{i,\tau}\cdot\vec{S}_{i,\tau'},\qquad(1)$$

where i and j enumerate the rungs, τ, τ' label the legs, and the sum marked by $\leftrightarrow$ ($\updownarrow$) runs over nearest neighbors along legs (rungs). Periodic boundary conditions are chosen along the leg direction and open boundary conditions perpendicular to it. For the known materials we expect the superexchange to be roughly isotropic ($J_{\perp}=J_{\parallel}$). However, it is educational first to consider the strongly anisotropic limit ($J_{\perp}\gg J_{\parallel}$).

In the completely anisotropic limit ($J_{\parallel}/J_{\perp}=0$), each eigenfunction is a direct product of one-rung states whose lowest-lying multiplet is a spin doublet, separated by a gap of order $J_{\perp}$ from the first excited state. The ground state of the whole system is therefore 2^L-fold degenerate. A finite value of $J_{\parallel}$ lifts this degeneracy. Our goal is to formulate an effective Hamiltonian, $H_{\rm eff}$, in this 2^L-dimensional subspace $\mathcal{M}$ of rung doublets which describes the low-energy properties. For the case of the 3-leg ladder, to third order in $J_{\parallel}/J_{\perp}$, we get

$$H_{\rm eff}^{(3)}=\sum_{j=1}^{L}\left[\sum_{n=1}^{3}J_n\vec{S}_j^{\rm tot}\cdot\vec{S}_{j+n}^{\rm tot}+\widetilde{J}\left((\vec{S}_j^{\rm tot}\cdot\vec{S}_{j+3}^{\rm tot})\times(\vec{S}_{j+1}^{\rm tot}\cdot\vec{S}_{j+2}^{\rm tot})-(\vec{S}_j^{\rm tot}\cdot\vec{S}_{j+2}^{\rm tot})(\vec{S}_{j+1}^{\rm tot}\cdot\vec{S}_{j+3}^{\rm tot})\right)\right],\qquad(2)$$

where $\vec{S}_j^{\rm tot}=\vec{S}_{j,1}+\vec{S}_{j,2}+\vec{S}_{j,3}$ is the total spin of the jth rung, $J_n = J_{\perp}\sum_{\lambda} a_{n,\lambda}(J_{\parallel}/J_{\perp})^{\lambda}$, with $a_{1,1}=1$, $a_{1,2}=-1/9$, $a_{1,3}=-103/243$, $a_{2,1}=0$, $a_{2,2}=-8/27$, $a_{2,3}=-49/162$, $a_{3,1}=a_{3,2}=0$, $a_{3,3}=32/243$, and $\widetilde{J}=(16/81)\,J_{\parallel}^3/J_{\perp}^2$.[5]

The last term in Eq. (2) will be neglected, since the corrections in the energy of the low-lying energy states due to this term are small. $H_{\rm eff}^{(3)}$ has then the form of a single chain with effective nearest neighbor (NN) coupling J_1, next-nearest neighbor (NNN) coupling J_2, and with exchange coupling J_3 between rung spins separated by three unit cells. Therefore the low-lying energy states of the 3-leg ladder can be mapped onto those of a J_1-J_2-J_3 chain. In this effective system the NNN interactions are F ($J_2<0$), while the NNNN interactions are AF ($J_3>0$). Consequently, both the second and the third term in Eq. (2) enhance the overall AF quasilong-range order. Note, that the third-order corrections in Eq. (2) affect J_1 and J_2 strongly since the corresponding coefficients are large. So one must perform the calculations at least up to third order.

To test $H_{\rm eff}^{(3)}$, we calculate the temperature-dependent uniform susceptibility, $\chi(T)$, for 3-leg ladders[6] using the Quantum Monte Carlo (QMC) loop algorithm,[7–9] and compare to susceptibilities obtained for the effective J_1-J_2-J_3 model. We consider large enough systems, such that finite-size effects are negligible. All results are extrapolated to a Trotter time interval $\Delta\tau\rightarrow 0$. Further, we compare with recent results obtained by Greven *et al.*[10] using the same algorithm.

