Quantum criticality in dimerized spin ladders

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We analyze the possibility of quantum criticality (gaplessness) in dimerized antiferromagnetic two- and three-leg spin-$\frac{1}{2}$ ladders. Contrary to earlier studies of these models, we examine different dimerization patterns in the ladder. We find that ladders with the columnar dimerization order have lower zero-temperature energies, and they are always gapped. For the staggered dimerization order, we find the quantum critical lines, in agreement with earlier analyses. The bond mean-field theory we apply demonstrates its quantitative accuracy and agrees with available numerical results. We conclude that unless some mechanism for locking dimerization into the energetically less favorable staggered configuration is provided, the dimerized ladders do not order into the phase where the quantum criticality occurs.

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I. INTRODUCTION

There has been a lot of interest in spin ladders for more than a decade now, mainly due to their very intriguing critical properties. One of the most peculiar ones is that the existence of a gap (i.e., mass) depends on the number of legs. The spin excitations in an m-leg spin ladder are gapped if m is even, and the system is gapless (quantum critical) if the number of legs m is odd. For reviews see Refs. 1 and 2. The even-m-leg ladders provide a very interesting example of systems where the gap (mass) generation is not accompanied by a long-range order or apparent symmetry breaking. Such systems, known as spin liquids, are under enormous scrutiny. They are notoriously difficult to realize in more than one dimension and are believed to be relevant to the physics of high-T_c superconductors.[3] Broadly speaking, spin ladders are interesting for studying gap (mass) generation; needless to say, this a very deep question in all physics.

The particular question we address in this study is the possibility of "restored quantum criticality" (or gaplessness) in a system (ladder) built from gapped blocks (dimerized chains).[4–12] Let us explain the issue, taking a dimerized two-leg ladder as an example.[13] It is well known that a single Heisenberg spin-$\frac{1}{2}$ chain with alternating spin exchange (a.k.a. the dimerized Heisenberg chain) is gapped.[2] When two chains are coupled into a ladder, the system is gapped even without dimerization. However, quite remarkably and counterintuitively, the dimerized two-leg ladder can be gapless, as was conjectured in Ref. 4. The subsequent numerical work[5–7,9] confirmed the critical (gapless) line proposed by Martin-Delgado *et al.*[4] Similarly, the originally conjectured critical line in a dimerized three-leg ladder[4] was confirmed in the very recent density-matrix renormalization-group (DMRG) calculations.[11,12]

We need to stress one very important point: In the earlier work[5–9,11,12] on the *intrinsically dimerized* ladders, the intrachain dimerization, as well as the (staggered) dimerization ordering pattern of the whole ladder (cf. Figs. 1 and 6 below), is taken for granted, i.e., as the *model built-in assumptions*. In the absence of a physical mechanism, which would lock a ladder with dimerized chains into a particular dimerization order, it is natural and physically more reasonable to consider various possible ordering patterns on the same footing. It means that the possibility of quantum criticality (gaplessness) has to be addressed in this broader setting. A strong motivation comes from the recent work on the three-leg ladder coupled to phonons.[14] It turns out that the phonon-induced intrachain dimerizaton, appearing in this ladder at the spin-Peierls transition, occurs into the columnar dimerization order (cf. Fig. 6 below). The latter, and not the staggered order, minimizes the spin-phonon Hamiltonian. The columnar dimerized three-leg ladder is always gapped.

So, we begin from the study of the dimerized two-leg ladder in Sec. II. In the present study the dimerization parameter is considered as a given fixed ("external") parameter of the model, and it is not a subject of self-consistency or minimization conditions. From analyses of the limits where the behavior of the two-leg ladder is known exactly, we conjecture that the gapped columnar dimerized phase has lower energy. This is confirmed by the subsequent treatment within the bond mean-field theory.[15–17] The latter approach, when applied to the case of staggered dimerization, demonstrates a good agreement with available numerical results and also yields quite simple formulas for analytical treatments of the problem. A similar program with analogous conclusions is carried out for the three-leg ladder in Sec. III.

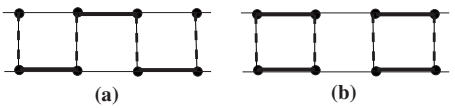

FIG. 1. Dimerized two-leg ladder. The bold and/or thin and/ or dashed lines represent the stronger and/or weaker chain coupling $J(1 \pm \delta)$ and rung coupling $J_\perp$, respectively. Dimerization patterns: (a) staggered and (b) columnar.

