Ground-state properties of two-dimensional dimerized Heisenberg models

J. Sirker,* A. Klümper,† and K. Hamacher‡
Theoretische Physik I, Universität Dortmund, Otto-Hahn-Strasse 4, D-44221 Dortmund, Germany
(Received 27 June 2001; revised manuscript received 20 November 2001; published 15 March 2002)

The purpose of this paper is to investigate the ground-state properties of two-dimensional Heisenberg models on a square lattice with a given dimerization. Our aim is threefold. First, we want to investigate the dimensional transition from two to one dimension for three models consisting of weakly coupled chains for large dimerizations. Simple scaling arguments show that the interchain coupling is always relevant. The ground states of two of these models therefore have one-dimensional nature only at the decoupling point. The third considered model is more complicated, because it contains additional relevant intrachain couplings leading to a gap, as shown by scaling arguments and numerical investigations. Second, we investigate at which point the dimerization destroys the Néel-ordered ground state of the isotropic model. Within a mapping to a nonlinear sigma model and linear spin-wave theory (LSWT), we conclude that the stability of the Néel-ordered state depends on the microscopic details of the model. Third, the considered models also can be regarded as effective models for a spin system with spin-phonon coupling. This leads to the question if a spin-Peierls transition, i.e., a gain of total energy due to lattice distortion, is possible. LSWT shows that such a transition is possible under certain conditions, leading to a coexistence of long-range order and spin-Peierls dimerization. We also find that the gain of magnetic energy is largest for a stairlike distortion of the lattice.

DOI: 10.1103/PhysRevB.65.134409 PACS number(s): 75.10.Jm, 75.50.Ee, 75.40.Cx

I. INTRODUCTION

For many years there has been considerable interest, both experimentally and theoretically, in the subject of low-dimensional quantum spin systems, because their properties are strongly affected by quantum fluctuations. The generic model to theoretically study such systems is the well-known Heisenberg model.

In one spatial dimension the model with nearest-neighbor exchange of spin-1/2 objects, known to be exactly solvable by the Bethe ansatz,[1] shows an algebraic decay of its correlation functions at zero temperature and constitutes thereby a quantum critical system. For arbitrary spin s, Haldane[2] has mapped the spin chain onto a nonlinear sigma (NLσ) model with a topological term for half-integer s and without such a term for integer s. From this result he conjectured that half-integer spin chains are critical whereas integer spin chains have a gap, a scenario that is well established by now. Another interesting aspect of the spin-1/2 Heisenberg chain is its instability towards a structural transition known as the spin-Peierls transition.[3]

Much less is known for the isotropic two-dimensional Heisenberg antiferromagnet with nearest-neighbor exchange on a square lattice. Contrary to one dimension no exact solution is available in any limit. Linear spin-wave theory (LSWT), which does not work in one dimension because of infrared divergencies, is applicable and predicts a Néel-ordered ground state for the spin-1/2 case, but with a magnetic moment reduced to nearly 50% of its classical value.[4] This result is also supported, qualitatively and also quantitatively, by numerical work.[5,6] For $s \geqslant 1$ Dyson, Lieb, and Simon[7] proved a theorem, which shows that the ground state is Néel ordered. As in one dimension it is also possible to map the system onto a NLσ model. From a renormalization-group (RG) treatment it is known[8] that this model exhibits in $2+1$ dimensions a nontrivial critical point g_c, which separates a phase with Néel-like long-range order ($g<g_c$) from a quantum disordered phase ($g>g_c$) at $T=0$. It has been shown that there is excellent agreement between theoretical results for this model and experimental measurements on La_2CuO_4 in the low-temperature regime if $g<g_c$ is assumed.[9] An interesting problem has been the question of whether there is also a topological term in two dimensions, which was finally answered by Haldane[10] who concluded that such a term is always absent if the order parameter field is smooth on the scale of the lattice spacing. However, there are tunneling events, which are crucial for an understanding of the disordered phase.[11]

In this work we want to consider two-dimensional Heisenberg models on a square lattice with a given alternation of the coupling between nearest-neighbor spins. In each spatial direction the coupling should be changing from bond to bond between $J(1+\delta)$ and $J(1-\delta)$ with $J>0$ and $\delta \in [0,1]$ so that the coupling is always antiferromagnetic. There are three topologically different possibilities (see Figs. 1–3) for arranging such ''dimerized chains'' on a square lattice if periodicity in each spatial direction is assumed.

These systems are described by the following Hamiltonian:

$$H = J \sum_i \left[1+(-1)^{i(+j)}\delta\right] \boldsymbol{S}_{i,j} \cdot \boldsymbol{S}_{i+1,j} + J \sum_j \left[1+(-1)^{j(+i)}\delta\right] \boldsymbol{S}_{i,j} \cdot \boldsymbol{S}_{i,j+1}, \qquad (1)$$

where $\boldsymbol{S}_{i,j}$ denotes the spin operator acting on the lattice site (i,j). Choosing both exponents equal to $i+j$ leads to the model shown in Fig. 1, whereas setting the first one equal to i and the second one to $i+j$ or vice versa leads to the model shown in Fig. 2. The third considered model (see Fig. 3) is described by Eq. (1) with the first exponent set to i and the second set to j.

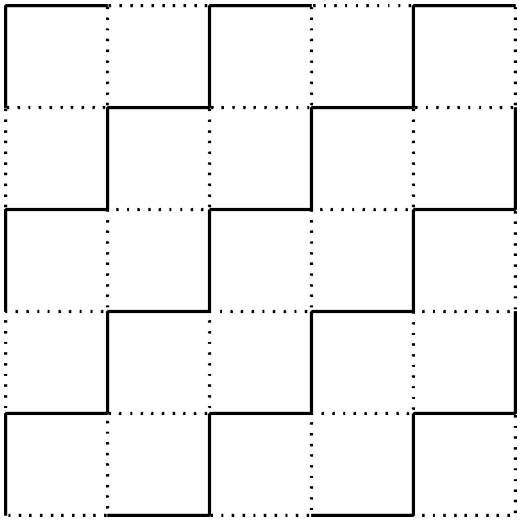

FIG. 1. (Stair model). A thick solid line indicates a strong bond $J(1+\delta)$ and a dashed line a weak bond with strength $J(1-\delta)$. This distortion of the lattice is caused by one transversal phonon with wave vector (π,π).

The models in Figs. 1 and 2, which we will refer to as the stair model and meander model, decouple into spin chains at $\delta=1$. This means that there is a transition from two to one dimension depending on the value of the dimerization δ. Because a model with a coupling J_x in the x direction and a coupling J_y in the y direction (see Fig. 4) is the simplest model showing such a transition, we want to reexamine this model although it has been studied intensively before. The model in Fig. 3 is different from the other three models, because it decouples into plaquettes consisting of four spins for $\delta=1$.

The dimerized models can also be regarded as effective models for a spin system with a spin-phonon coupling treated adiabatically. In such a system the exchange coupling J between nearest neighbors depends linearly on their distance. This is expressed through the deformation parameter of the horizontal bond extending from site (i,j) to the right

$$\delta^h(i,j)=\frac{1}{J}\sum_{\boldsymbol{k},s}\lambda_{\boldsymbol{k},s}(\langle \boldsymbol{u}_{i,j}(\boldsymbol{k},s)\rangle-\langle \boldsymbol{u}_{i+1,j}(\boldsymbol{k},s)\rangle)_{\parallel} \quad (2)$$

with the deformation parameter of the vertical bond $\delta^v(i,j)$ defined analogously. Here $\lambda_{\boldsymbol{k},s}$ is the microscopic spin-phonon coupling constant and $\boldsymbol{u}_{i,j}(\boldsymbol{k},s)$ the local displacement of the atom at the position (i,j) with respect to the phonon wave vector $\boldsymbol{k}$ and branch s. In the considered models δ^h and δ^v are equal to $\pm\delta$. Note that the lattice distortion is static due to the mean-field approach leading to a classical elastic energy.

In Sec. II, we study the models, which decouple into chains at $\delta=1$. We address the question of whether there is already a transition from two- to one-dimensional behavior

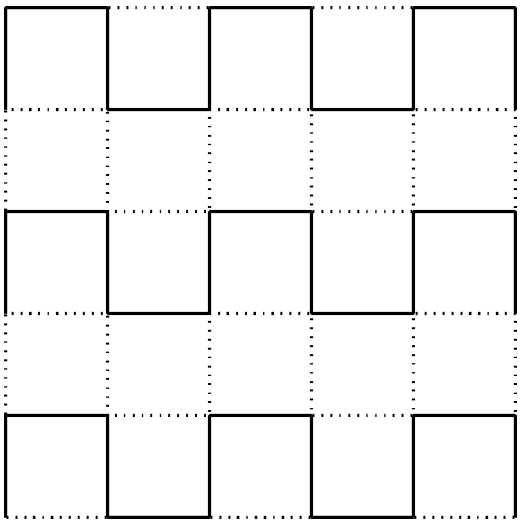

FIG. 2. (Meander model). Three phonons, a longitudinal and a transversal (π,π) phonon together with a longitudinal $(0,\pi)$ phonon.

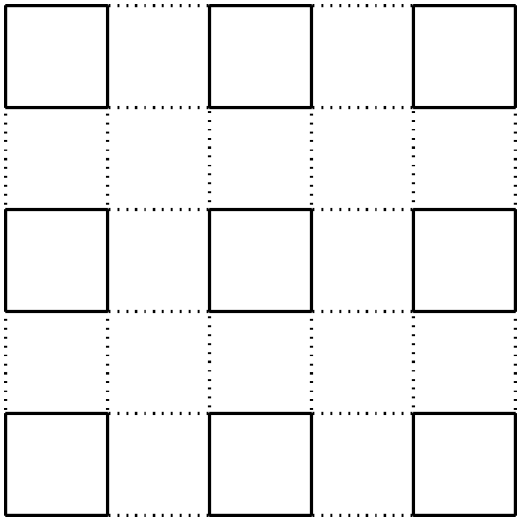

FIG. 3. (Plaquette model). Two longitudinal phonons, one with wave vector $(\pi,0)$, the other with $(0,\pi)$.