At low temperatures, where only the states in $\mathcal{M}$ are relevant, the susceptibilities of the 3-leg ladders with small $J_{\parallel}/J_{\perp}$ coincide with those of the corresponding J_1-J_2-J_3 chain. This can be seen in the inset of Fig. 1, where we show the susceptibility per rung of the 3-leg ladder with $J_{\parallel}/J_{\perp}=0.2$ together with the susceptibilities of the corresponding effective models in first, second, and third order in

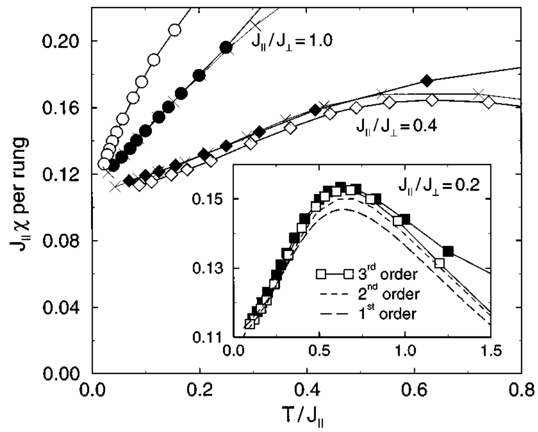

FIG. 1. Susceptibility of the 3-leg ladder for different $J_{\parallel}/J_{\perp}$ and of the corresponding effective models. The filled symbols show the data for the 3-leg ladders and the open symbols those of the corresponding third-order effective model. The crosses show the susceptibility of the corresponding J_1-J_2 chains in the mapping of the 3-leg ladders to J_1-J_2 chains (for details see text). The inset shows the susceptibility per rung of the 3-leg ladder with $J_{\parallel}/J_{\perp}=0.2$ together with those of the corresponding effective models in first, second, and third order in $J_{\parallel}/J_{\perp}$. The error bars are smaller or in order of the symbols.

$J_{\parallel}/J_{\perp}$. While the first-order effective model (a single chain with only NN interactions) gives only a qualitative description of the 3-leg ladder at low temperatures, $\chi(T)$ of the effective model in third order in $J_{\parallel}/J_{\perp}$ coincides with the susceptibility per rung of the 3-leg ladder up to a crossover temperature. Above this temperature, $\chi(T)$ of the 3-leg ladder is larger, due to the presence of additional states in the 3-leg ladder which are not included in the subspace $\mathcal{M}$.

The crossover temperature is of the order of the gap Δ to the higher lying states in the 3-leg ladder. It can be estimated best by considering the entropy of both the 3-leg ladder and the corresponding effective model[11] (Fig. 2). Just above the crossover temperature, the additional states lead to a rise $\propto e^{-\Delta/T}$ in the entropy. Consequently, fitting the form $e^{-\Delta/T}$ to the difference of the entropy per rung of the 3-leg ladder and the entropy of the corresponding effective model gives a rough estimate of Δ. We find $\Delta \approx J_{\perp}$ more or less independent of $J_{\parallel}/J_{\perp}$.

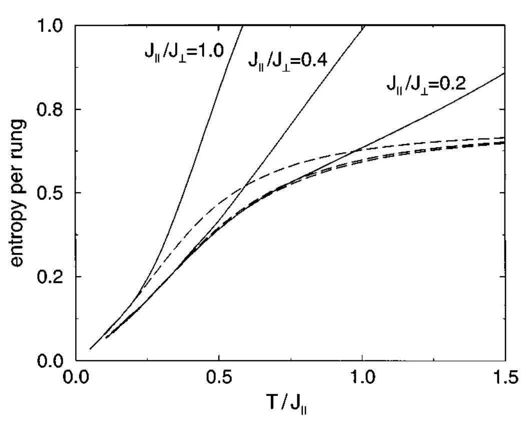

FIG. 2. Entropy of the 3-leg ladder for different $J_{\parallel}/J_{\perp}$ (solid lines) and of the corresponding effective models (dashed lines).

From Fig. 1, it is clear that with increasing $J_{\parallel}/J_{\perp}$ the quality of the description of the 3-leg ladder by the third-order effective model becomes worse. The *qualitative* features of the temperature dependence of the susceptibility, however, are correctly given even in the isotropic case $J_{\parallel}/J_{\perp}=1$, e.g., the slope of $\chi(T)$ is increasing, while the zero-temperature value $\chi(0)$ remains more or less constant, as $J_{\parallel}/J_{\perp}$ increases (see Fig. 1).

