# Probable absence of a quadrupolar spin-nematic phase in the bilinear-biquadratic spin-1 chain

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We study numerically the ground-state phase diagram of the bilinear-biquadratic spin-1 chain near the ferromagnetic instability point, where the existence of a gapped or gapless nondimerized quantum nematic phase has been suggested. Our results, obtained by a highly accurate density-matrix renormalization-group calculation, are consistent with the view that the order parameter characterizing the dimer phase vanishes only at the point where the system becomes ferromagnetic, although the existence of a gapped or gapless nondimerized phase in a very narrow parameter range between the ferromagnetic and the dimerized regimes cannot be ruled out.

## I. INTRODUCTION

In the past two decades, a large number of papers was devoted to the study of various properties of quantum spin chains. This was inspired to a large extent by Haldane's conjecture,[1] which states that isotropic antiferromagnetic spin chains with half-odd-integer or integer spin values behave completely differently. While the excitation spectrum is gapless in the first case, a gap, the so-called Haldane gap, is generated in the other case.

The most general form of isotropic coupling for $S=1/2$ spins is the usual Heisenberg model. For higher spin values, higher powers of the spins may appear in the Hamiltonian and this gives rise to a richer phase diagram. For $S=1$ spins, assuming the most general isotropic nearest-neighbor interaction, the Hamiltonian has bilinear and biquadratic terms in the spin operators and it can be written in the form

$$\mathcal{H} = \sum_i \mathcal{H}_{i,i+1} = \sum_i [\cos\theta (\mathbf{S}_i \cdot \mathbf{S}_{i+1}) + \sin\theta (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2].$$

(1)

In this parametrization, $\theta=0$ corresponds to the antiferromagnetic model where the spectrum has a finite Haldane gap, while at $\theta=\pm\pi$ the system is ferromagnetic. In fact, both phases have a finite extension in the parameter space. The massive Haldane phase is stable for $-\pi/4 < \theta < \pi/4$, while ferromagnetism exists for $\pi/2 < \theta < \pi$ and $-\pi < \theta < -3\pi/4$. The phase boundaries $\theta=\pm\pi/4$, $-3\pi/4$, and $\pi/2$ are in fact special points, where the model can be solved exactly.[2–5]

The Haldane gap vanishes at $\theta=\pi/4$ and three soft modes appear at $k=0$ and $\pm 2\pi/3$. The system remains critical for $\pi/4 < \theta < \pi/2$ with the soft modes remaining at $k=0, \pm 2\pi/3$ (Refs. 6 and 7). This gives rise to a power-law decay of correlations with a $3a$ periodic oscillation, hence the name "trimerized" phase, although the translation symmetry is not broken.

The gap vanishes also at the other end of the Haldane phase, at $-\pi/4$, but it reopens for $\theta < -\pi/4$ and a massive dimerized phase with spontaneously broken translational symmetry is found. A possible definition of the dimer order parameter $D$ is

$$D = \lim_{N\to\infty} |D_{N/2}|; \quad D_i = \langle \mathcal{H}_{i-1,i} \rangle - \langle \mathcal{H}_{i,i+1} \rangle,$$

(2)

where chains are considered with open boundary condition. Dimerization is measured as the alternation in the bond energy in the middle of a long enough open chain.

The properties of this phase are best known for $\theta=-\pi/2$, where a partial mapping[8–10] to the nine-state quantum Potts model allows to calculate exactly the ground-state energy, the gap, the correlation length, and also the dimer order.[11]

While the properties and boundaries of the ferromagnetic, Haldane, and critical "trimerized" phases have been well established, there has been a long debate in the literature as for the boundary of the dimerized phase and the eventual existence of another phase between this dimerized phase and the ferromagnetic one near $\theta=-3\pi/4$, as seen in Fig. 1.