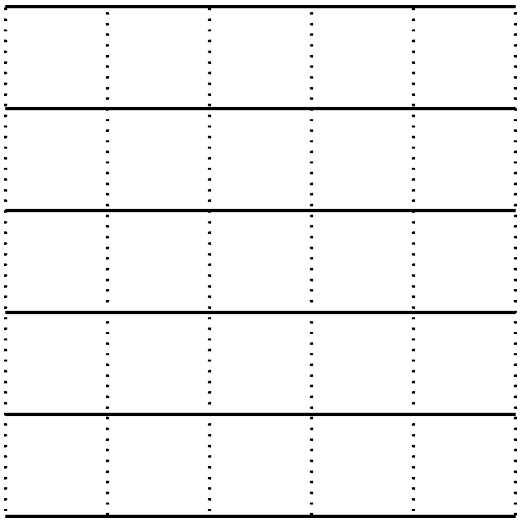

FIG. 4. $(J_x/J_y$ model). Two longitudinal phonons, one with wave vector $(-q,0)$, the other with $(0,+q)$, where q is infinitesimal $(q=2\pi/\sqrt{N}a)$.

at a δ smaller than 1 on the basis of some scaling arguments. Because the situation in the meander model is much more complicated than in the other models due to third-nearest-neighbor (NNNN) couplings, we show in Sec. III numerical results from density-matrix renormalization group (DMRG) and transfer-matrix DMRG (TMRG) to confirm the conclusions drawn from the simple scaling arguments in Sec. II. In Sec. IV, we show that it is possible to map all models onto a $(2+1)$-dimensional NLσ model. We use the known RG results for this model to discuss the magnetic properties of the spin models. In Sec. V, LSWT is applied to support the picture from the RG arguments and to determine a value for the critical dimerization δ_c, where the magnetic order vanishes. Also from this, we get a condition for the spin-Peierls transition and an answer to the question of which structure is energetically prefered. Sections IV and V consist of separate subsections for each model. However, in Sec. V we have interchanged the order of the first two subsections in comparison with Sec. IV to keep calculations as simple as possible. In Sec. VI we discuss our results and give some conclusions.

II. SCALING ARGUMENTS

At $\delta=1-\epsilon$ with $\epsilon \ll 1$, the models in Figs. 1, 2, 4 consist of weakly coupled Heisenberg chains. Such a Heisenberg chain with $s=1/2$ is a critical system and the additional weak interchain and intrachain couplings are small perturbations of this critical system. If we pick two such chains from each model with the corresponding interchain coupling proportional to ϵ, we can determine the relevance of the perturbation by calculating the energy-energy correlation function and from this the scaling dimension of the perturbation operator. Let us start with the simplest case, the J_x/J_y model, where $J_y=J(1-\delta)$ and $J_x=J(1+\delta)$. The Hamiltonian of the weak interchain coupling is given by

$$\tilde{H}=J_y\sum_r \boldsymbol{S}_r^1\boldsymbol{S}_r^2, \tag{3}$$

where the upper index labels the two chains. The energy-energy correlation function of this perturbation can be calculated as follows:

$$\begin{aligned}\langle\sigma_0\sigma_r\rangle_0 &= J_y^2\sum_{\alpha,\beta}\langle S_0^{\alpha,1}S_0^{\alpha,2}S_r^{\beta,1}S_r^{\beta,2}\rangle_0\\ &= J_y^2\sum_{\alpha}\langle S_0^{\alpha,1}S_r^{\alpha,1}\rangle\langle S_0^{\alpha,2}S_r^{\alpha,2}\rangle\\ &= \frac{J_y^2}{3}\langle \boldsymbol{S}_0\cdot\boldsymbol{S}_r\rangle^2=\frac{J_y^2}{3}\left(\frac{(-1)^r}{r}\right)^2,\end{aligned} \tag{4}$$

where $\sigma_r=J_y\boldsymbol{S}_r^1\cdot\boldsymbol{S}_r^2$ and α, β label the components of the spin operator. The subscript "0" represents the calculation in the case of vanishing interchain coupling and in the last relation the known result for the spin correlation function of the homogenous Heisenberg chain is used.[12] From conformal field theory it is known that this correlation function decays algebraically as $1/r^{2x}$, where x is the scaling dimension when we disregard multiplicative logarithmic corrections. We therefore conclude that the scaling dimension of the interchain coupling is $x=1$ and represents a relevant perturbation of the critical system. From scaling relations we find, again ignoring logarithmic corrections, the ground-state energy E_0 of this system behaving as

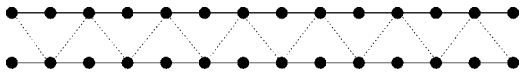

FIG. 5. Two chains from the stair model with the corresponding interchain coupling

$$E_0\propto J_y^{d/(d-x)}=J_y^2 \tag{5}$$

and a gap Δ is opening with

$$\Delta\propto|J_y|^{1/(d-x)}=|J_y|, \tag{6}$$

where $d=1+1$ is the dimension of the corresponding classical model. The existence of a gap for the two-leg ladder has also been shown numerically.[13] In general, there seems to be a gap for an even number of coupled chains, whereas a system with an odd number of chains is gapless. However, it is not possible to determine from scaling arguments if there is a gap or not for an infinite number of arbitrarily weakly coupled chains. Nevertheless, the relevance of the interchain coupling clearly shows that the system scales away from decoupled chains and therefore even at very large, however, not perfect dimerization does not behave as decoupled chains. We conclude that the ground state of this model has two-dimensional nature if $J_y\neq 0$ as has been stated before.[14]

Also we can pick two chains out of the stair model and after smoothing the chains, we get the configuration shown in Fig. 5. Here the interchain coupling is described by the Hamiltonian

$$\tilde{H}=\tilde{J}\sum_{r=1}^{N/2}\boldsymbol{S}_{2r}^1(\boldsymbol{S}_{2r-1}^2+\boldsymbol{S}_{2r+1}^2) \tag{7}$$

and by calculating again the energy-energy correlation function, we find that this perturbation also has scaling dimension $x=1$. That leads to the same conclusions as in the J_x/J_y model. The situation is much more complicated in the meander model, because there is not only interchain coupling, but also a coupling between third-nearest neighbors within every chain as shown in Fig. 6. First, we want to investigate the intrachain coupling. The operator of this perturbation is given by

$$\tilde{H}=\tilde{J}\sum_{r=0}^{N/2}\boldsymbol{S}_{2r}\cdot\boldsymbol{S}_{2r+3} \tag{8}$$

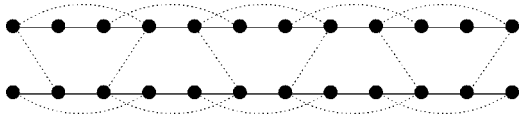

FIG. 6. Two smooth chains from the meander model.

and we can calculate the corresponding energy-energy correlation function

$$\langle \sigma_0 \sigma_r \rangle_0 = \tilde{J}^2 \langle \boldsymbol{S}_0 \cdot \boldsymbol{S}_3 \cdot \boldsymbol{S}_{2r} \cdot \boldsymbol{S}_{2r+3} \rangle_0 \propto \frac{(-1)^{2r}}{2r}, \qquad (9)$$

where the value $x=1/2$ of the scaling dimension of the singlet operator $\boldsymbol{S}_{2r} \cdot \boldsymbol{S}_{2r+3}$ has been employed.[12] This means that the NNNN coupling is relevant. By simply applying the scaling relations, we conclude that it destroys criticality and a gap opens with $\Delta \propto |\tilde{J}|^{2/3}$. But there might be some doubt if this scenario is correct, because if we suggest a short-range Néel order on the critical chain the NNNN coupling is not frustrating. On the other hand, if the NNNN coupling is as strong as the NN coupling, this chain is equivalent to a two-leg ladder, which does show a gap. We therefore have used the transfer-matrix DMRG and the standard DMRG to test numerically the predictions from scaling. Before we enter the numerical part, we have to analyze the other perturbation in the meander model caused by the interchain coupling. It turns out that this is again relevant with a scaling dimension $x=1$ as in the other two models.

The conclusion from scaling arguments is therefore that the J_x/J_y model and the stair model show one-dimensional behavior only at the decoupling point. Because in the meander model the intrachain is more relevant than the interchain coupling, the scaling arguments suggest the existence of a disordered phase between the decoupling point and the phase with two-dimensional antiferromagnetic long-range order. This will be further investigated in Secs. III and IV.

III. NUMERICAL INVESTIGATIONS

To prove the scaling argument for the NNNN coupling in the meander model, we have used two numerical methods. The first one is the so-called transfer-matrix DMRG (TMRG), which combines White's DMRG idea[15] with the transfer-matrix approach.[16] This method has been applied to different quantum chains before[17–19] and yields very accurate results for finite temperature. It is particularly suited, because the thermodynamic limit in quantum space can be performed exactly. Before we state the results, we write down the considered Hamiltonian explicitly:

$$H = J_1 \sum_{r=0}^{N} \boldsymbol{S}_r \cdot \boldsymbol{S}_{r+1} + J_2 \sum_{r=0}^{N/2} \boldsymbol{S}_{2r} \cdot \boldsymbol{S}_{2r+3}. \qquad (10)$$

The relevant case in this context is a NNNN coupling J_2, which is much smaller than the NN coupling J_1.