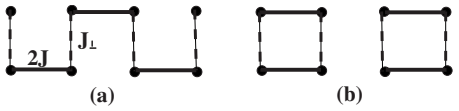

FIG. 2. Completely dimerized ladder, $\delta=1$. (a) Alternated staggering reduces model (1) to a snakelike dimerized Heisenberg chain of $2N$ spins. (b) Columnar order degenerates into a set of $N/2$ decoupled plaquettes.

II. TWO-LEG LADDER

We consider the two-leg dimerized spin ladder given by the Hamiltonian

$$H_{2L} = \sum_{\alpha=1,2} \sum_{n=1}^{N} J_\alpha(n) \mathbf{S}_\alpha(n) \cdot \mathbf{S}_\alpha(n+1) + J_\perp \sum_{n=1}^{N} \mathbf{S}_1(n) \cdot \mathbf{S}_2(n). \tag{1}$$

The m-leg ladder has N rungs and $m \cdot N$ spins. We consider the situation when dimerization occurs along the chains ($\alpha = 1,2$) only, while the coupling $J_\perp$ is constant on each rung. One needs to consider two possible dimerization patterns: alternated, when staggering occurs in both directions

$$J_\alpha(n) = J[1 + (-1)^{n+\alpha}\delta], \tag{2}$$

and columnar, when

$$J_\alpha(n) = J[1 + (-1)^n \delta]. \tag{3}$$

The two patterns are shown in Fig. 1,

A. Analytical limits

Let us discuss the points on the $(\delta, J_\perp)$-plane where the properties of model (1) are known:

(i) $\delta=0$, $J_\perp=0$—two decoupled critical (gapless) Heisenberg chains;

(ii) $\delta=0$, $J_\perp>0$—uniform gapped ladder; and

(iii) $\delta=1$—complete dimerization. In this limit the model reduces to:

(a) the snakelike dimerized Heisenberg chain of $2N$ spins in case of the alternated staggered pattern [Fig. 2(a)] and

(b) a set of $N/2$ decoupled four-spin plaquettes in case of the columnar dimerization pattern [Fig. 2(b)].

For a four-spin plaquette, where its nearest-neighbor spins interact via the Heisenberg couplings J_1 and J_2, the spectrum is known.[18] The ground-state singlet has the energy

$$\mathcal{E}_\square = -\frac{J_1 + J_2}{2} - \sqrt{J_1^2 + J_2^2 - J_1 J_2} \tag{4}$$

and is separated by a gap from the closest triplet state with the energy $\mathcal{E}_t = -\frac{J_1+J_2}{2}$.

As was first noted in Ref. 4, at the critical point $2J = J_\perp \equiv J_c$ the snakelike chain [Fig. 2(a)] becomes just a uniform (*gapless*) Heisenberg model. Its ground-state energy is

$$E_{HC} = -2\left(\log 2 - \frac{1}{4}\right) J_c N \approx -0.88 J_c N. \tag{5}$$

The set of $N/2$ plaquettes (4) has a lower ground-state energy

$$E_\square = -J_c N. \tag{6}$$

The simple results [Eqs. (5) and (6)] question the very existence of the critical line predicted in Ref. 4. That line was conjectured essentially from a continuity argument and analysis of the model in the two solvable (integrable) points $\delta=0$, $J_\perp=0$ and $\delta=1$, $J_\perp=2J$. The latter was assumed to be a critical (gapless) point since the alternated staggering pattern (thus the snakelike chain in the limit $\delta=1$) was assumed to be a ground state. The subsequent analyses addressed the issue of the critical line (within the alternated staggering pattern) more quantitatively,[5–9] while to the best of our knowledge, comparisons with the energy of the columnar pattern were not done. As one can see from Eqs. (5) and (6), the gapped plaquettes have lower energy than the critical (gapless) snakelike Heisenberg chain. Note that the decoupled plaquettes at $\delta=1$ evolve smoothly from the columnar dimerization pattern at $\delta<1$.