By studying fluctuation effects near the end point of the ferromagnetic phase, Chubukov[12] claimed that there should be a gapped nondimerized nematic phase between the ferromagnetic and the dimerized phases. In fact, both ferromagnetism and dimerization involves spontaneous symmetry breaking: for ferromagnetism SU(2) is broken, whereas for dimerization it is translation invariance. These symmetries are largely unrelated, and there seems to be no *a priori* rea-
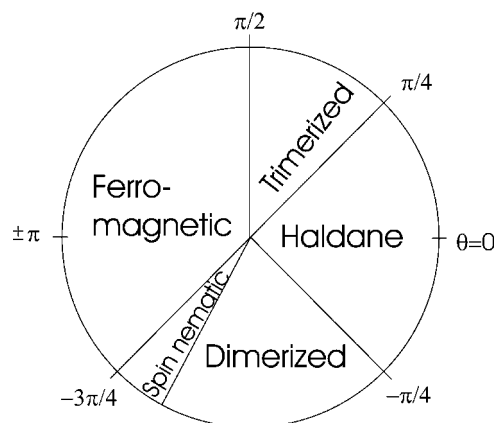


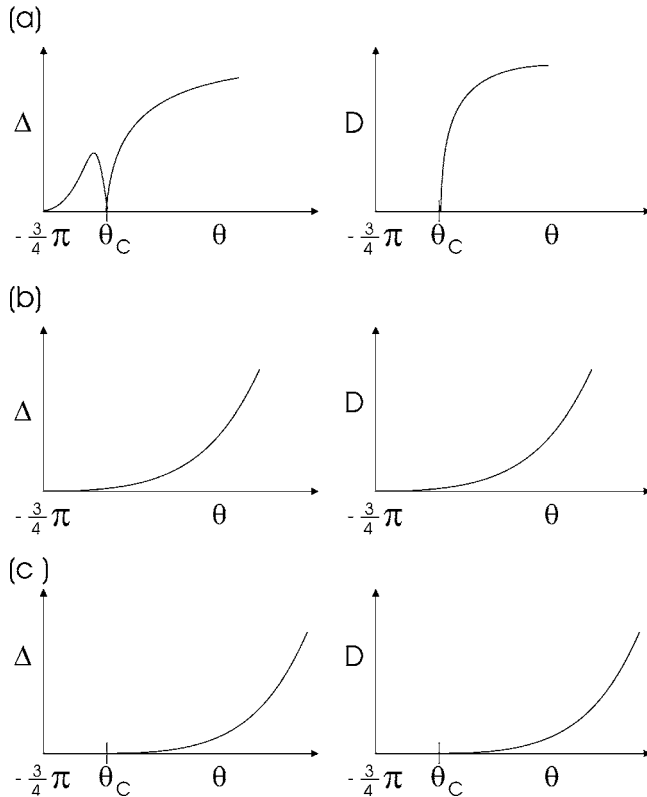FIG. 1. Schematic plot of the phase diagram of the bilinear-biquadratic $S=1$ model as a function of $\theta$.

FIG. 2. Schematic plot of the excitation gap ($\Delta$) and the dimer order parameter $D$ as a function of $\theta$ around the phase boundary of the ferromagnetic and dimerized phases. (a) Chubukov's suggestion; (b) the result of earlier numerical work; (c) the case of a critical nondimerized phase.

son why the two should be broken hand in hand in one single transition.

According to Chubukov's scenario the dimer order parameter is finite in the dimerized phase and vanishes together with the gap at a $\theta_c$ close to, but definitely above, $-3\pi/4$. The gap reopens for $\theta < \theta_c$ and closes again at $-3\pi/4$, but the dimer order parameter remains zero in this whole range of $\theta$. In this extended region, the system would have a non-degenerate singlet ground state and unbroken translational symmetry. Since the higher-dimensional counterpart of Chubukov's phase would have quadrupolar order, this phase is usually called the "spin-nematic" phase. The behavior of the gap and the dimer order parameter according to this scenario are shown schematically in Fig. 2(a). Other field-theoretic calculations based on a nonlinear $\sigma$-model approach for the director field also supported this scenario.[13] Note, however, that all these field-theoretic calculations assumed a translation invariant ground state and did not check its stability against a possible spontaneous breaking of translation invariance.

In our earlier numerical calculations,[14,15] where the vanishing of the gap was studied, we found no evidence for a closing and reopening gap. In these works both the gap and the dimer order parameter, indicating broken translation invariance, were reported to vanish at $\theta_c = -3\pi/4$ only. This scenario, the absence of the nematic phase, is shown in Fig. 2(b).