The free energy as calculated with the TMRG for $J_2/J_1=0.25$ is shown in Fig. 7. We can now determine if there is a gap or not, because we know from scaling relations that in the low-temperature limit the free energy of a gapless, critical system scales as $f(T) \propto e_0 - aT^2$ with e_0 being the ground-state energy, whereas $f(T) \propto e_0 - aT^{3/2} e^{-\Delta/T}$ if there is a gap. We tried to fit a quadratic function to the data and noted that this is impossible, whereas a function as expected for the gapped case fits perfectly with values e_0

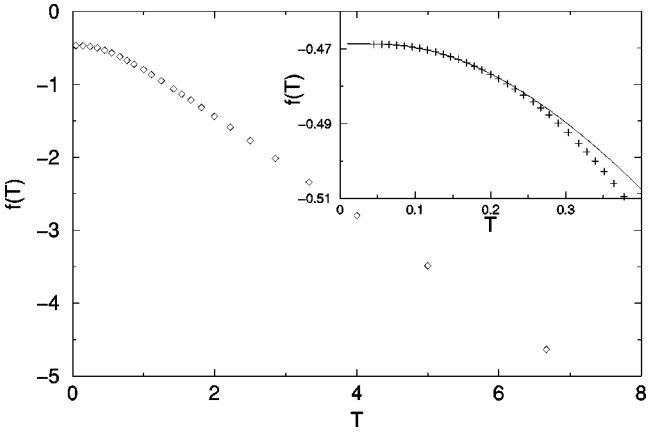

FIG. 7. Free energy for the Heisenberg chain with NNNN coupling calculated by TMRG with $J_2/J_1=0.25$, $m=40$ states kept in the DMRG, and a Trotter parameter of $\epsilon=\beta/M=0.05$. The inset shows a low-temperature fit with $f \propto e_0 - aT^{3/2} e^{-\Delta/T}$ and $T \in [0,0.2]$.

$=-0.46873 \pm 0.00002$, $a=0.29 \pm 0.03$, $\Delta=0.23 \pm 0.02$ and errors, which are determined by a variation of the fit region (see inset of Fig. 7).

This means that at this strength the NNNN coupling has really destroyed criticality. To test the scaling argument further, we also applied a standard DMRG program to this problem. When using the same parameters $J_2/J_1=0.25$, we find a gap depending on the length of the chain as shown in Fig. 8. An extrapolation $L \to \infty$ then leads to a gap $\Delta_{\mathrm{PBC}} = 0.23652 \pm 0.00064$ and a ground-state energy $e_{\mathrm{PBC}} = -0.46841 \pm 0.00816$ if periodic boundary conditions (PBC's) are applied. For open boundary conditions (OBC's), we find a gap $\Delta_{\mathrm{OBC}}=0.23834 \pm 0.00027$ and a ground-state energy $e_{\mathrm{OBC}}=-0.46843 \pm 0.00003$. Consequently, there is a good agreement between the numerical results from the two different methods. Up to now, we have only stated that the

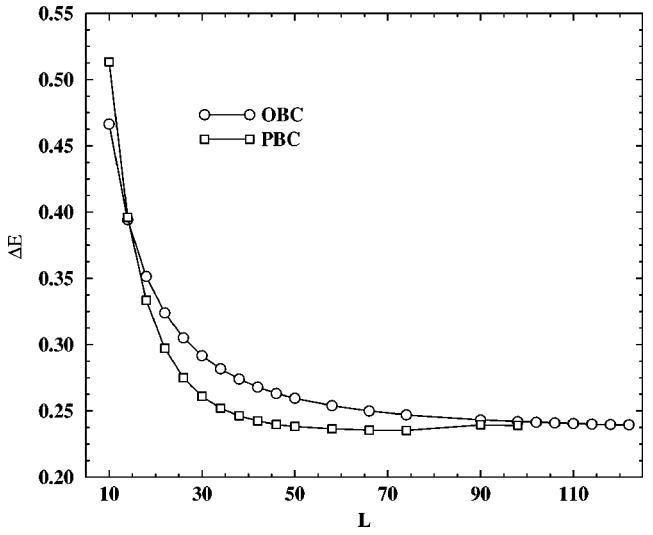

FIG. 8. DMRG calculation of the gap ΔE for finite chains with length L for open and periodic boundary conditions using an extrapolation in the number of states m. The lines are guides to the eye.

system has a gap for one special choice of parameters. Because the infinite chain with $J_2=0$ is a critical system, we can use the RG to study the behavior of the free energy depending on the length of the chain and of the NNNN coupling J_2. In general, we can linearize the RG transformation in the vicinity of a critical Hamiltonian, which is a fixed point of the RG flow, and find that the free energy per lattice site for a classical system scales as $f(g_1,\ldots,g_n)=b^{-ld}f(b^{l\lambda_1}g_1,\ldots,b^{l\lambda_n}g_n)$ if the RG is applied l times. Here g_i denotes a linear scaling field, λ_i is the eigenvalue of the RG transformation, and b is the scaling factor. Because the quantum chain with length L is equivalent to a classical system with volume $V=L\times\beta$, with β being the inverse temperature, the dimension d is equal to 2 and the relevant scaling fields at $T=0$ are $1/L$ and J_2. It follows that

$$f(L,J_2)=b^{-ld}f\left(b^{\lambda_1 l}\frac{1}{L},b^{\lambda_2 l}J_2\right) \tag{11}$$

and by choosing $b^{\lambda_1 l}=L$ we get

$$f(L,J_2)=\left(\frac{1}{L}\right)^{d/\lambda_1}f\left(1,\frac{J_2}{L^{-\lambda_2/\lambda_1}}\right). \tag{12}$$

At $J_2=0$ this reduces to $f(L,0)=\text{const}L^{-d/\lambda_1}$ and because the ground-state energy per lattice site scales as L^{-2}, we conclude that $\lambda_1=1$.

By setting $b^{\lambda_2 l}=J_2^{-1}$ we find the relation

$$f(L,J_2)=J_2^{d/\lambda_2}f(L^{-1}J_2^{-\lambda_1/\lambda_2},1). \tag{13}$$

When inserting the known result $\lambda_2=3/2$, we can state that there must exist an universal scaling function Φ with

$$J_2^{-4/3}f(L,J_2)=\Phi(L^{-1}J_2^{-2/3}). \tag{14}$$

We can do similar calculations for the gap Δ and get from $\Delta(L,J_2)=b^{-l}\Delta(b^{\lambda_1 l}L^{-1},b^{\lambda_2 l}J_2)$ the scaling relation

$$J_2^{-2/3}\Delta(L,J_2)=\tilde{\Phi}(LJ_2^{2/3}). \tag{15}$$

To test this, we have applied the DMRG to 862 different chains with lengths up to 122 sites and $J_2\in[0.00005,0.8]$ (see Fig. 9). By these calculations the scaling relation (15) is confirmed in a convincing way. Note that practically all data points collapse on a one-dimensional manifold. Some minor deviations are noticeable and can be explained by higher order terms in the finite size scaling and an effective exponent 0.662 instead of 2/3 (see inset of Fig. 9). It is also possible to determine two scaling regions. For large lengths L of the chain the plotted function saturates, indicating that the relation $\Delta E\propto J_2^{2/3}$, derived from scaling arguments for the infinite chain, really holds. For small $LJ_2^{2/3}$ there is a linear regime, showing that the finite size gap proportional to $1/L$ is the dominant contribution in this region.

IV. MAPPING ONTO A NLσ MODEL

In this section, we want to discuss the possible transition from the magnetically ordered phase to a disordered phase driven by the dimerization δ by using the NLσ model as a low-energy effective theory. The easiest way to get a path integral for the considered models is the use of coherent states.[20–23] Spin coherent states $|n\rangle$ form an overcomplete basis set and are generated by a SU(2) rotation of the highest weight state $|s,s\rangle$

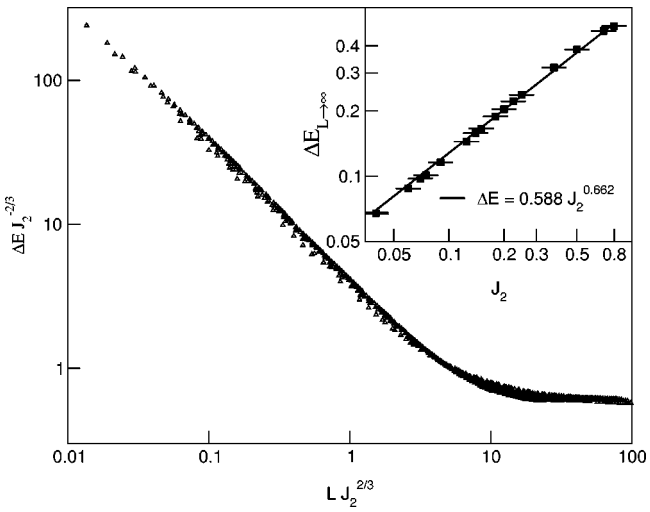

FIG. 9. DMRG results for 862 chains with different length L and NNNN coupling J_2. Two scaling regimes are visible as discussed in the text. The inset shows the gap extrapolated to the thermodynamic limit versus coupling J_2.

$$|\boldsymbol{n}\rangle := e^{i\phi(\boldsymbol{n}_0\times\boldsymbol{n})\boldsymbol{S}}|s,s>, \tag{16}$$

where $\boldsymbol{n}_0$ is an unit vector along the quantization axis and $\cos(\phi)=\boldsymbol{n}\cdot\boldsymbol{n}_0$. By using the Trotter formula and inserting the identity operator, the partition function can be written as $Z=\int D\boldsymbol{n}e^{-S_E[\boldsymbol{n}]}$ with an Euclidian action given by

$$S_E[\boldsymbol{n}]=-isS_{\text{WZ}}+\int_0^\beta dt\langle\boldsymbol{n}|H|\boldsymbol{n}\rangle. \tag{17}$$

S_{WZ} is a topological term (Wess-Zumino term), which arises from Berry phases and can be expressed as

$$S_{\text{WZ}}[\boldsymbol{n}]=\sum_{\boldsymbol{r}}\int_0^1 d\tau\int_0^\beta dt\,\boldsymbol{n}(\partial_t\boldsymbol{n}\times\partial_\tau\boldsymbol{n}) \tag{18}$$

with the boundary conditions $\boldsymbol{n}(t,0)=\boldsymbol{n}(t)$, $\boldsymbol{n}(t,1)=\boldsymbol{n}_0$, and $\boldsymbol{n}(0,\tau)=\boldsymbol{n}(\beta,\tau)$.