Calculating the effective Hamiltonian of the 3-leg ladders to nth order leads to a spin-chain Hamiltonian with interaction terms between spins which are separated by up to n unit cells. All these interactions are invariant under translations and rotations. Consequently, for very low temperatures the 3-leg ladders can be mapped onto the $k=1$ Wess-Zumino-Witten (WZW) nonlinear σ model,[6,12] which is determined by a spinon velocity, v, and an energy scale parameter, T_0. For $T \ll T_0$, $\chi(T)$ of this model reads[12,13] up to $O((\ln T)^{-3})$

$$\chi(T)=\frac{1}{2\pi v}+\frac{1}{4\pi v}\left[\frac{1}{\ln(T_0/T)}-\frac{\ln(\ln(T_0/T)+1/2)}{2\ln^2(T_0/T)}\right] \tag{3}$$

$\chi(T)$ approaches its $T=0$ value $\chi(0)=1/(2\pi v)$ with infinite slope. T_0 should be $\lesssim \Delta$, and characterizes the interactions between the spinons. The smaller T_0, the stronger the interactions, and the faster $\chi(T)$ increases with temperature.

The low-temperature regime of the universality class of spin chains with a rotationally and translationally invariant Hamiltonian (to which also the 3-leg ladders belong) is determined by only two parameters, v and T_0. However, the determination of v and T_0 for the 3-leg ladder is difficult. QMC calculations cannot be performed down to low enough temperatures such that a fit to the above form (3) gives reliable estimates for v and T_0. Especially T_0 is considerably underestimated in all cases.

To overcome this problem we first map the 3-leg ladder to a J_1-J_2 chain and then study the one-to-one mapping of this J_1-J_2 chain to the WZW model: $(J_1, J_2)\leftrightarrow(v, T_0)$. The mapping to J_1-J_2 chains is always possible since the low-T range is characterized by only two parameters which can be chosen as J_1, J_2 instead of v, T_0. The mapping of the 3-leg ladder to J_1-J_2 chains is done as follows. For small $J_{\parallel}/J_{\perp}$ we can use the third-order result for J_1 and J_2 [Eq. (2)], neglecting J_3, since J_3 is small. Otherwise we fit $\chi(T)$ of J_1-J_2 chains for low T to $\chi(T)$ of the 3-leg ladder (see Fig. 1) which gives estimates of the values J_1 and J_2 (see Table I).

The mapping $(J_1,J_2)\leftrightarrow(v,T_0)$ can be studied, using exact diagonalization methods. v and T_0 are determined by the finite-size scaling of the energy gap between the excited state $E(k=\pi,\ S_z=1)$ and the ground state $E(k=0,\ S_z=0)$:[13]

$$E(k=\pi,\ S_z=1)-E(k=0,\ S_z=0)$$
$$=\frac{\pi\ v}{L}\left(1-\frac{1}{2\ln(L/L_0)}+\frac{\ln(\ln(L/L_0)+1/2)}{4\ln^2(L/L_0)}\right), \tag{4}$$

where $E(k,S_z)$ is the lowest energy with wave vector k and z component of spin S_z for a chain of length L. L_0 is the characteristic scaling length of the chain. As a consequence

TABLE I. For low temperatures, 3-leg ladders can be mapped onto J_1-J_2 chains. The corresponding coupling constants, J_1 and J_2, are given for different $J_\parallel/J_\perp$. The spinon velocity v and the energy scale parameter T_0 for the 3-leg ladders are also listed. The value enclosed in brackets was obtained by fitting the ξ-data (Ref. 10) to Eq. (7).

$J_\parallel/J_\perp$	$J_1/J_\parallel$	$J_2/J_\parallel$	$v/J_\parallel$	$T_0/J_\parallel$
0	1	0	$\pi/2$	2.6
0.1	0.985	−0.033	1.61	1.64
0.2	0.961	−0.071	1.63	1.28
0.4	0.86	−0.17	1.63	0.78
0.6	0.76	−0.30	1.65	0.57
0.8	0.67	−0.47	1.73	0.47
1.0	0.61	−0.61	1.81	0.41[0.34]

of the equivalence of the imaginary time direction and the space direction, $L_0=v/T_0$. Fitting Eq. (4) for different lengths using exact diagonalization gives v as well as T_0. The results for different fractions J_2/J_1 are plotted in Fig. 3.