Let us now look at the line $\delta=1$, $J_\perp \neq 2J$. It is convenient to parametrize the couplings as

$$2J \equiv J_\circ(1 + \delta_{\text{eff}}), \tag{7}$$

$$J_\perp \equiv J_\circ(1 - \delta_{\text{eff}}). \tag{8}$$

The plaquette pattern results in the ground-state energy

$$E_\square = -\frac{1}{2} J_\circ N(1 + \sqrt{1 + 3\delta_{\text{eff}}^2}). \tag{9}$$

The energy minimum of the snakelike configuration is given by the ground-state energy of the dimerized Heisenberg chain. The latter is known to be equivalent to the massive sine-Gordon (integrable) model, perturbed by the marginal (logarithmic) corrections.[19,20] A leading order ansatz reads as

$$E_{\text{DHC}} \approx -2J_\circ N\left(\log 2 - \frac{1}{4} + a_\circ \frac{\delta_{\text{eff}}^{4/3}}{\ln \frac{\delta_\circ}{\delta_{\text{eff}}}}\right), \tag{10}$$

where from the recent numerical calculations,[21] $a_\circ \approx 2.2$ and $\delta_\circ \approx 110$. To get a more accurate analytical expression for E_{DHC} is an involved problem (for a recent analysis and more references, see Ref. 22). However numerically, the ansatz [Eq. (10)] or even the unperturbed sine-Gordon formula[22]

$$E_{\text{SG}} \approx -2J_\circ N\left(\log 2 - \frac{1}{4} + 0.2728\,\delta_{\text{eff}}^{4/3}\right) \tag{11}$$

work quite well. A direct inspection of Eqs. (9)–(11) (e.g., plots) clearly shows that the plaquettes again provide the lower energy state on the line $\delta=1$ near the point $J_\perp = 2J \Leftrightarrow \delta_{\text{eff}}=0$.[23]

B. Mean-field equations

Away from integrable points we need to resort to approximations. We will treat the dimerized ladders in the framework of the bond mean-field theory.[15,16] This approach for the case of the dimerized three-leg ladder is described in detail in Ref. 14, and the case of two legs is essentially a simplified version of the former. First, the spin Hamiltonian

is mapped onto an interacting fermion problem via a two-dimensional (2D) version of the Jordan-Wigner transformation, proposed by one of us.[15] Then, the phase differences due to hopping of the fermions around any given elementary plaquette is approximated by π. The quartic fermionic terms $c^{\dagger}_{i,}c_{i,\alpha}c^{\dagger}_{i+1,\alpha}c_{i+1,\alpha}$ are treated within the Hartree-Fock approximation, i.e., are decoupled using the single-particle (bond) parameters. The latter are defined as

$$Q_{+} = \langle c_{2i,\alpha}c^{\dagger}_{2i+1,\alpha}\rangle, \quad Q_{-} = \langle c_{2i+1,\alpha}c^{\dagger}_{2i+2,\alpha}\rangle, \tag{12}$$

with $\alpha=1,2$. A single bond parameter suffices in the rung direction: $P=\langle c_{2i,\alpha}c^{\dagger}_{2i,\alpha+1}\rangle$. With the Fourier transforming along the chain direction and using the Nambu formalism, the mean-field theory results in the single-particle effective Hamiltonian

$$H^{\mathrm{s/c}} = \sum_{k} \Psi^{\dagger}_{k}\mathcal{H}^{(\mathrm{s/c})}\Psi_{k} + NC_{2}, \tag{13}$$

where the Hamiltonian density $\mathcal{H}^{\mathrm{s/c}}$ is a 4×4 matrix and the Nambu spinor $\Psi^{\dagger}_{k} \equiv (c^{A\dagger}_{1k}c^{B\dagger}_{1k}c^{A\dagger}_{2k}c^{B\dagger}_{2k})$. Here $c^{\sharp}_{\alpha k}$ is the Fourier transform of $c^{\sharp}_{i\alpha}$. To account for the dimerization (doubling of the lattice spacing), the lattice is subdivided into two sublattices, A and B. The explicit form of the effective Hamiltonian [Eq. (13)] depends on the dimerization pattern (staggered or columnar), which is accounted for by an extra label (s,c) in the above equation and

$$C_{2} = J_{+}|Q_{+}|^{2} + J_{-}|Q_{-}|^{2} + J_{\perp}|P|^{2}. \tag{14}$$

Diagonalization of $\mathcal{H}^{\mathrm{s/c}}$ yields four energy eigenvalues $\pm E^{\mathrm{s}}_{n}(k)$, $n=1,2$,