A. J_x/J_y model

With a_0 being the lattice constant, a site on the lattice G can be described by $i=o+a_0\Sigma_{a=1}^2 i_a\boldsymbol{e}^a$ with spatial unit vectors $\boldsymbol{e}^a$. Using this notation, which is more suitable for the following calculations than Eq. (1), the Hamiltonian of the model can be represented as

$$H=\sum_{i\in G}\{J_x\boldsymbol{S}(i)\boldsymbol{S}(i+a_0\boldsymbol{e}^x)+J_y\boldsymbol{S}(i)\boldsymbol{S}(i+a_0\boldsymbol{e}^y)\}. \tag{19}$$

We assume periodic boundary conditions and an even number of sites N in each direction. By defining $R=J_y/J_x$ and

using the coherent state relation $\langle \boldsymbol{n}|\boldsymbol{S}|\boldsymbol{n}\rangle = s\cdot\boldsymbol{n}$, the second term in Eq. (17) can now be easily calculated leading to the Euclidian action

$$S_E[\boldsymbol{n}] = -isS_{\mathrm{WZ}}[\boldsymbol{n}] + J_x s^2 \sum_{i\in G}\int_0^\beta dt\{\boldsymbol{n}(i)\boldsymbol{n}(i+a_0\boldsymbol{e}^x) + R\boldsymbol{n}(i)\boldsymbol{n}(i+a_0\boldsymbol{e}^y)\}. \tag{20}$$

Now we use the well-known ansatz[8,2]

$$\boldsymbol{n}(i) = p(i)\boldsymbol{m}(i)\cdot\sqrt{1-a_0^{2d}\boldsymbol{l}^2(i)} + a_0^d\boldsymbol{l}(i) \tag{21}$$

with

$$p(i) = (-1)^{\sum_{a=1}^{2} i_a}, \tag{22}$$

taking into account the short-range Néel order due to the antiferromagnetic exchange. Here $\boldsymbol{m}$ is the order parameter field and $\boldsymbol{l}$ represents the rapidly varying but small part. The constraint $\boldsymbol{n}^2=1$ leads to $\boldsymbol{m}^2=1$ and $\boldsymbol{m}\cdot\boldsymbol{l}=0$ and we will expand Eq. (21) up to quadratic order. Because the Wess-Zumino term is independent of the microscopic details of the spin model, we want to discuss this term more generally in d dimensions. Starting with Eq. (18) and using the ansatz (21) leads to

$$isS_{\mathrm{WZ}}[\boldsymbol{n}] = is\int_V d^dx\int_0^\beta dt\boldsymbol{l}(\boldsymbol{m}\times\partial_t\boldsymbol{m}) + i\theta\sum_{i_2,\ldots,i_d=1}^{N}(-1)^{i_2+\cdots+i_d}k(i_2,\ldots,i_d), \tag{23}$$

where $\theta = 2\pi s$ and $k(i_2,\ldots,i_d)$ is the winding number or Pontryagin index of the field $\boldsymbol{m}$ defined by

$$k(i_2,\ldots,i_d) = \frac{1}{4\pi}\int dx_1\int dt\,\partial_{x_1}\boldsymbol{m}(\boldsymbol{m}\times\partial_t\boldsymbol{m}). \tag{24}$$

In one spatial dimension the second term in Eq. (23) is responsible for the different physics of chains with integer and half-integer spin. If the $\boldsymbol{m}$ field is smooth, the integer-valued Pontryagin index $k(i_2,\ldots,i_d)$ must be a constant and hence this term cancels out in higher dimensions.[10] Note that we have to treat this term more carefully for the anisotropic models considered here, because the $\boldsymbol{m}$ field may no longer be smooth in each direction. Using the same ansatz (21) for the part of the action depending on the Hamiltonian of the system and integrating out the $\boldsymbol{l}$ field, results in an effective action for the low-lying excitations

$$S[\boldsymbol{m}] = \frac{\rho_s}{2}\int_V d^2x\int_0^\beta dt\left\{(\partial_x\boldsymbol{m})^2 + R(\partial_y\boldsymbol{m})^2 + \frac{1}{v_s^2}(\partial_t\boldsymbol{m})^2\right\} \tag{25}$$

with a spin stiffness $\rho_s = J_x s^2$, a transversal magnetic susceptibility $\chi_\perp = 4J_x a_0^2(1+R)$, and a spin-wave velocity $v_s = \sqrt{\rho_s\chi_\perp}$. We now rescale the imaginary time by $x_0 = v_s t$ leading to

$$S_{nl\sigma}[\boldsymbol{m}] = \frac{1}{2a_0 g_0}\int d^3x\{(\partial_{x_0}\boldsymbol{m})^2 + (\partial_x\boldsymbol{m})^2 + R(\partial_y\boldsymbol{m})^2\}, \tag{26}$$

where the dimensionless coupling g_0 is defined by

$$g_0 = \frac{2}{s}\sqrt{1+R}. \tag{27}$$

We want to discuss Eq. (26) following some arguments given by Affleck and Halperin.[24] Because the coupling in the y direction may be arbitrarily weak, a continuum representation may not be justified and we therefore rewrite the action as

$$S_{nl\sigma}[\boldsymbol{m}] = \frac{1}{2g_0}\sum_n\int d^2x\left\{(\partial_{x_0}\boldsymbol{m}_n)^2 + (\partial_x\boldsymbol{m}_n)^2 + \frac{R}{a_0^2}(m_{n+1}-m_n)^2\right\}. \tag{28}$$

After a rescaling $y' = y/\sqrt{R}$ the momentum space UV cutoff in the y direction is now smaller than the cutoff in the other directions. In a Wilsonian RG step, where the higher momentum modes are integrated out, only k_0 and k_x contribute, so that the RG is essentially two dimensional. Only if the momentum scale has been lowered so that also k_y has components in the shell, we have to switch to the three-dimensional RG. During the two-dimensional RG, we also have to consider the rescaling of the $\boldsymbol{m}$ field which is given by $\boldsymbol{m}_n \rightarrow (\Lambda'/\Lambda)^x\boldsymbol{m}_n$. Here Λ is the UV cutoff before renormalization and Λ' the reduced one after a RG step. x is the scaling dimension of the $\boldsymbol{m}$ field which is equal to 1/2 for the Heisenberg model.

The scale Λ', where we have to switch from two- to three-dimensional RG, is therefore given by the condition

$$R(\Lambda'/\Lambda)^{2x}\Lambda^2/2g_0 \approx \Lambda'^2/2g(\Lambda'). \tag{29}$$

Here $g(\Lambda')$ is the renormalized coupling constant when the momentum modes have been integrated out down to the cutoff Λ'. Note that the assumption that the $\boldsymbol{m}$ field is smooth on the scale of the lattice spacing is no longer justified in the y direction. Instead of canceling out, the second part of Eq. (23) leads to an independent winding number for each chain with topological angle $\theta=\pi$. Therefore g flows in two dimensions to the marginally stable fixed point $g_2(0)$ of the $s=1/2$ chain. As a consequence $g_0/g(\Lambda')$ is always of order one and Eq. (29) simplifies to $\Lambda' = R\Lambda$. The coupling constant $g(\Lambda')$ then acts as bare coupling constant for the three-dimensional RG flow. Therefore the ground state is ordered if $g(\Lambda')$ is smaller than the critical fixed point g_c of the three-dimensional RG, whereas it is disordered if $g(\Lambda') > g_c$. If even $g_2(0) < g_c$, the system is always ordered for a nonvanishing R. Numerical calculations using different

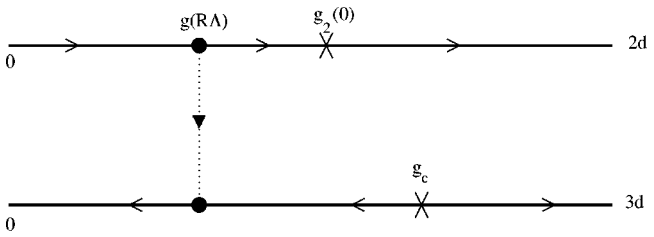

FIG. 10. RG flow for the J_x/J_y model.

methods[14,25,26] give strong evidence that this model orders for arbitrarily weak R, meaning in the language of RG that $g_2(0)$ seems to be smaller than g_c (see the corresponding flow diagram Fig. 10).