An alternate possibility to determine v and T_0 is to map the J_1-J_2 chains onto the $O(3)$ nonlinear σ model with $\theta=\pi$. For the coupling constant g one finds $g=4(1-4J_2/J_1)^{-1/2}$.[14] Therefore the spinon velocity can be written as

$$v=\frac{\pi J_1}{2}\sqrt{1-\frac{4J_2}{J_1}}. \tag{5}$$

Logarithmic corrections, on the other hand, depend on a mass scale Λ, which is generated dynamically in the σ model, and for small g, $\Lambda=1/a\exp(-2\pi/g)$, where a is the lattice spacing.[15] Since $T_0\propto\Lambda$,

$$T_0\propto\exp\left[-\frac{\pi}{2}\sqrt{1-\frac{4J_2}{J_1}}\right]. \tag{6}$$

The results for v and T_0 [Eqs. (5) and (6)] are plotted in Fig. 3 together with those obtained by finite-size scaling.

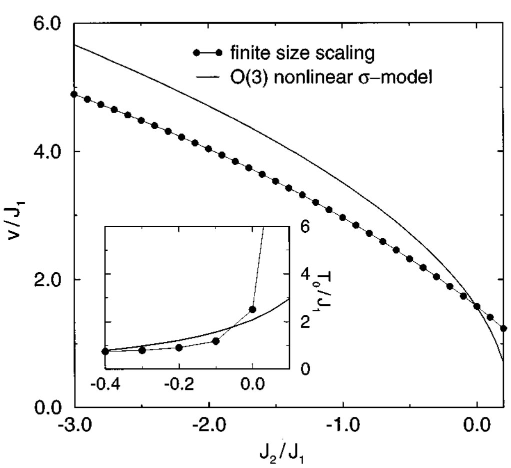

FIG. 3. Spinon velocity, v, and energy scale parameter, T_0, of the J_1-J_2 chains, determined by finite-size scaling analysis (circles) respectively by mapping to the $O(3)$-nonlinear σ model.

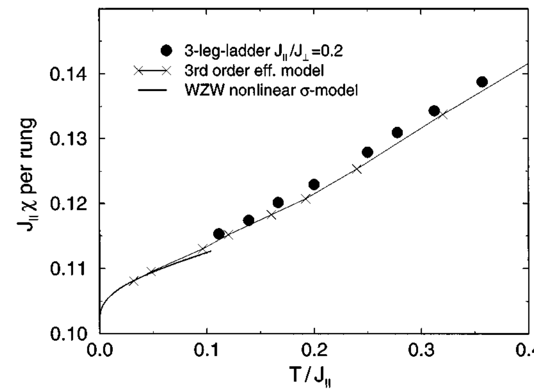

FIG. 4. Susceptibility of the 3-leg ladder with $J_\parallel/J_\perp=0.2$ and its effective models. The error bars are smaller or in order of the symbols.

In Table I, the estimated values v,T_0 (following the above-described procedure) are given for various 3-leg ladders. The spinon velocity increases, while T_0 decreases with increasing $J_\parallel/J_\perp$.

The values for v and T_0 can now be put back into Eq. (3) which gives the low-temperature susceptibilities of the corresponding 3-leg ladders. This is shown in the example of $J_\parallel/J_\perp=0.2$ in Fig. 4. Together with the QMC data for the 3-leg ladder itself and its third-order effective model, we get the susceptibility for the 3-leg ladder with good precision on the whole temperature range from zero temperature to high T.

Greven *et al.* recently calculated the correlation length ξ of isotropic ladders,[10] using also the QMC loop algorithm. For $T\ll T_0$ the inverse of the correlation length in the WZW-model can be written as[16]

$$\frac{1}{\xi(T)}\approx T\left(2-\frac{1}{\ln(T_0/T)}+\frac{1}{2}\frac{\ln(\ln(T_0/T)+1/2)}{\ln^2(T_0/T)}\right). \tag{7}$$

Fitting the data[10] for $n_l=3$ to the above form [Eq. (7)] also gives an estimate of T_0. In the isotropic case we find $T_0=0.34J_\parallel$ which is in good agreement with our result (see Table I). For the 5-leg-ladder T_0 is already $\lesssim 0.1J_\parallel$.