Recent quantum Monte Carlo[16] and density-matrix renormalization-group (DMRG) (Ref. 17) calculations have indicated that although Chubukov's proposal may not be completely correct in a closing and reopening gap, an exotic, *critical* phase with quadrupolar correlations may exist between the ferromagnetic and dimerized phases for $-3\pi/4 < \theta < \theta_c$. The behavior of the gap and the dimer order in this scenario is shown in Fig. 2(c). Läuchli *et al.*[17] estimated the value of $\theta_c$ to be $-0.67\pi$.

The aim of the present paper is to find further numerical evidence for the possible existence of this nondimerized phase. For this purpose we have studied finite spin chains up to 1000 lattice sites with open (OBC) and periodic boundary conditions (PBC) for various $\theta$ values using the DMRG method.[18] We have analyzed the behavior of the excitation gap and the dimer order parameter given by Eq. (2).

## II. NUMERICAL PROCEDURE

The numerical calculations were performed using the DMRG algorithm. Since the numerical accuracy is of crucial importance in the present study, this section is devoted to the problem of how the accuracy of our calculations could be determined and controlled.

We have performed DMRG calculations both by using the standard technique,[18] i.e., by keeping the number of block states fixed, and by using the dynamic block state selection (DBSS) approach.[19,20] All eigenstates of the model have been targeted independently using two or three DMRG sweeps.

In the standard procedure $M = 500 - 1000$ block states have been used. It was found that for the largest systems built up of $N = 500 - 1000$ lattice sites the truncation error varied in the range $10^{-8} - 10^{-9}$ for OBC and $10^{-5} - 10^{-7}$ for PBC. The following numbers are indicative of the accuracy: for OBC using $M = 300$ or $M = 500$ block states the ground-state energies at $\theta = -0.7\pi$ differ in the fifth digit, $\delta E(300, 500) < 10^{-5}$, and the accuracy improved one order of magnitude when $M = 1000$ block states were kept, $\delta E(500, 1000) < 10^{-6}$.

The DBSS approach[19] allows for a more rigorous control of numerical accuracy, and we set the threshold value of the quantum information loss $\chi$ to $10^{-8}$. The minimum number of block states $M_{min}$ has been set to 256. The entropy sum rule was checked for all finite chain lengths for each DMRG sweep, and it was found that the sum rule was satisfied after the second sweep already. The maximum number of block states varied in the range 600–1400 for OBC and 1000–2500 for PBC, respectively.

After accomplishing the infinite lattice procedure and using White's wave-function transformation method[21] the largest value of the fidelity error of the starting vector $\Psi_{stv}$, $\delta\epsilon_{\Psi_{stv}} = 1 - \langle \Psi_T | \Psi_{stv} \rangle$ was of the order of $10^{-10}$, where $\Psi_T$ is the target state determined by the diagonalization of the superblock Hamiltonian.