$$E^{\mathrm{s}}_{1/2}(k) = \frac{1}{2}\sqrt{W + J^{2}_{\perp 1} \mp 2J_{\perp 1}(J_{1+} - J_{1-})\cos k} \tag{15}$$

for the staggered phase. We define

$$J_{1\pm} = J(1 \pm \delta)(1 + 2Q_{\pm}), \quad J_{\perp 1} = J_{\perp}(1 + 2P), \tag{16}$$

$$W = J^{2}_{1+} + J^{2}_{1-} - 2J_{1+}J_{1-}\cos(2k). \tag{17}$$

For the columnar pattern we obtain two doubly degenerate energy eigenvalues $\pm E^{c}(k)$:

$$E^{c}(k) = \frac{1}{2}\sqrt{W + J^{2}_{\perp 1}}, \tag{18}$$

The partition function of the single-particle Hamiltonian [Eq. (13)] can be found in a closed form, and the free energy per spin is

$$F^{\sharp} = \frac{1}{m}C_{m} - \frac{\log 2}{\beta} - \frac{2\mathfrak{g}}{m\pi\beta}\sum_{n}\int_{0}^{\pi/2}\log\cosh\frac{\beta E^{\sharp}_{n}(k)}{2}dk, \tag{19}$$

where $\beta=1/k_{B}T$ and $\mathfrak{g}$ is the eigenvalue's degeneracy. We gave the above formula valid for the m legs. The mean-field equations are derived from minimization of the free energy [Eq. (19)] with respect to the mean-field parameters $Q_{\pm}$ and P. These self-consistent integral equations are solved numerically.

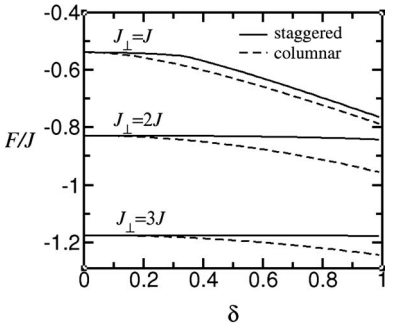

FIG. 3. Two-leg ladder: the energies of staggered and columnar dimerization configurations at $T=0$.

C. Analysis

To start with, let us make the following observation: In the antiferomagnetic two-leg ladder [Eq. (1)] with intrinsically dimerized chains, we cannot think of a particular mechanism to enforce a specific (i.e., staggered or columnar) dimerization pattern. So having the dimerized chains, the ladder must admit the pattern which minimizes its free energy. Using Eq. (19), we compared the zero-temperature energies of two configurations in various parameter ranges. The characteristic results are given in Fig. 3. The columnar pattern corresponds to the lower energies in all cases, so it is the thermodynamically stable state (phase).

Now let us analyze the excitation spectra of two phases. We will identify the minimal band gap of the eigenvalues [Eq. (15) or Eq. (18)] with the spin gap of the corresponding phase. To demonstrate that this is true, it suffices, e.g., to calculate the uniform spin susceptibility from the free energy [Eq. (19)] with an external magnetic field added.

We find that the columnar phase is *always gapped* with the gap $\Delta_{c}=E^{c}(0)$ given by

$$\Delta_{c} = J\sqrt{u^{2}\delta^{2} + \left(\frac{J_{\perp}}{2J}\right)^{2}p^{2}}, \tag{20}$$

where

$$u = 1 + (Q_{+} + Q_{-}) + \frac{Q_{+} - Q_{-}}{\delta}, \tag{21}$$

$$p = 1 + 2P. \tag{22}$$

Qualitatively, the columnar phase is similar to the uniform two-leg ladder, i.e., gapped. The gap [Eq. (20)] persists in the limit of the decoupled chains $J_{\perp}\to0$, as it must be, and disappears only together with the vanishing chain dimerization $\delta\to0$. If the latter limit is taken first, then the uniform ladder is gapped with $\Delta_{c}=J_{\perp}p/2$.