Finally, we examine the static structure factor $C(\pi,\pi)$, defined by (N_s=number of sites)

$$C(k_x,k_y)=\frac{1}{N_s}\sum_{i,j,\tau,\tau'} e^{ik_x(i-j)+ik_y(\tau-\tau')}\langle\vec{S}_{i,\tau}\cdot\vec{S}_{j,\tau'}\rangle$$

and show that it can be calculated from the effective model without introducing additional physical parameters. $C(\pi,\pi)$ can be written as $\Sigma_{i,j}(-1)^{i+j}\langle\vec{S}_i^{\rm st}\cdot\vec{S}_j^{\rm st}\rangle/3L$, where $\vec{S}_i^{\rm st}=\vec{S}_{i,1}-\vec{S}_{i,2}+\vec{S}_{i,3}$ is the staggered spin of one rung. In the limit $J_\parallel=0$ the correlations of the staggered rung spins are simply related to those of the uniform rung spins by

$$\langle\vec{S}_i^{\rm st}\cdot\vec{S}_j^{\rm st}\rangle_{i\neq j}=\lambda\langle\vec{S}_i^{\rm tot}\cdot\vec{S}_j^{\rm tot}\rangle_{i\neq j}, \tag{8}$$

with $\lambda=25/9$ for all temperatures, where only the states in $\mathcal{M}$ are relevant. For $J_\parallel\neq 0$ the ‘‘wave function’’ of the spin-$\frac{1}{2}$ degree of freedom at each rung is spread out over a certain number of unit cells. On one hand, this gives rise to the longer range interactions, described above, and on the other

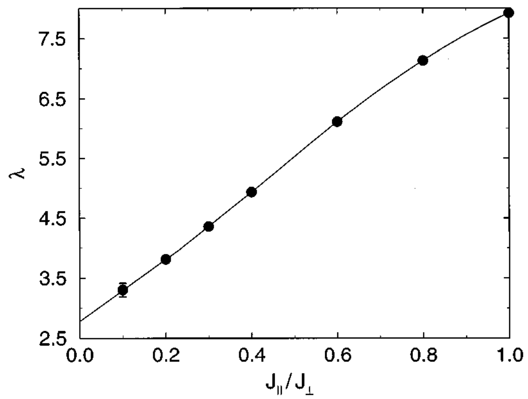

FIG. 5. The fraction $\lambda=\langle\vec{S}_i^{st}\cdot\vec{S}_j^{st}\rangle/\langle\vec{S}_i^{tot}\cdot\vec{S}_j^{tot}\rangle$ at $|i-j|\gg 1$ for different $J_\parallel/J_\perp$.

hand, it affects the correlations $\langle\vec{S}_i^{st}\cdot\vec{S}_j^{st}\rangle$ and $\langle\vec{S}_i^{tot}\cdot\vec{S}_j^{tot}\rangle$. For large distances $|i-j|\gg 1$, however, $\langle\vec{S}_i^{st}\cdot\vec{S}_j^{st}\rangle$ and $\langle\vec{S}_i^{tot}\cdot\vec{S}_j^{tot}\rangle$ are still related by Eq. (8) but with a renormalized value of λ.

Here, we calculate λ numerically, using QMC simulations. The values are plotted in Fig. 5 for different $J_\parallel/J_\perp$ and extrapolating to $J_\parallel=0$ leads to a value $\lambda=2.78$ which agrees with the analytical result 25/9. At low T, the correlation length $\xi\gg 1$ and $C(\pi,\pi)$, as well as $C(\pi,0)=\Sigma_{i,j}(-1)^{i+j}\langle\vec{S}_i^{tot}\cdot\vec{S}_j^{tot}\rangle/3L$ are dominated by correlations with $|i-j|\gg 1$. Additionally, $C(\pi,0)$ per rung of the 3-leg ladder differs only slightly from $C(\pi)$ of the single chain. Consequently at low temperature, $C(\pi,\pi)_{\text{3-leg}}=\lambda C(\pi,0)_{\text{3-leg}}\approx\lambda C(\pi)_{\text{single ch.}}/3$. Greven *et al.* have calculated $C(\pi,\pi)_{\text{3-leg}}$ for $J_\parallel=J_\perp$ and $C(\pi)_{\text{single ch.}}$.[10] From their data we determine $C(\pi,\pi)_{\text{3-leg}}/C(\pi)_{\text{single ch.}}=2.55$, which is in good agreement with our value $\lambda/3=2.64$ (see Fig. 5).