As another test of the accuracy we calculated the dimer order profile $D_i$ using PBC. In theory, this should vanish identically for all finite chain lengths. Using the DBSS approach with $\chi = 10^{-6}$, $M_{min} = 256$ for chains up to $N = 200$ sites, in the parameter range $-0.75\pi \leq \theta \leq -0.5\pi$, the value
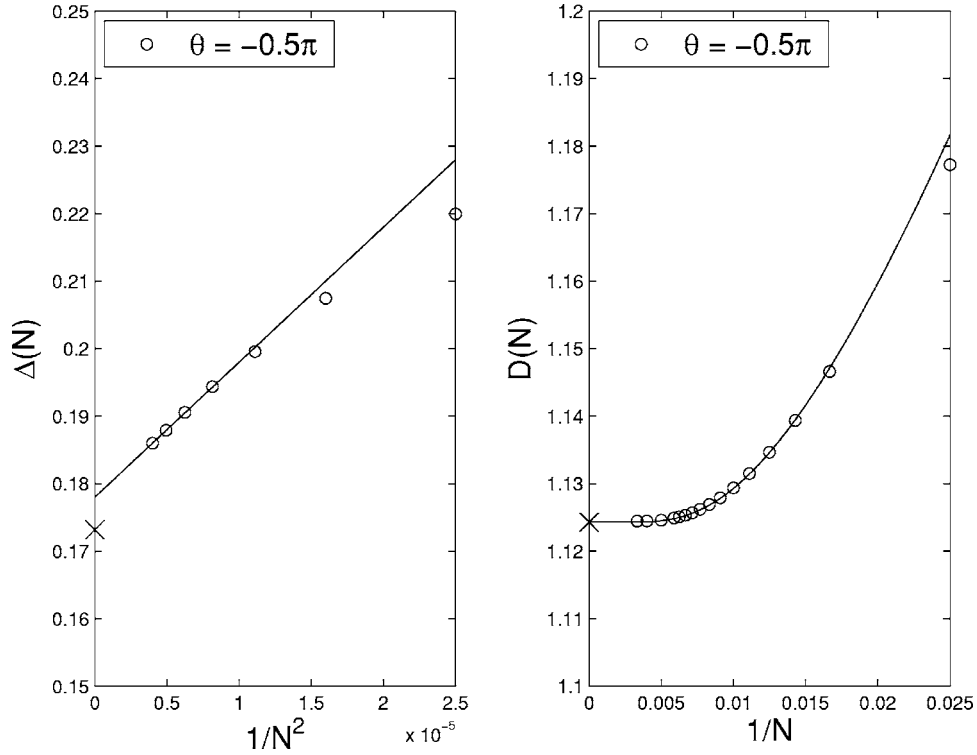
FIG. 3. The excitation gap ($\Delta$) and dimer order parameter ($D$) at $\theta=-0.5\pi$ as a function of $1/N^2$. The symbol $\times$ denotes the exact value. The solid lines are least-square fits using the scaling forms discussed in the text.

obtained for $D_i$ was less than $10^{-5}$ for all $i=1,\ldots,N$. The ratio of the DMRG block energy and the number of bonds within the block agreed up to five digits with the bond energy obtained between the two DMRG blocks. These results indicate that the finite dimer order parameter calculated with OBC is probably accurate at least up to four digits.

### III. GAP VERSUS DIMER ORDER PARAMETER

In order to obtain the energy gap $\Delta$ and the dimer order parameter $D$ in the thermodynamic limit $N\to\infty$, a finite-size scaling analysis has to be performed. In this section, as a benchmark case, we study in detail the exactly solvable point $\theta=-\pi/2$. We demonstrate that for OBC, which is usually preferred in DMRG, the dimer order parameter is a better quantity to be analyzed, as it provides much more accurate results. At the special point $\theta=-\pi/2$ most of the quantities of special interest have been determined exactly.[8–11] The gap is $\Delta_{\text{exact}}=0.173\,178$, the dimer order parameter reads $D_{\text{exact}}=1.124\,378$, and the coherence length is $\xi_{\text{exact}}=21.072$.

#### A. Energy gap

In a noncritical model with PBC the gap $\Delta(N)$ is expected to scale in leading order as

$$\Delta(N) = \Delta + c\frac{1}{N^{1/2}}\exp(-N/\xi). \qquad (3)$$

For OBC, however, the corrections are algebraic, and $\Delta(N)$ is expected to vary as

$$\Delta(N) = \Delta + a/N^2 + \mathcal{O}(N^{-4}), \qquad (4)$$

where $a$ is a suitable constant. A qualitative argument for this scaling ansatz can be given as follows.[22] The magnon dispersion is quadratic around its minimum, $\epsilon(k)=\sqrt{\Delta^2+v^2k^2}$. Due to the boundary condition, however, the magnon wave function should have nodes on the boundary, which constrains the lowest possible magnon momentum to be $k=\pm\pi/N$. Consequently, the lowest possible excitation energy (the gap) is $\Delta(N)=\sqrt{\Delta^2+v^2(\pi/N)^2}\approx\Delta+\pi^2v^2/2\Delta N^2+\mathcal{O}(N^{-4})$, giving Eq. (4).