B. Stair model

We generalize the stair model to d dimensions assuming a hypercubic, bipartite lattice $G=A\oplus B$ with periodic boundary conditions, and an even number N of sites in each spatial direction. We do this, because the model reduces in one dimension to a dimerized chain and we want to compare the results, especially the topological terms, for the dimerized chain and for the two-dimensional model. Using the same notation as for the J_x/J_y model with the sum in Eq. (22) now running up to d, the Hamiltonian can be expressed by

$$H=J\sum_{i\in G}\sum_{a=1}^{d}[1+p(i)\delta]\boldsymbol{S}(i)\boldsymbol{S}(i+a_0\boldsymbol{e}^a). \tag{30}$$

Using again relation (17) and also the ansatz (21), an Euclidian action for this model depending on the unit vector field $\boldsymbol{m}$ and the orthogonal vector field $\boldsymbol{l}$ is derived. By the same arguments given in the chapter before, the Wess-Zumino term vanishes in spatial dimensions greater than 1 under the assumption that $\boldsymbol{m}$ is smooth on the scale of the lattice spacing, but is important in one dimension. Again, we integrate out the rapidly varying but small $\boldsymbol{l}$ fields. The result is an effective action

$$S[\boldsymbol{m}]=\frac{\rho_s}{2}\int_V d^dx\int_0^\beta dt\left[\gamma_s^{ab}(\partial_a\boldsymbol{m})(\partial_b\boldsymbol{m})+\frac{1}{v_s^2}(\partial_t\boldsymbol{m})^2\right] \tag{31}$$

with a spin stiffness $\rho_s=Js^2a_0^{2-d}(1-\delta^2/d)$, an induced anisotropy $\gamma_s^{ab}=\delta^{ab}-\delta^2(1-\delta^{ab})/(d-\delta^2)$, a transversal magnetic susceptibility $\chi_\perp=4Jda_0^d$ and a spinwave velocity $v_s=\sqrt{\rho_s\chi_\perp}$. But there arises also an imaginary contribution proportional to δ from the $\boldsymbol{l}$-field integration, which can be expressed as

$$\begin{aligned}&\frac{i\theta\delta}{d}\sum_{i_2,\ldots,i_d}\int dx_1\int dt\,\partial_{x_1}\boldsymbol{m}(\boldsymbol{m}\times\partial_t\boldsymbol{m})+\cdots\\&\quad+\frac{i\theta\delta}{d}\sum_{i_1,\ldots,i_{d-1}}\int dx_d\int dt\,\partial_{x_d}\boldsymbol{m}(\boldsymbol{m}\times\partial_t\boldsymbol{m})\\&=\frac{i\theta\delta}{d}\sum_{i_2,\ldots,i_d}k_1(i_2,\ldots,i_d)+\cdots\\&\quad+\frac{i\theta\delta}{d}\sum_{i_1,\ldots,i_{d-1}}k_d(i_1,\ldots,i_{d-1}).\end{aligned} \tag{32}$$

If the $\boldsymbol{m}$ field is smooth, every k_i must be a constant. Under this assumption the topological term simplifies to

$$S_{\text{top}}=\frac{i\theta\delta}{d}N^{d-1}\sum_{a=1}^{d}k_a. \tag{33}$$

In one dimension, where the stair model corresponds to the dimerized chain, we find a total topological contribution of $S_{\text{top}}=i\theta(1+\delta)k$ as has been calculated before.[27] Before we discuss the two topological terms (23) and (32) in two dimensions, we look at the additional anisotropy in the action (31) expressed by the matrix γ_s^{ab}. This matrix is symmetric and becomes the identity if δ goes to zero.

In two dimensions a 45° rotation diagonalizes this matrix and with $x_0=v_st$ the action of the two-dimensional model is given by

$$S_{\text{eff}}[\boldsymbol{m}]=\frac{1}{2}\int_\Omega d^3x\frac{\rho_s^a}{v_s}(\partial_a\boldsymbol{m})^2. \tag{34}$$

There are now different spin stiffnesses in the spatial directions given by

$$\rho_s^1=Js^2=\rho_s\frac{2}{2-\delta^2},\quad \rho_s^2=\rho_s\frac{2-2\delta^2}{2-\delta^2}, \tag{35}$$

and $\rho_s^0=\rho_s$. By a rescaling of the imaginary time, Eq. (34) is transformed into

$$S[\boldsymbol{m}]=\frac{1}{2a_0g_0}\int d^3\tilde{x}\{(\partial_{\tilde{x}}\boldsymbol{m})^2+(1-\delta^2)(\partial_{\tilde{y}}\boldsymbol{m})^2+(\partial_{x_0}\boldsymbol{m})^2\} \tag{36}$$

with a bare coupling given by

$$g_0=\frac{2\sqrt{2}}{s}. \tag{37}$$

Again the coupling in $\tilde{y}$ direction may be arbitrarily weak, and we therefore have to use a discrete version of Eq. (36) as for the J_x/J_y model. As a consequence a two-dimensional RG has to be used until the UV cutoff is lowered to $\Lambda'=(1-\delta^2)\Lambda$. The coupling $g(\Lambda')$ is then the bare coupling for the three-dimensional RG. Now, we have to remember that there are also two topological terms (23) and (33) present. Because we have stated that it is necessary to use a discrete representation instead of derivatives for the weak

couplings, neither the winding number in the x nor the winding number in the y direction is well defined any longer. We therefore have performed an alternative mapping to a NLσ model starting with a slightly modified version of this model, where the chains formed by strong bonds are smooth and along the x axis and the weak bonds form zigzag chains (see Fig. 5). The result is again an anisotropic NLσ model such as Eq. (26), but now without a topological contribution proportional to δ and with a winding number in the topological part of Eq. (23) calculated along the strong bonds. The situation is therefore exactly the same as in the J_x/J_y-model and if we accept $g_2(0)<g_c$ as an universal property, we conclude that the ground state of this model is always antiferromagnetically ordered for $\delta\in[0,1)$, and this order only vanishes at $\delta=1$, where the model consists of uncoupled critical chains.

C. Plaquette model

The model is described by the following Hamiltonian:

$$H=J\sum_{i,j}\{[1+p_x(i)\,\delta]\boldsymbol{S}_{i,j}\cdot\boldsymbol{S}_{i+1,j}+[1+p_y(i)\,\delta]\boldsymbol{S}_{i,j}\cdot\boldsymbol{S}_{i,j+1}\}, \tag{38}$$

where we have defined $p_x(i)=(-1)^{i_x}$ and $p_y(i)=(-1)^{i_y}$. Substituting Eq. (38) into Eq. (17), we derive again a path integral formulation. By using the same ansatz as before, we notice that the dimerization δ does only contribute in $(\partial_a\boldsymbol{m})^3\cdot\boldsymbol{l}$ and higher orders. This is not surprising, because the relevant low energy modes are not only near wave vectors (π,π) and $(0,0)$ but also near $(0,\pi)$ and $(\pi,0)$. We therefore generalize Eq. (21) in the following way:

$$\boldsymbol{n}(i)=p(i)\boldsymbol{m}(i)\sqrt{1-a_0^{2d}[\boldsymbol{l}_0(i)+p_x(i)\boldsymbol{l}_x(i)+p_y(i)\boldsymbol{l}_y(i)]^2}+a_0^d[\boldsymbol{l}_0(i)+p_x(i)\boldsymbol{l}_x(i)+p_y(i)\boldsymbol{l}_y(i)]. \tag{39}$$

The constraint $\boldsymbol{n}^2=1$ implies $\boldsymbol{m}^2=1$ and $\boldsymbol{m}\cdot\boldsymbol{l}_i=0$, where $\boldsymbol{l}_i$ denotes any of the three fluctuation fields. By an expansion up to quadratic order in $\boldsymbol{l}_i$, $\partial_a\boldsymbol{m}$, and $\partial_t\boldsymbol{m}$, we get again the effective action (25) but now $R=1$ and the other parameters are defined by $\rho_s=Js^2(1-\delta^2)$, $\chi_\perp=8Ja_0^2$ and $v_s=\sqrt{\rho_s\chi_\perp}$. By rescaling the imaginary time axis this is transformed to the standard NLσ model

$$S[\boldsymbol{m}]=\frac{1}{2a_0g_0}\int_\Omega d^3x(\partial_\mu\boldsymbol{m})(\partial^\mu\boldsymbol{m}) \tag{40}$$

with a bare coupling

$$g_0=\frac{2\sqrt{2}}{s}\,\frac{1}{\sqrt{1-\delta^2}}. \tag{41}$$

All topological terms vanish for this model and—different from the two models considered before—the action is isotropic in the spatial directions. So the 3D RG has to be used from the beginning and whether or not the model has an ordered ground state depends on whether or not $g_0<g_c$. Because $g_0\to\infty$ for $\delta\to1$, the order vanishes already before the plaquettes decouple. The precise value of $\delta_c\in(0,1)$ cannot be determined within the RG treatment.