The above considerations can be generalized to an arbitrary odd-leg ladder with n_l legs. There are no qualitative differences. The overall AF quasilong-range order, however, increases with increasing n_l. Therefore, especially the ratio $|J_2/J_1|$ of the effective Hamiltonian H_{eff} is larger. The logarithmic corrections increase markedly (T_0 decreases) and the $T\to 0$ behavior sets in at lower temperature as n_l increases. The zero temperature value $\chi(0)$, on the other hand, is almost independent of n_l. This implies that the spinon velocity of odd-leg ladders depends only slightly on the number of legs.

In conclusion, we have proposed an effective spin-$\frac{1}{2}$ chain model which describes the low-energy properties of odd-leg ladders. The temperature dependence of χ, ξ, and $C(\pi,\pi)$ for the effective system is shown to be consistent with that of the original model at low enough temperatures. The effective model requires two parameters, e.g., a spinon velocity v and an energy scale, T_0. With an increasing number of legs, v does not change, but T_0 decreases rapidly. The exchange interactions of the corresponding effective model become longer ranged, and antiferromagnetic correlations are enhanced.

The calculations were performed on the Intel Paragon of the ETH Zürich. The support of the Schweizerischer Nationalfond was gratefully acknowledged.

[1] E. Dagotto, J. Riera, and D. J. Scalapino, Phys. Rev. B **45**, 5744 (1992).
[2] For a review, see E. Dagotto and T. M. Rice, Science **271**, 618 (1996).
[3] D. C. Johnston, J. W. Johnson, D. P. Goshorn, and A. J. Jacobson, Phys. Rev. B **35**, 219 (1987).
[4] Z. Hiroi, M. Azuma, M. Takano, and Y. Bando, J. Solid State Chem. **95**, 230 (1991); M. Azuma *et al.*, Phys. Rev. Lett. **73**, 3463 (1994).
[5] In comparison with the case of the 5-leg ladder, where to second order in $J_\parallel/J_\perp$, we get $a_{1,1}=1.0169$, $a_{1,2}=-0.2371$, $a_{2,1}=0$, $a_{2,2}=-0.5697$.
[6] B. Frischmuth, B. Ammon, and M. Troyer, Phys. Rev. B **54**, R3714 (1996).
[7] H. G. Evertz, G. Lana, and M. Marcu, Phys. Rev. Lett. **70**, 875 (1993).
[8] H. G. Evertz and M. Marcu, Nucl. Phys. B **30**, 277 (1993).
[9] U. J. Wiese and H. P. Ying, Z. Phys. B **93**, 147 (1994).
[10] M. Greven, R. J. Birgeneau, and U.-J. Wiese (unpublished).
[11] The entropy is calculated numerically from the internal energy, using $S(\beta_2)-S(\beta_1)=\beta_2U(\beta_2)-\beta_1U(\beta_1)-\int_{\beta_1}^{\beta_2}U(\beta)d\beta$, where $\beta=1/T$.
[12] S. Eggert, I. Affleck, and M. Takahashi, Phys. Rev. Lett. **73**, 332 (1994).
[13] K. Nomura, Phys. Rev. B **48**, 16 814 (1993).
[14] I. Affleck, in *Field, Strings, and Critical Phenomena,* edited by E. Brezin and J. Zinn-Justin, Les Houches Lecture Notes (North-Holland, Amsterdam, 1988).
[15] G. Sierra, J. Math. Phys. (N.Y.) **A29**, 3299 (1996).
[16] K. Nomura and M. Yamada, Phys. Rev. B **43**, 8217 (1991).