Since in the region of interest the ground state is a singlet and the lowest-lying excited state is in the $S_{\text{tot}}=2$ total spin sector, the excitation gap is calculated from the energy difference between the lowest-lying levels of the $S_{\text{tot}}=2$ and $S_{\text{tot}}=0$ sectors,

$$\Delta(N) = E^{(0)}_{S_{\text{tot}}=2}(N) - E^{(0)}_{S_{\text{tot}}=0}(N). \qquad (5)$$

We used OBC and the DBSS approach with $\chi=10^{-8}$, $M_{\text{min}}=256$. Our results for the gap as a function of $1/N$ up to $N=500$ are shown in the first panel of Fig. 3. A quadratic fit using the form in Eq. (4) for $250\leqslant N\leqslant500$ yields $\Delta=0.177$ and $a=2300$. The gap is about 2% higher than the exact result.

#### B. Dimer order

For finite open chains with an even number of lattice sites the two typical valence-bond configurations of the dimerized phase are shown in Fig. 4. Due to the boundary condition these two singlet states are separated by a finite-energy gap
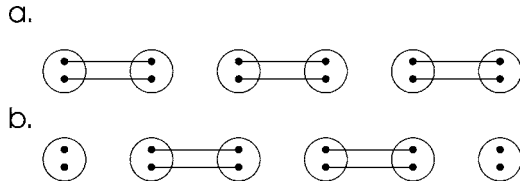
a.

b.

FIG. 4. Typical valence-bond configurations for chains with even lattice sites.

even in the thermodynamic limit. The ground state retains a high overlap with the configuration depicted in Fig. 4(a) as $N \to \infty$. This allows us to measure the possible dimer order by considering $D(N)$ and take the limit $N \to \infty$. Note that this is only possible for OPB. For PBC the two possible dimerized configurations mix up and restore translation invariance for any finite $N$. In this case dimer order could only be measured by considering the dimer (four-point bond-bond) correlation function. In fact, this was the quantity measured numerically in Ref. 17. Since calculations with PBC give less accurate results in DMRG than with OPB, we do not pursue here this approach.

Accordingly, in our numerical calculations we used OBC with $\chi \simeq 10^{-8}$, $M_{\min} = 256$, and determined $D(N)$ as defined in Eq. (2) at the center of the chain. Two DMRG sweeps were taken and we checked that the entropy sum rule was satisfied. Our result is shown in the second panel of Fig. 3. The upward curvature of the data points as a function of $1/N$ is apparent for very short chain lengths ($N \simeq 40 - 80$) and already for $N > 200$ $D(N)$ agrees up to three digits with the infinite chain-length limit.

For noncritical models the characteristic behavior of the system is determined by a finite correlation length. Therefore, the end effects decay exponentially and the *local* quantity $D(N)$ is expected to vary in leading order according to

$$D(N) = D + dN^{-\beta} \exp(-N/2\xi), \qquad (6)$$

which is qualitatively similar to the PBC scaling of the gap in Eq. (3), except that the scaling variable is the distance of the middle of the chain from the boundary, $N/2$, and the exponent of the algebraic prefactor is *a priori* unknown. Nevertheless, knowing the exact value of $D$ for $\theta = -0.5\pi$, a least-square fit provided $\beta$ very close to 1. Using this, our numerical data for $N > 60$ can be fitted with $D = 1.124\,375$, $\xi = 20.2$, and $a = 5.9$ (see the solid line in the second panel of Fig. 3). The correlation length is off by 4%, but the numerical value of $D$ has an excellent relative accuracy of $3 \times 10^{-6}$. The exponential convergence of local quantities such as the dimer order parameter $D(N)$ makes the extrapolation to the thermodynamic limit very reliable. Our general conclusion is that—because of their different scaling behavior—the dimer order parameter is a much better quantity to analyze than the energy gap. In the next section we pursue this idea to investigate the phase diagram as a function of $\theta$.

## IV. NUMERICAL RESULTS

For the reasons presented above, the highest chance to find the subtle nondimerized spin-nematic phase near

$\theta = -3\pi/4$ is by studying the dimer order in open chains. Therefore, we calculated $D(N)$ using OBC up to 1000 lattice sites for various $\theta$ values between $-3\pi/4$ and $-\pi/2$. We have set $\chi \simeq 10^{-8}$, $M_{\min} = 256$, and used three DMRG sweeps. Due to the very large correlation length in the vicinity of the ferromagnetic phase boundary the maximum value of $M$ is varied in the range of 600–1400 for our longest chains. Our numerical results are shown in Fig. 5 for two different $\theta$ values. The numerical error is much smaller than the size of the symbols.