The staggered phase is more interesting. Its gap $\Delta_{s}=E^{\mathrm{s}}_{1}(0)$ reads as[24]

$$\Delta_{s} = J\left|u\delta - \frac{J_{\perp}}{2J}p\right|. \tag{23}$$

It vanishes on a certain critical line, even if neither dimerization δ nor rung coupling $J_{\perp}$ is zero. Thus, the mean-field theory confirms the earlier conjecture,[4] which has been so far

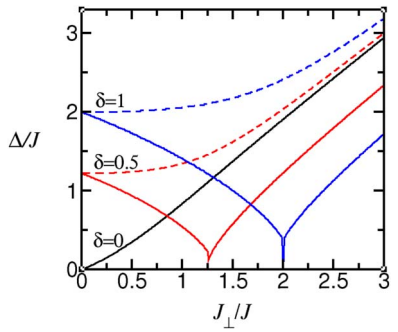

FIG. 4. (Color online) Two-leg ladder: the gaps of the staggered and columnar phases as functions of couplings for different dimerizations. For a fixed dimerization δ, gaps of the staggered (solid lines) and columnar (dashed lines) configurations coincide only at $J_\perp=0$; the columnar gap grows monotonously with $J_\perp/J$, while the staggered gap demonstrates critical behavior and vanishes at the quantum critical point. The gap in the uniform ladder $\delta=0$ is also shown for comparison.

corroborated only by numerical calculations.[5–7,9] With the bond parameters $Q_\pm$, P determined from the mean-field equations, we plot the gaps $\Delta_{c,s}$ given by Eqs. (20) and (23) as functions of the coupling ratio $J_\perp/J$ for several dimerizations in Fig. 4. Note that the gaps Δ_c and Δ_s coincide at "the decoupled chains line" $J_\perp/J=0$, as well as in the absence of dimerization. The qualitative differences between the gaps in the columnar and staggered phases are clearly seen. The former is always nonzero if the chains are dimerized and increases with the growth of $J_\perp/J$. The latter behaves nonmonotonously, passing through a critical point. It is worth noting that the known analytical limits (discussed above) are recovered exactly by the mean-field equations. In particular, on the "decoupled" axis $J_\perp=0$, the mean-field parameter $Q_\pm$ whose physical meaning is the average of the dimerization operator $\mathbf{S}_\alpha(n)\cdot\mathbf{S}_\alpha(n+1)$ behaves almost as that in the dimerized XY chain, coinciding with the exact values of that quantity at the ends of the interval $\delta\in[0,1]$. For the dimerized XY chain

$$Q_\pm=\langle \mathbf{S}_n\cdot\mathbf{S}_{n+1}\rangle \equiv t\pm\delta\cdot\eta, \tag{24}$$

the uniform term t and the dimerization susceptibility η at $T=0$ are given in terms of the elliptic functions and can be found, e.g., in Ref. 25. In particular,

$$\delta=0:\quad Q_\pm=\frac{1}{\pi}, \tag{25}$$

$$\delta=1:\quad Q_+=\frac{1}{2},\quad Q_-=0. \tag{26}$$

For instance, at $\delta=1$ ($J_\perp=0$), the ladder reduces to the set of decoupled dimers with the Heisenberg exchange $2J$. Our Eqs. (20)–(26) result in the exact value of the gap $\Delta=2J$ for this case. Similarly, at the integrable quantum critical point $\delta=1$, $J_\perp=2J$ (uniform snakelike chain), we have $Q_+=P$ and the mean field [Eq. (23)] correctly predicting a vanishing gap.

We plot in Fig. 5 the mean-field critical line given by

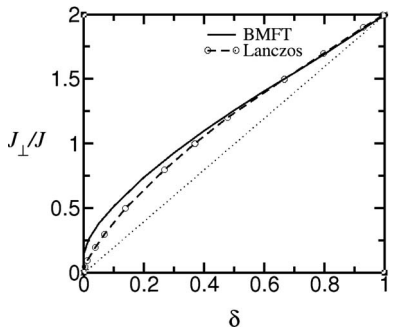

FIG. 5. Two-leg ladder: the critical line where the gap of the staggered phase vanishes. Along with the present bond mean-field theory predictions, the numerical diagonalization data from Ref. 9 are shown.

$$\frac{J_\perp}{J}=\frac{2u}{p}\delta, \tag{27}$$

along with the numerical results of Ref. 9. As one can see, the mean field works quite well quantitatively. It is surprising, but the mean field does much better than, e.g., the nonlinear sigma model (NLσM). The latter fails to predict the correct critical line.[4] The analysis of the topological term of the NLσM predicts that the line ends at $\delta=\frac{1}{2}$, $J_\perp=0$. The dotted line in Fig. 5 corresponds to the case when in the gap equations we set the bond parameters to their maximal values $Q_\pm=P=\frac{1}{2}$ (i.e., $u=p=2$), so $J_\perp/J=2\delta$. Such a naive "uniform isotropic limit" simplifies drastically the formulas and provides a decent approximation.