D. Meander model

The Hamiltonian looks quite similar to Eq. (38), but instead of an alternation with $p_x(i)$ in the x direction there is one with $p(i)$. As a result the $\boldsymbol{l}_y$ field is unnecessary and can be left out. By using this reduced form of Eq. (39) and integrating out the $\boldsymbol{l}_0$ and $\boldsymbol{l}_x$ fields an effective theory is derived:

$$S_{\mathrm{eff}}[\boldsymbol{m}]=\frac{i\theta}{2}\delta\sum_{i=1}^{N}k_x(i)+\int_V d^2x\int_0^\beta dt\left\{\frac{\rho_s}{2}\left[\left(1-\frac{\delta^2}{2}\right)(\partial_x\boldsymbol{m})^2+(1-\delta^2)(\partial_y\boldsymbol{m})^2+\frac{1}{v_s^2}(\partial_t\boldsymbol{m})^2\right]\right\}, \tag{42}$$

where $\rho_s=Js^2$, $\chi_\perp=8Ja_0^2$, and $v_s=\sqrt{\rho_s\chi_\perp}$. Like in the stair model there are different spin stiffnesses in the spatial directions and also a topological contribution proportional to δ such as Eq. (33), but in this model only the winding number in the x direction is involved. As in the stair model, this winding number is not well defined. The same calculations within the modified model, where the chains formed by strong bonds are again smooth and along the x axis (see Fig. 6), show that the topological term proportional to δ vanishes and the winding number in Eq. (23) is calculated along the strong bonds. We therefore ignore the topological term in Eq. (42) from now on and use a 2D RG flow with $\theta=\pi$ later on. A rescaling of the imaginary time axis then leads to

$$S[\boldsymbol{m}]=\frac{1}{2a_0g_0}\int_\Omega d^3x\left\{(\partial_x\boldsymbol{m})^2+\frac{2-2\delta^2}{2-\delta^2}(\partial_y\boldsymbol{m})^2+(\partial_t\boldsymbol{m})^2\right\}, \tag{43}$$

where the bare coupling is given by

$$g_0(\delta)=\frac{2\sqrt{2}}{s}\sqrt{\frac{2}{2-\delta^2}}. \tag{44}$$

Because of the anisotropy in the y direction the RG is, as in the J_x/J_y and stair models, two dimensional at the beginning. But here the bare coupling $g_0(\delta)$ is increased with increasing δ. Therefore two scenarios are possible: If a δ_c exists so that $g_0(\delta)>g_2(0)$ if $\delta>\delta_c$, the coupling is driven by the 2D RG flow towards infinity and $g(\Lambda')$ with $\Lambda'=(2-2\delta^2)/(2-\delta^2)\Lambda$, which is the bare coupling for the 3D RG, is then greater than g_c. Therefore the ground state is disordered for $\delta>\delta_c$. If, however, even for $\delta\to1$, $g_0(\delta)$ remains smaller than $g_2(0)$, the ground state is always ordered for a nonvanishing interchain coupling. In summary, we cannot decide within the RG treatment if an extended disordered phase exists or if there is long-range order for all $\delta\in[0,1)$ as in the J_x/J_y and the stair models.

V. LINEAR SPIN-WAVE THEORY (LSWT)

In the section before, we have mentioned that it is impossible to determine a value for the critical coupling g_c, or

equivalent a value for the criticial dimerization δ_c, for the plaquette and the meander model from RG. This is one reason to apply LSWT onto the considered models. The second reason is that we are interested in the question if these models can be the result of a dynamical process, i.e., a spin-Peierls transition. Because the calculated ground-state energy for the isotropic two-dimensional Heisenberg antiferromagnet of $E_0/NJ \approx -0.6579$ deviates less than 3% from the best numerical results[5,6] and also the sublattice magnetization $m = 0.3034$ agrees very well, we expect that LSWT gives reliable results near the isotropic point. On the other hand, the results for large dimerizations have to be regarded with care, because LSWT fails in one dimension.

We use the Holstein-Primakoff transformation[28] to map the spin operators onto Bose operators

$$S^z = s - a^+ a, \quad S^- = \sqrt{2s}\, a^+ \sqrt{1 - \frac{a^+ a}{2s}}. \tag{45}$$

By expanding the square root in $1/s$ and taking only the lowest order into account, LSWT is reached.

A. Stair model

As before, we want to consider the stair model generalized to d dimensions. Because the lattice $G = A \oplus B$ is bipartite, it is possible to write the Hamiltonian as

$$H = \sum_{i \in A} \sum_{a=1}^{d} [J(1+\delta)\boldsymbol{S}(i) \cdot \boldsymbol{S}(i + a_0 \boldsymbol{e}^a) + J(1-\delta)\boldsymbol{S}(i) \cdot \boldsymbol{S}(i - a_0 \boldsymbol{e}^a)], \tag{46}$$

which is useful for LSWT. Starting point is again a Néel ordered state, and we therefore apply independent Holstein-Primakoff transformations to the two sublattices A, B:

$$x \in A: S^z(x) = s - a^+(x)a(x), \quad S^-(x) = \sqrt{2s}\, a^+(x), \tag{47a}$$

$$x \in B: S^z(x) = -s + b^+(x)b(x), \quad S^-(x) = \sqrt{2s}\, b(x). \tag{47b}$$

Taking the Fourier transform the Hamiltonian is bilinear and given by

$$H = -NJs^2 d + 2Jsd \sum_{\boldsymbol{k}} \{a_{\boldsymbol{k}}^+ a_{\boldsymbol{k}} + b_{\boldsymbol{k}}^+ b_{\boldsymbol{k}} + A a_{\boldsymbol{k}} b_{\boldsymbol{k}} + A^* a_{\boldsymbol{k}}^+ b_{\boldsymbol{k}}^+\}, \tag{48}$$

where the definitions $\gamma_{\boldsymbol{k}} = (1/d)\Sigma_{l=1}^{d} \cos(k_l a_0)$, $\beta_{\boldsymbol{k}} = (i/d)\Sigma_{m=1}^{d} \sin(k_m a_0)$, and $A = \gamma_{\boldsymbol{k}} + \delta\beta_{\boldsymbol{k}}$ have been used. By means of a Bogoliubov transformation this is easily diagonalized leading to

$$H = -NJds(s+1) + 2Jsd \sum_{\boldsymbol{k}} \sqrt{1 - (\gamma_{\boldsymbol{k}}^2 - \delta^2 \beta_{\boldsymbol{k}}^2)}\,(c_{\boldsymbol{k}}^+ c_{\boldsymbol{k}} + d_{\boldsymbol{k}}^+ d_{\boldsymbol{k}} + 1). \tag{49}$$

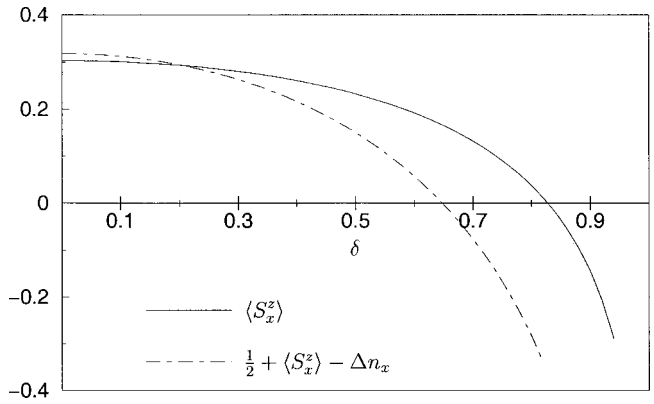

FIG. 11. Sublattice magnetization and condition (51) for the validity of the LSWT, both for the stair model.

1. Sublattice magnetization

The sublattice magnetization m is given by

$$m = \langle S_A^z \rangle = \frac{N}{2}s - \sum_{\boldsymbol{k}} \langle a_{\boldsymbol{k}}^+ a_{\boldsymbol{k}} \rangle = \frac{N}{2}s - \frac{1}{2}\sum_{\boldsymbol{k}} \left\{ \frac{1}{\sqrt{1 - (\gamma_{\boldsymbol{k}}^2 - \delta^2 \beta_{\boldsymbol{k}}^2)}} - 1 \right\}. \tag{50}$$

By replacing the sum by an integral this can be evaluated in principle in any dimension d. However, in one dimension this integral is divergent. This is not astonishing due to Coleman's theorem[29] stating that the continuous SU(2) symmetry cannot be broken in one dimension.

In two dimensions the dimerization δ reduces the magnetization as expected and at $\delta = 1$ there is again the one-dimensional infrared divergence. Nevertheless, we can take the value of the dimerization where m vanishes as indication for the breakdown of Néel order. For the stair model we get $\delta_c = 0.8286$ or $R_c = (1-\delta)/(1+\delta) = 0.094$ (see Fig. 11).

To check the validity of the LSWT, we want to use an argument given by Sakai and Takahashi.[25] In spin-wave theory the number n_x of bosons per lattice site is not restricted. That means that there are unphysical states in this theory, because in the original spin system the condition $n_x \leqslant 2S$ holds. A possible estimation for the validity of LSWT may therefore be given by

$$\langle n_x \rangle + \Delta n_x < 2s \Leftrightarrow \langle S_x^z \rangle - \Delta n_x > -s. \tag{51}$$

This predicts that LSWT is valid for this model from $\delta = 0$ up to $\delta \approx 0.65$ (see Fig. 11). Therefore the calculated δ_c is in a region, where LSWT is not reliable. We can only conclude that δ_c must be greater than 0.65.

2. Distortion due to spin-phonon coupling

The dimerization leads to a gain in magnetic energy on the one hand, on the other hand it costs elastic energy. To answer the question of whether a spin-Peierls transition towards a distorted lattice is possible, we expand the calculated ground-state energy up to quadratic order. Because the linear term vanishes for symmetry reasons, we get

$$\frac{E(\delta)}{NJ} = e_0 - A\delta^2 \tag{52}$$

with $e_0 = -0.6579$ and $A = 0.261$. As mentioned in the Introduction, Eq. (2), the displacement of an atom is proportional to δ and the mean-field treatment of the phonons leads to a classical elastic energy proportional to δ^2. Therefore the lattice is only distorted if

$$\frac{m}{2}\frac{J^2\omega^2_{\text{trans}}(\pi,\pi)}{\lambda^2_{\text{trans}}(\pi,\pi)} < 0.261, \tag{53}$$

whereas the lattice is unchanged otherwise. Here m is the mass of the moved atom and ω the phonon frequency of the responsible phonon mode. If this condition is fulfilled, there is a coexistence of spin-Peierls dimerization and Néel-like long-range order. The situation here is quite different from that in one dimension. For the dimerized chain the magnetic energy scales as $E_{\text{mag}} \propto \delta^{4/3}$ and because the elastic energy is proportional to δ^2, there is always a distortion. In the two-dimensional stair model the magnetic and elastic energy behave as δ^2 and therefore a distortion of the lattice is only possible if certain conditions are fulfilled. Because we expand around the isotropic point where LSWT results agree well with numerical results, the quantitative results for the condition of dimerization are expected to be reliable.