It is seen in the figure that for large $N$ the data points show an upward curvature as a function of $1/N$ for all $\theta$ values. On the other hand, the inflexion point shifts towards very long chain lengths with decreasing $\theta$ values. The extrapolated value $D$ of the dimer order parameter was determined using Eq. (6). These values are shown in Fig. 6 as a function of $\theta$. In fact, we found a finite, nonzero $D$ for all $\theta$ shown. However, we have no results for $\theta < 0.7\pi$, where $D(N)$ is so small that it is comparable to the numerical error. Although the dimer order parameter decreases very rapidly for $\theta < -0.64\pi$, the smooth behavior of $D$ as a function of $\theta$ and the upward curvature observed suggests that it vanishes at $\theta = -3\pi/4$.

It is also apparent from Fig. 6 that the dimer order parameter resembles the form of the Berezinskii-Kosterlitz-Thouless (BKT) transition, thus it opens exponentially slowly as a function of $\theta$,

$$D(\theta) = a \exp[-c(\theta - \theta_c)^{-\sigma}], \quad \theta_c = -3\pi/4, \qquad (7)$$

for $\theta > \theta_c$. In Eq. (7), $a$ and $c$ are nonuniversal constants and $\sigma$ is a characteristic exponent, which was estimated by a least-square fit to be $\sigma = 1.3 \pm 0.3$ (see Fig. 6). This functional form is in qualitative agreement with our earlier numerical result.[14]

Based on our calculations we conclude that there is no sign of any phase transition to either a gapped or a gapless nondimerized phase in the vicinity of $\theta \simeq -0.67\pi$, and thus a direct phase transition takes place between the ferromagnetic and the dimerized phases.

## V. CONCLUSION

In summary, we have performed a density-matrix renormalization-group calculation on the spin-1 bilinear-biquadratic spin chain model in the vicinity of the ferromagnetic phase in order to search for a nondimerized quantum nematic phase suggested by Chubukov[12] or an extended critical region reported recently by Läuchli *et al.*[17] We took special care of the numerical accuracy since it has special importance in the present problem. We used the DBSS approach with the maximum number of block states varying between 1000 and 2000, and performed calculations on very long chains up to $N = 1000$ lattice sites.

As a benchmark case we analyzed in detail the exactly solvable point $\theta = -\pi/2$. We have found that the dimer order
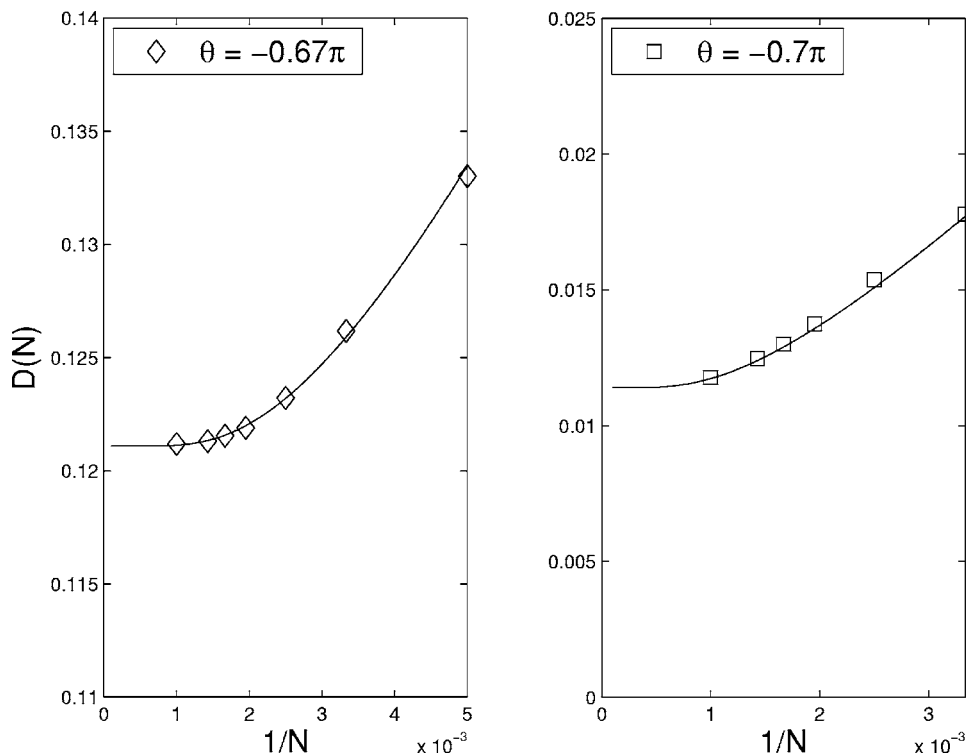
FIG. 5. Finite-size scaling of the dimer order parameter at $\theta = -0.67\pi$ and $-0.70\pi$ for $100 \leqslant N \leqslant 1000$.