III. THREE-LEG LADDER

The three-leg dimerized ladder is defined by the Hamiltonian

$$H_{3L}=\sum_{\alpha=1,2}\sum_{n=1}^{N}J_\alpha(n)\mathbf{S}_\alpha(n)\cdot\mathbf{S}_\alpha(n+1)+J_\perp\sum_{n=1}^{N}[\mathbf{S}_1(n)\cdot\mathbf{S}_2(n)+\mathbf{S}_2(n)\cdot\mathbf{S}_3(n)]. \tag{28}$$

Similar to the two-leg case, we consider dimerizations of the whole ladder [Eqs. (2) and (3)], which follow the staggered or columnar patterns, as shown in Fig. 6.

Contrary to the previous case, we do not have limits where the behavior of this ladder is known *exactly*. Although the nondimerized limit $\delta=0$ is known to be gapless, and the three-leg ladder, roughly speaking, can be described as a "renormalized" spin-$\frac{1}{2}$ Heisenberg chain.[1,17] One can easily

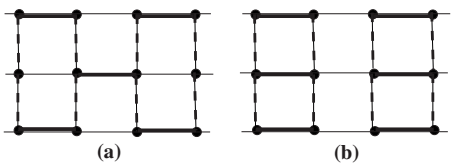

FIG. 6. Dimerized three-leg ladder. The line notations are the same as in Fig. 1. Dimerization patterns: (a) staggered and (b) columnar.

see from Fig. 6 that in the totally dimerized limit $\delta=1$, the columnar dimerized ladder becomes a set of $N/2$ decoupled six-spin plaquettes, while the staggered pattern evolves into a "decorated" chain. The latter, to the best of our knowledge, was not analyzed earlier.

We treat the problem in the bond mean-field approach as above. In fact, we will use directly our earlier results for the three-leg ladder coupled to phonons,[14] with minor modifications. Along with a couple of the bond parameters $Q_{\pm}$, defined by Eq. (12) with $\alpha=1,3$, one needs an extra couple of parameters $Q'_{\pm}$ for the chain in the middle, defined by the same equation with $\alpha=2$. The effective Hamiltonian density $\mathcal{H}^{s/c}$ [cf. Eq. (13)] is now a 6×6 matrix, and the Nambu spinor $\Psi_k^{\dagger}=(c_{1k}^{A\dagger}c_{1k}^{B\dagger}c_{2k}^{A\dagger}c_{2k}^{B\dagger}c_{3k}^{A\dagger}c_{3k}^{B\dagger})$. The constant term

$$C_3 = J_+|Q_+|^2 + J_-|Q_-|^2 + \frac{1}{2}J_-|Q'_+|^2 + \frac{1}{2}J_+|Q'_+|^2 + 2J_\perp|P|^2. \tag{29}$$

Diagonalization of $\mathcal{H}^{s/c}$ results in six energy eigenvalues $\pm E_j^{s/c}(k)$, $j=1,2,3$ for each configuration

$$E_1^s(k) = E_1^c(k) = \frac{1}{2}\sqrt{W}, \tag{30}$$

and

$$E_n^{s/c}(k) = \frac{1}{2^{3/2}}[(-1)^n\sqrt{(W-W')^2+8J_{\perp 1}^2(W+W'+2Y^{s/c})}+W + W'+4J_{\perp 1}^2]^{1/2}, \quad n=2,3, \tag{31}$$

where

$$Y^s = (J_{1+}J'_{1+}+J_{1-}J'_{1-})\cos(2k)-(J_{1+}J'_{1-}+J_{1-}J'_{1+}),$$

$$Y^c = (J_{1+}J'_{1-}+J_{1-}J'_{1+})\cos(2k)-(J_{1+}J'_{1+}+J_{1-}J'_{1-}),$$

and $J'_{1\pm}$ and W' are given by Eqs. (16) and (17), where $Q_{\pm}\to Q'_{\pm}$. The mean-field equations are obtained via minimization of the free energy, given by Eq. (19) with $m=3$. Our analysis here follows the steps of the above two-leg case, so we will be brief.