B. J_x/J_y model

Because this model is well known and LSWT has already been applied to it,[25] we only want to briefly state the results. The bosonic Hamiltonian is again easily diagonalized by a Bogoliubov transformation and can be written as

$$H = -N(J_x + J_y)s(s+1) + 2sJ_x(1+R) \times \sum_{\boldsymbol{k}} \gamma_{\boldsymbol{k}}(c^+_{\boldsymbol{k}}c_{\boldsymbol{k}} + d^+_{\boldsymbol{k}}d_{\boldsymbol{k}} + 1) \tag{54}$$

with

$$\gamma_{\boldsymbol{k}} = \sqrt{1 - \left(\frac{1}{1+R}\right)^2 [\cos(k_x) + R\cos(k_y)]^2}$$

and $R = J_y/J_x$.

1. Sublattice magnetization

If we again calculate the sublattice magnetization and take its vanishing as an indication for the breakdown of Néel order, we find a critical $R_c = 0.0337$. We also proved by using condition (51) the reliability of the spin-wave approach. It seems to be valid if $R > 0.1$ and therefore we only can conclude that the critical coupling R_c must be smaller than 0.1. As mentioned before, numerical studies such as series expansions[14] and Monte Carlo studies[26] seem to indicate that R_c is equal to zero.

2. Distortion due to spin-phonon coupling

By using the relation $\delta = (1-R)/(1+R)$ we switch again to the description of the model with the parameter δ. In the expansion of the ground-state energy (52) the parameter A is now given by $A = 0.146$. A spin-Peierls transition is only possible if the gain of magnetic energy is larger than the cost of elastic energy leading to the condition

$$m\frac{J^2}{\lambda^2}[2c^2_{\text{long}}(1,0) + c^2_{\text{trans}}(1,1) - c^2_{\text{long}}(1,1)] < 0.146, \tag{55}$$

where $c(1,0)$ and $c(1,1)$ are the phonon velocities in directions (1,0) and (1,1).

C. Plaquette model

The situation is more complicated for this model, because the unit cell includes four sites. Therefore we have to introduce four kinds of bosons. This happens as follows:

A: $r \in (2i,2j)$, $S^z = s - a^+_r a_r$, $S^- = \sqrt{2s}a^+_r$,

B: $r \in (2i+1,2j+1)$, $S^z = s - b^+_r b_r$, $S^- = \sqrt{2s}b^+_r$,

C: $r \in (2i,2j+1)$, $S^z = -s + c^+_r c_r$, $S^- = \sqrt{2s}c_r$,

D: $r \in (2i+1,2j)$, $S^z = -s + d^+_r d_r$, $S^- = \sqrt{2s}d_r$,

where A, B, C, D enumerate the four sublattices.

In principle it is possible to diagonalize every Hamiltonian of an assembly of N bilinearly interacting bosons or fermions what has been well known for a long time.[30] But especially for bosons it is often complicated to construct the transformation matrix T between new and old operators, because the transformation is not unitary. We therefore add an ''antiferromagnetic field'' B^z_A, which allows us to calculate the sublattice magnetization without doing this canonical transformation explicitly. After taking the Fourier transform the Hamiltonian with additional field is given by

$$H = -2NJs^2 - NB^z_A s + 4Js\sum_{\boldsymbol{k}} \Big\{ a^+_{\boldsymbol{k}}a_{\boldsymbol{k}} + b^+_{\boldsymbol{k}}b_{\boldsymbol{k}} + c^+_{\boldsymbol{k}}c_{\boldsymbol{k}} + d^+_{\boldsymbol{k}}d_{\boldsymbol{k}} + A^x_{\boldsymbol{k}}[a_{\boldsymbol{k}}c_{\boldsymbol{k}} + b^+_{\boldsymbol{k}}d^+_{\boldsymbol{k}}] + \text{H.c.} + A^y_{\boldsymbol{k}}[a_{\boldsymbol{k}}d_{\boldsymbol{k}} + b^+_{\boldsymbol{k}}c^+_{\boldsymbol{k}}] + \text{H.c.} + \frac{B^z_A}{4Js}[a^+_{\boldsymbol{k}}a_{\boldsymbol{k}} + b^+_{\boldsymbol{k}}b_{\boldsymbol{k}} + c^+_{\boldsymbol{k}}c_{\boldsymbol{k}} + d^+_{\boldsymbol{k}}d_{\boldsymbol{k}}] \Big\}, \tag{56}$$

where $\gamma^a_{\boldsymbol{k}} = \frac{1}{2}\cos(\boldsymbol{k}a_0 \cdot \boldsymbol{e}^a)$, $\beta^a_{\boldsymbol{k}} = (i/2)\sin(\boldsymbol{k}a_0 \cdot \boldsymbol{e}^a)$, and $A^a_{\boldsymbol{k}} = \gamma^a_{\boldsymbol{k}} + \delta\beta^a_{\boldsymbol{k}}$.

This has to be diagonalized under the subcondition that the new operators fulfill again Bose commutation relations leading to[31]

$$\text{(I)} \quad T^{-1}\mathcal{H}JT = \mathcal{H}_D J \tag{57a}$$

and

$$\text{(II)} \quad T^+JTJ = 1, \tag{57b}$$

where $\mathcal{H}_D$ denotes the diagonalized Hamilton matrix and J is given by

$$J=\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{57c}$$

From Eq. (57b) it follows that T is an element of the pseudounitary group U(2,2), whereas Eq. (57a) implies the secular equation

$$\det(\mathcal{H}J-\lambda_i 1)=0 \tag{58}$$

for the diagonalization problem. The eigenvalues of $\mathcal{H}$ are then given by $|\lambda_i|$. By solving the secular equation (58) we get the diagonalized Hamiltonian of the plaquette model in LSWT:

$$H=-2NJs(s+1)-NB_A^z\left(s+\frac{1}{2}\right)+4Js\sum_{\mathbf{k}}\{\lambda_{\mathbf{k}}^1[\mathcal{A}_{\mathbf{k}}^+\mathcal{A}_{\mathbf{k}}+\mathcal{C}_{\mathbf{k}}^+\mathcal{C}_{\mathbf{k}}+1]+\lambda_{\mathbf{k}}^2[\mathcal{B}_{\mathbf{k}}^+\mathcal{B}_{\mathbf{k}}+\mathcal{D}_{\mathbf{k}}^+\mathcal{D}_{\mathbf{k}}+1]\}, \tag{59a}$$

$$\lambda_{\mathbf{k}}^1=\sqrt{(1+\tilde{B}_A^z)^2-(|A_{\mathbf{k}}^x|+|A_{\mathbf{k}}^y|)^2},$$

$$\lambda_{\mathbf{k}}^2=\sqrt{(1+\tilde{B}_A^z)^2-(|A_{\mathbf{k}}^x|-|A_{\mathbf{k}}^y|)^2} \tag{59b}$$

with the new Bose operators $\mathcal{A}_{\mathbf{k}}$, $\mathcal{B}_{\mathbf{k}}$, $\mathcal{C}_{\mathbf{k}}$, $\mathcal{D}_{\mathbf{k}}$ and $\tilde{B}_A^z=B_A^z/4Js$.

1. Sublattice magnetization

The ground-state sublattice magnetization per lattice site is now easily calculated from Eq. (59a) by the derivative $(1/N)\langle\partial H/\partial B_A^z\rangle|_{B_A^z=0}$. Setting $s=1/2$ and replacing the sum through an integral the sublattice magnetization is given by

$$\langle S^z\rangle=1-\frac{1}{4\pi^2}\int_{-\pi/2}^{\pi/2}\int_{-\pi/2}^{\pi/2}\left\{\frac{1}{\tilde{\lambda}_{\mathbf{k}}^1}+\frac{1}{\tilde{\lambda}_{\mathbf{k}}^2}\right\}, \tag{60}$$

where $\tilde{\lambda}_{\mathbf{k}}^i=\lambda_{\mathbf{k}}^i(\tilde{B}_A^z=0)$. This decreases with increasing δ and vanishes at $\delta_c=0.798$ or aquivalently $R_c=0.112$. This value agrees with that given in a paper by Koga, Kumada, and Kawakami.[32] The same authors have also used a series expansion[33] starting from uncoupled plaquettes to determine the critical coupling and get $\delta_c\approx 0.3$. This value is in good agreement with results from Monte Carlo calculations, showing again that the results in LSWT at high dimerizations have to be considered with care, because of the unphysical states in this approach.

2. Distortion due to spin-phonon coupling

We set $\tilde{B}_A^z=0$ and expand again the ground-state energy up to quadratic order. For this model the parameter A is equal 0.174. Therefore the lattice is distorted if the condition

$$\frac{m}{4}\left(\frac{J^2\omega_{\text{long}}^2(\pi,0)}{\lambda_{\text{long}}^2(\pi,0)}+\frac{J^2\omega_{\text{long}}^2(0,\pi)}{\lambda_{\text{long}}^2(0,\pi)}\right)<0.174 \tag{61}$$

is fulfilled.