parameter is a quantity, which can be determined numerically much more accurately than the energy gap, because of their unequal finite-size scaling forms. Whereas the gap scales algebraically in open chains, the dimer order parameter, which is a local quantity measured in the middle of the chain, becomes highly independent of end effects and scales exponentially.

The phase diagram of the model was explored in general by computing the dimer order parameter as a function of $\theta$. We have found strong indications that the dimer order, which characterizes the dimer phase, only vanishes at the phase boundary of the ferromagnetic phase $\theta = -3\pi/4$. The behav-



FIG. 6. The extrapolated value of the dimer order parameter as a function of $\theta/\pi$. The solid curve is a least-square fit using the form in Eq. (7) with $a = 2.4 \pm 0.6$, $c = 0.11 \pm 0.05$, and $\sigma = 1.3 \pm 0.3$.

ior resembles that of Berezinskii-Kosterlitz-Thouless transition, i.e., the order parameter opens exponentially slowly as we move away from the transition point. Our findings are in agreement with the exponentially slow opening of the energy gap reported earlier.[14] Nevertheless, the actual transition itself is of first order as it involves direct level crossings, as well. It is noteworthy that at $\theta = -3\pi/4$ the model has an extra SU(3) symmetry,[3] which causes extra degeneracies in the spectrum. We are tempted to speculate that this extra symmetry may play a role in that the two phases with seemingly unrelated broken symmetries, SU(2) and translation invariance, meet in this special point without an intermediate phase.

We could not find any trace of a nondimerized regime, at least surely not above $\theta \approx -0.7\pi$. Below this limit numerical precision is a crucial issue since the quantities of interests are extremely small. If the intermediate phase exists, it should be constrained in a very narrow region near $\theta = -3\pi/4$, certainly much narrower than predicted by Läuchli *et al.* The more likely alternative interpretation, i.e., the nonexistence of the intermediate phase, is clearly at odds with current field-theory analysis. A reconciliation of the numerical results with field theory would be very welcome in the future.
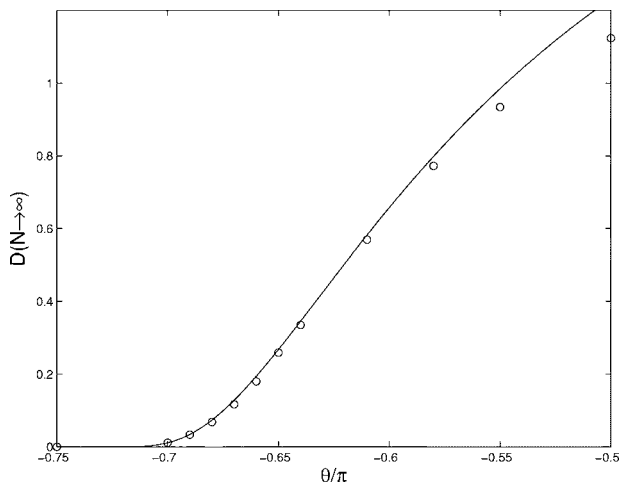
**ACKNOWLEDGMENTS**

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