Similar to the two-leg case, the columnar order corresponds to a state with lower energy of the dimerized three-leg ladder, thus this is a thermodynamically stable state. We present several plots of the zero-temperature energies for the two types of dimerization order in Fig. 7.

The columnar phase of the three-leg ladder is *always gapped* when $\delta\neq0$. The gap $\Delta_c=E_1^c(0)$ is given by

$$\Delta_c = Ju\delta. \tag{32}$$

In the limit $\delta\to0$, this mean-field approach correctly predicts gaplessness,[17] in accordance with the general results for odd-m-leg ladders.[1,2] We should however point out that the gapless limit $\Delta_c\to0$ when $\delta\to0$ is recovered only if we set $(Q_-^{\sharp}-Q_+^{\sharp})\to0$. The latter limit, obviously correct from a physical point of view [cf. Eq. (24)], is not automatically fulfilled in the bond mean-field equations. This is an artifact of the particular bond mean-field decoupling scheme and is not intrinsic for any mean-field decoupling, as one can see, e.g., from the (classical) mean-field results in Ref. 26. It is worth noting that the simple analytical approximations we derived are free of these flaws.

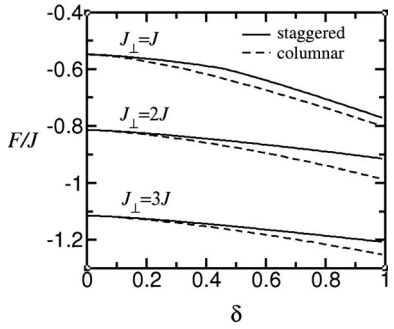

FIG. 7. Three-leg ladder: the energies of staggered and columnar dimerization configurations at $T=0$.

The staggered phase is gapped everywhere, except for the critical line of vanishing gap when $\delta\neq0$, $J_\perp\neq0$. Thus, we confirm the original conjecture,[4] which has been corroborated by the recent DMRG calculations of Almeida *et al.*[12] The gap of the staggered phase, found from $E_3^s(0)$, reads as

$$\Delta_s^{<} = \frac{J}{\sqrt{2}}\left[\delta^2(u^2+u'^2)+\left(\frac{J_\perp p}{J}\right)^2 - (u+u')\sqrt{(u-u')^2\delta^2+2\left(\frac{J_\perp p}{J}\right)^2}\right]^{1/2}, \tag{33}$$

where u' is given by Eq. (21) with the replacement $Q_{\pm}\to Q'_{\pm}$. The columnar gap Δ_c and the (critical) staggered gap Δ_s, directly calculated from the mean-field equations, are plotted in Fig. 8.

There is one subtlety related to the staggered gap, absent in the case of the two-leg ladder. Recall that we defined gap in a given phase as a *minimal* band gap of the energy eigenvalues of the effective single-particle Hamiltonian. What happens here is that the staggered gap [Eq. (33)] is determined from the eigenvalue E_3^s, which has minimal band gap at small $J_\perp/J$. However with the increase in $J_\perp/J$ it reaches

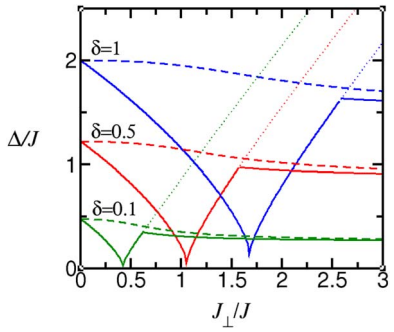

FIG. 8. (Color online) Three-leg ladder: the gaps of the staggered (solid lines) and columnar (dashed lines) phases for three values of dimerization. Contrary to the monotonous gap dependence on couplings in the columnar phase, the staggered gaps vanish at the quantum critical points. The dotted lines correspond to the numerical solution given by Eq. (33) and should be distinguished from the physically defined gaps. For more details, see the text.

