Search for the nondimerized quantum nematic phase in the spin-1 chain

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Abstract

Chubukov's proposal concerning the possibility of a nondimerized quantum nematic phase in the ground-state phase diagram of the bilinear-biquadratic spin-1 chain is studied numerically. Our results do not support the existence of this phase, but they rather indicate a direct transition from the ferromagnetic into the dimerized phase.

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I. INTRODUCTION

The general isotropic spin-1 model with nearest neighbor interactions on a d-dimensional lattice is described by the Hamiltonian

$$H = \sum_{<i,j>} h_{i,j} = \sum_{<i,j>} \left[\cos\theta \ (\boldsymbol{S}_i \cdot \boldsymbol{S}_j) + \sin\theta \ (\boldsymbol{S}_i \cdot \boldsymbol{S}_j)^2 \right] \ , \tag{1}$$

where the parameter θ governs the ratio of the bilinear and biquadratic terms. This model has been the subject of several studies in the last decade [1–11]. The existence of a variety of phases has been demonstrated. The complete characterization of these phases and of the phase transitions between them is, however, not yet entirely solved.

For $d \geq 2$ the semiclassical approximation gives a rather good description of the ground state [1]. The zero temperature phase diagram obtained in this way is sketched in Fig. 1(a). It consists of four different phases. The usual ferromagnetic ($\pi/2 < \theta < 5\pi/4$) and antiferromagnetic ($-\pi/2 < \theta < \pi/4$) phases are separated on both sides by rather exotic phases, where *collinear* or *orthogonal nematic* ordering appears. In all phases the original $SU(2)$ symmetry of the model is spontaneously broken. The order can be characterized by different long range order parameters. In the nematic phases, e.g., the expectation value of the spin operators vanishes,

$$\langle S_i^\alpha \rangle = 0 \ , \qquad \alpha = x, y, z \ , \tag{2}$$

while some of the quadrupole operators have finite expectation values with

$$\langle (S_i^x)^2 \rangle = \langle (S_i^y)^2 \rangle \neq \langle (S_i^z)^2 \rangle \ . \tag{3}$$

Quantum effects, that appear most strongly in one dimension (1D), can drastically modify this phase diagram. Coleman's theorem [12] (the quantum analog of the Mermin-Wagner theorem) states that, unless the order parameter is a conserved quantity, quantum fluctuations will restore the continuous symmetry of the Hamiltonian. This means that apart from the ferromagnetic state, whose domain of stability is the same in the classical and quantum calculations, in 1D the ground state of the model in Eq. (1) should be disordered for any

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other value of θ. Within this quantum disordered regime, however, there could still be several phases. The semiclassical phase diagram in Fig. 1(a) should therefore be replaced by a rather different *quantum* phase diagram.

The quantum analog of the classical Néel state is the Haldane phase [13], where dynamic mass generation leads to a unique disordered ground state with hidden order [14]. There is a finite gap (Haldane gap) to the excitations. This phase is thought to exist in the region $-\pi/4 \leq \theta \leq \pi/4$.

The orthogonal nematic phase in $\pi/4 \leq \theta \leq \pi/2$ is replaced by a tripled periodic phase. There are strong numerical indications [7] that this phase is critical due to three soft modes at $k = 0$ and $\pm 2\pi/3$, as is the case in the integrable Lai-Sutherland [15] model corresponding to $\theta = \pi/4$.

Far less understood is the behavior on the other side of the ferromagnetic regime. In a recent series of papers Chubukov [5,6] has shown by using perturbational calculation on a specially chosen "vacuum" state with nematic long range order and by applying the standard renormalization group method, that in 1D in the vicinity of the ferromagnetic instability point quantum fluctuations restore the $SU(2)$ symmetry, the ground state remains unique, and the interaction between the Goldstone bosons leads to dynamic mass generation. The opening of the gap is exponentially slow as θ departs from θ_F.

Chubukov [6] has emphasized that this disordered phase is different from the Haldane phase. In fact, the two phases are separated by a dimerized phase in which translational invariance is broken. This dimerized phase is believed to exist for $\theta < -\pi/4$. The spontaneous breakdown of the translational invariance leads to a pair of singlet ground states and a finite excitation gap above it. This behavior has been proven rigorously at $\theta = -\pi/2$, where the system is again integrable and hence the spectrum can be determined exactly [3,4]. The value of the gap at this point is 0.173178, a rather small value, while the correlation length is large, about 21 lattice units [4]. This explains the early numerical difficulties in identifying this phase [2].

As a further support for the existence of the new disordered phase Chubukov [6] has

pointed out that at $\theta_F \equiv -3\pi/4$, where the ferromagnetic state becomes unstable, the magnon spectrum has no soft mode at $k = \pi$. Neither is there any interesting feature at $k = \pi$ in the spectrum of bound states of two, three, etc., magnons. There does not seem to exist any mode that could drive a direct transition from the ferromagnet into a dimerized state. In fact, his study of the effect of quantum fluctuations on the dimerized state, using appropriate bosonization, led him to conclude that the stability region of the dimerized phase is $\theta_c \leq \theta \leq -\pi/4$, where $\theta_c \approx -.7\pi$, thus the disordered phase could exist in the range $-3\pi/4 \leq \theta \leq \theta_c$.