D. Meander model

The sublattice structure of this model is similar to that of the plaquette model and it is again necessary to introduce four kinds of bosons. With the same definitions as before the Hamiltonian of the model is given by

$$H=-2NJs^2-NB_A^z s+4Js\sum_{\mathbf{k}}\Big\{a_{\mathbf{k}}^+a_{\mathbf{k}}+b_{\mathbf{k}}^+b_{\mathbf{k}}+c_{\mathbf{k}}^+c_{\mathbf{k}}+d_{\mathbf{k}}^+d_{\mathbf{k}}+A_{\mathbf{k}}^x[a_{\mathbf{k}}c_{\mathbf{k}}+b_{\mathbf{k}}d_{\mathbf{k}}]+\text{H.c.}+A_{\mathbf{k}}^y[a_{\mathbf{k}}d_{\mathbf{k}}+b_{\mathbf{k}}^+c_{\mathbf{k}}^+]+\text{H.c.}+\frac{B_A^z}{4Js}[a_{\mathbf{k}}^+a_{\mathbf{k}}+b_{\mathbf{k}}^+b_{\mathbf{k}}+c_{\mathbf{k}}^+c_{\mathbf{k}}+d_{\mathbf{k}}^+d_{\mathbf{k}}]\Big\}. \tag{62}$$

By solving the secular equation (58) this is diagonalized leading to a Hamiltonian in the new Bose operators $\mathcal{A}_{\mathbf{k}}$, $\mathcal{B}_{\mathbf{k}}$, $\mathcal{C}_{\mathbf{k}}$, $\mathcal{D}_{\mathbf{k}}$ as in Eq. (59a) but now with eigenvalues

$$\lambda_{\mathbf{k}}^1=\sqrt{(1+\tilde{B}_A^z)^2-|A_{\mathbf{k}}^x|^2-|A_{\mathbf{k}}^y|^2-2|A_{\mathbf{k}}^y|\text{Re}(A_{\mathbf{k}}^x)}, \tag{63}$$

$$\lambda_{\mathbf{k}}^2=\sqrt{(1+\tilde{B}_A^z)^2-|A_{\mathbf{k}}^x|^2-|A_{\mathbf{k}}^y|^2+2|A_{\mathbf{k}}^y|\text{Re}(A_{\mathbf{k}}^x)}.$$

1. Sublattice magnetization

Analogous to the plaquette model the sublattice magnetization can be calculated by a derivative. The value for the critical dimerization determined by this calculation is $\delta_c=0.898$ or $R_c=0.054$. This is similar to all the other models in a region where the spin-wave approach is no longer justified.

2. Distortion due to spin-phonon coupling

The parameter in the expansion is given by $A=0.160$ and therefore the condition for the spin-Peierls transition is

$$\frac{m}{4}\left(\frac{J^2\omega^2(\pi,\pi)}{\lambda^2(\pi,\pi)}+\frac{J^2\omega_{\text{long}}^2(0,\pi)}{\lambda_{\text{long}}^2(0,\pi)}\right)<0.160, \tag{64}$$

where we have assumed that the phonon frequencies and spin-phonon coupling constants for the longitudinal and transversal (π,π) phonon are identical.

VI. CONCLUSIONS

By using simple scaling arguments we have shown that for the J_x/J_y model and the stair model, which consist of weakly coupled Heisenberg chains for large dimerizations, the interchain coupling is a relevant operator. Therefore only at $\delta=1$ the ground state is of one-dimensional nature. Also in the meander model the interchain coupling is relevant, but there is also a relevant intrachain coupling. By numerical calculations (DMRG + TMRG) we have shown in this more complicated case that the scaling behavior for the intrachain coupling is predicted correctly by the simple scaling argument. We also showed that it is possible to map all four

models onto a NLσ model. By applying the known results for the RG flow in two and three dimensions we have concluded that the ground state of the J_x/J_y and the stair models is Néel-like ordered for all $\delta \in [0,1)$, whereas an extended disordered phase exists for the plaquette model. However, it was not possible to determine the critical dimerization $\delta_c \in (0,1)$ for the plaquette model within the RG treatment. For the meander model the RG gave no unique result. A phase diagram such as for the J_x/J_y and stair models, but also an extended disordered phase as in the plaquette model are both possible scenarios. The second possibility seems to be more probable, as the intrachain coupling has scaling dimension $x=1/2$ and is therefore more relevant than the interchain coupling with $x=1$. If we start from $\delta=1$ and reduce the dimerization, we might expect that there arises first a system consisting of weakly coupled two-leg ladders. Because a two-leg ladder with $s=1/2$ is a gapped system, a small coupling between these ladders can be treated within normal perturbation theory and does not change the global properties drastically. At lower dimerization the gap closes and the system orders antiferromagnetically. If this picture is correct, δ_c must be smaller than 1.

To investigate this further and to determine a value for the critical dimerizations δ_c, we also applied LSWT to the models. The following values for δ_c are derived.

Model	δ_c
J_x/J_y model	0.935
meander model	0.898
stair model	0.829
plaquette model	0.798

All these values have to be regarded with great care, because LSWT allows also unphysical states and a simple argument has shown that there is a large contribution of these states at such high dimerizations.

This problem does not occur near $\delta=0$, where LSWT gives very precise results. We therefore believe that the conditions for the spin-Peierls transition, which we have obtained within LSWT, are qualitatively and quantitatively useful. For all models we have found that elastic and magnetic energies scale as δ^2 at small dimerizations. A phase transition leading to a coexistence of spin-Peierls dimerization and antiferromagnetic long-range order is therefore only possible for certain values of the microscopic coupling constants. From an expansion of the magnetic ground-state energy $E(\delta)=e_0-A\delta^2$ we have got the following values for the parameter A.

Model	A
stair model	0.261
plaquette model	0.174
meander model	0.160
J_x/J_y model	0.146

The gain of magnetic energy is therefore largest for a stairlike distortion of the lattice, which is caused by a transversal (π,π) phonon. What kind of distortion is energetically prefered, depends also on the elastic energy, which in general is different for each model. However, if we assume that the elastic energy is equal for all models, we would conclude that the stairlike distortion is energetically prefered. This is in contradiction to a result by Tang and Hirsch,[34] who have studied the plaquettelike and stairlike distortion by an exact diagonalization of a 4×4 lattice and conclude by using the same assumption that the plaquette structure is prefered. However, the lattice they have considered is very small and they have not done any finite size scaling so that we believe our result is more reliable for the infinite lattice.

ACKNOWLEDGMENTS

J.S. thanks R. Raupach for doing the TMRG calculations and also J. Gruneberg for valuable discussions. K.H. gratefully acknowledges financial support by the Stipendienfonds im Verband der chemischen Industrie, BMBF and the Studienstiftung des dt. Volkes.

*Electronic address: sirker@fkt.physik.uni-dortmund.de
†Electronic address: kluemper@fkt.physik.uni-dortmund.de
‡Electronic address: kontakt@kay-hamacher.de

[1] H. Bethe, Z. Phys. **71**, 205 (1931).
[2] F. D. M. Haldane, Phys. Lett. **93A**, 464 (1983).
[3] M. C. Cross and D. S. Fisher, Phys. Rev. B **19**, 402 (1978).
[4] P. W. Anderson, Phys. Rev. **86**, 694 (1952).
[5] B. B. Beard, R. J. Birgeneau, M. Greven, and U.-J. Wiese, Phys. Rev. Lett. **80**, 1742 (1998).
[6] T. Barnes, Int. J. Mod. Phys. C **2**, 659 (1991).
[7] F. Dyson, E. H. Lieb, and B. Simon, J. Stat. Phys. **18**, 335 (1978).
[8] A. M. Polyakov, Phys. Lett. **1**, 79 (1975).
[9] S. Chakravarty, B. Halperin, and D. R. Nelson, Phys. Rev. Lett. **60**, 1057 (1988).
[10] F. D. M. Haldane, Phys. Rev. Lett. **61**, 1029 (1988).
[11] N. Read and S. Sachdev, Phys. Rev. B **42**, 4568 (1990).
[12] F. Woynarovich, Phys. Rev. Lett. **59**, 259 (1987).
[13] S. R. White, R. M. Noack, and D. J. Scalapino, Phys. Rev. Lett. **73**, 886 (1994).
[14] I. Affleck, M. P. Gelfand, and R. Singh, J. Phys. A **27**, 7313 (1994).
[15] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).
[16] M. Suzuki and M. Inoue, Prog. Theor. Phys. **78**, 787 (1987).
[17] X. Wang and T. Xiang, Phys. Rev. B **56**, 5061 (1997).
[18] N. Shibata, J. Phys. Soc. Jpn. **66**, 2221 (1997).
[19] A. Klümper, R. Raupach, and F. Schönfeld, Phys. Rev. B **59**, 3612 (1999).
[20] J. Klauder, Phys. Rev. D **19**, 2349 (1979).
[21] P. Wiegmann, Phys. Rev. Lett. **60**, 821 (1988).
[22] E. Fradkin and M. Stone, Phys. Rev. B **38**, 7215 (1988).
[23] A. Perelomov, *Generalized Coherent States and Their Applications* (Springer, Berlin, 1986).
[24] I. Affleck and B. I. Halperin, J. Phys. A **29**, 2627 (1996).
[25] T. Sakai and M. Takahashi, J. Phys. Soc. Jpn. **58**, 3131 (1989).

[26] Y. J. Kim and R. J. Birgeneau, Phys. Rev. B **62**, 6378 (2000).
[27] I. Affleck, Nucl. Phys. B **265**, 409 (1985).
[28] T. Holstein and H. Primakoff, Phys. Rev. **58**, 1098 (1940).
[29] S. Coleman, Commun. Math. Phys. **31**, 259 (1973).
[30] N. N. Bogoliubov, J. Phys. (Moscow) **11**, 23 (1947).
[31] C. Tsallis, J. Math. Phys. **19**, 277 (1978).
[32] A. Koga, S. Kumada, and N. Kawakami, J. Phys. Soc. Jpn. **68**, 642 (1999).
[33] A. Koga, S. Kumada, and N. Kawakami, J. Phys. Soc. Jpn. **68**, 2373 (1999).
[34] S. Tang and J. E. Hirsch, Phys. Rev. B **37**, 9546 (1988).