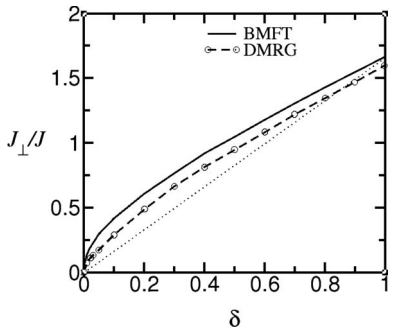

FIG. 9. Three-leg ladder: the critical line of the vanishing staggered gap. Our results are shown along with the DMRG data from Ref. 12.

a certain value where "a level crossing" occurs, i.e., the band gaps of E_3^s and E_1^s are equal. Then for bigger $J_\perp/J$, the staggered gap is determined by the (minimal) band gap of E_1^s. In addition, since $E_1^s=E_1^c$ [Eq. (30)], the staggered and columnar gaps are equal, and according to Eq. (32), $\Delta_s^>=\Delta_c=Ju\delta$ in that region. In fact, however, one can see differences between $\Delta_s^>$ and Δ_c. The reason is that the self-consistently determined mean-field parameters entering Eq. (21) for u are not necessarily equal for two configurations.

To get some analytically tractable formulas for the gap, let us approximate $u=u'$. Then

$$\Delta_s^< \approx J\left|u\delta-\frac{p}{\sqrt{2}}\frac{J_\perp}{J}\right|. \tag{34}$$

Making an even more drastic approximation for the bond mean-field parameters by their maximal values, i.e., $u=2$ and $p=1+1/\sqrt{2}$ $(P=2^{-3/2})$, we get

$$\Delta_s^< \approx 2J\left|\delta-\frac{1+\sqrt{2}}{4}\frac{J_\perp}{J}\right|. \tag{35}$$

We plot in Fig. 9 the critical line obtained from the "exact" mean-field gap Eq. (33) and the DMRG result in Ref. 12. The dotted line $J_\perp/J=1.6569\delta$ is the prediction of the simplified gap Eq. (35).

Note that contrary to the two-leg ladder, where we have exact predictions for the two integrable end points of the critical line, for this case we do not have an independent prediction for the critical ratio $J_\perp/J$ at $\delta=1$.[27] We can point out, however, a very good agreement between the mean field and DMRG. The former via Eq. (33) yields 1.67 [or 1.66 via Eq. (35)], while the latter yields 1.60.

IV. CONCLUSIONS

We analyze the possibility of quantum criticality (gaplessness) in the dimerized two- and three-leg ladders. Contrary to earlier studies of these models, we do not imply a particular ladder's dimerization pattern. In this work we restrict ourselves to the zero-temperature properties. We find that for a given intrinsic intrachain dimerization, the ladder has lower zero-temperature energy for the columnar dimerization order. This is true for both types of ladders (two and three legs) considered. For the columnar dimerization pattern the ladders are always gapped, i.e., there are no lines of quantum criticality on the $(\delta,J_\perp)$ plane.

For the staggered dimerization order, we find that the ladders possess the quantum critical lines, in agreement with earlier analyses of this problem.[5–9,11,12] The mean-field theory we apply in this study demonstrates its quantitative accuracy. For the two-leg ladder, the mean-field critical line passes through both integrable quantum critical points (0,0) and $(1,2J)$ on the $(\delta,J_\perp)$ plane and demonstrates a good agreement with the numerical diagonalization results[9] in between. For the case of the three-leg ladder, the mean-field critical line passes through (0,0) (the only integrable quantum critical point) and agrees well with the critical line determined through the DMRG calculations.[12]

Thus, from a more practical point of view, the very possibility of quantum criticality in dimerized ladders hinges on some mechanism, which would lock the dimerization order into a more energetically expensive staggered configuration. A realistic example of dimerization in the three-leg ladder through the spin-Peierls mechanism results in the columnar order and so, the gapful phase everywhere at nonzero dimerization.[14] At the moment we are not aware of any Hamiltonian that would provide such a mechanism for quantum criticality in dimerized ladders to occur.

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[27] Using the formula for the NLσM topological term derived in Ref. 4, we obtain the critical line located between two points: ($\delta=\frac{18}{35}=0.5142\ldots$, $J_\perp=0$) and ($\delta=1$, $J_\perp/J=1.9823\ldots$). So this approach does not result in adequate predictions.