In what follows this hypothesized phase will be referred to as the *nondimerized quantum nematic* or *Chubukov's phase*. The phase diagram expected to be valid in the 1D case is summarized in Fig. 1(b).

The main goal of the present paper is to find numerical evidence for the possible existence of Chubukov's phase. For this purpose we studied finite spin chains for various values of θ. Beside the usual Lánczos diagonalization method, which allowed us to study chains up to $L = 16$ sites with periodic boundary condition, we used White's density matrix renormalization group method (DMRG) [16] with open boundary condition up to $L = 48$. The data were analyzed by finite-size scaling techniques.

Since Chubukov's proposed phase is supposed to have a nondegenerate singlet ground state and unbroken translational symmetry, the transition to this phase from the dimerized phase can be located either by studying the ground state degeneracy, the appearance of soft modes at the transition point, or the behaviour of the dimerization order parameter. Our results for these quantities will be presented subsequently in the next three sections. Section V. contains some concluding remarks.

II. STUDY OF THE GROUND-STATE DEGENERACY

One possibility to see the difference between the dimerized and the nondimerized quantum nematic phases would be to study the degeneracy of the infinite volume ground state.

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For a finite system with even number of sites L the ground state is unique for any $\theta > \theta_{\mathrm{F}}$; it is an $S_T = 0$ spin singlet state. If periodic boundary condition is used, this state has momentum $k = 0$. In the dimerized phase there has to be another singlet state with momentum $k = \pi$ with an energy, which, for long enough chains, is exponentially close to the ground-state energy. This should not be the case, however, for the nondimerized quantum nematic phase, where the ground state is expected to be nondegenerate, even in the thermodynamic limit. Thus a gap has to be opened between the lowest singlet $k = 0$ and $k = \pi$ states. Therefore, we first studied the finite-size scaling behaviour of this gap.

The gaps were calculated by the Lánczos diagonalization method for chains with $L = 8, 10, \ldots 16$ sites. It is worth pointing out why we could not use the DMRG method to study this degeneracy problem, although it would have allowed us to consider much longer chains. Exactly at the point θ_{F} the model has an extra $SU(3)$ symmetry and the Hamiltonian can be written as a (negative) sum of permutation operators. Any totally symmetric state is a ground state. The ground-state sector is highly degenerate and belongs to the $D(L, 0)$ symmetric representation of $SU(3)$. This implies that for any finite even chain length L the ground-state sector consists of the $S_T = L, L - 2, \ldots, 2, 0$ spin multiplets, each once. Away from θ_{F} this degeneracy is lifted, the spin singlet becomes the ground state for $\theta > -3\pi/4$. However, in the interesting range of θ the other states remain still rather close in energy. For chains with $L = 48$ sites many of them lie still lower than the relevant lowest $k = \pi$ level. They could be separated by looking at their momentum, since we are interested in a $k = \pi$ level, while the others have momentum $k = 0$. Unfortunately the DMRG method does not allow to work in a definite momentum sector, and too many levels would have to be considered. Therefore, using this method, the interesting gap cannot be computed with a reasonable precision.

The scaled gaps for various chain lengths, ie. the gaps multiplied by the number of bonds in the chain are plotted in Fig. 2. Close to the point $\theta_{\mathrm{F}} = -3\pi/4$ the scaled gap increases monotonically with increasing chain length, while further away it decreases. In a critical model the scaled gap should asymptotically be independent of the chain length. Therefore,

according to the standard procedure the transition point θ_c could be located by looking at the crossing points between curves belonging to chain lengths L and $L+2$. They are marked by arrows and also shown in the inset of Fig. 2. As the chain length increases, the crossing points scale towards the ferromagnetic transition point. In fact, as the inset shows, the points fit well to a straight line on the L^{-2} scale, giving $\theta_c = -3\pi/4 = \theta_F$. This would mean that the gap vanishes everywhere above θ_F and Chubukov's phase does not exist.

Due to the limitations of the numerical calculations we cannot exclude the possibility that the crossing points converge to a $\theta_c > \theta_F$. However, the θ range where the quantum nematic phase exists, must then be very narrow with $\theta_c \lesssim -.74\pi$.

III. SEARCH FOR SOFT MODES

According to Chubukov's proposal the transition at θ_c between the nondimerized quantum nematic and the dimerized phases belongs to the Ising universality class. The lifting of the twofold degeneracy should be accompanied by the appearance of a soft mode and the vanishing of the gap. Therefore we have studied the behavior of the gap between the ground state and the lowest excited state. In the whole interesting region of θ this lowest excited state was found to have total spin $S_T = 2$.

For the calculation of this gap the abovementioned objection does not hold, and we could apply the DMRG method. Following the usual procedure, the open boundary condition was used, since it gives much better results than the periodic one. Now the ground state is expected to be unique even in the dimerized phase, if the number of sites L is even. This is easily understood by comparing the two dimerized valence-bond configurations, depicted in Fig. 3, which are believed to be good variational states in the dimerized region. Since the bond-strength oscillates in a dimerized state, clearly the configuration which has low-energy bonds at the ends has lower energy than the other one with high-energy bonds at the ends. (For odd L the two simple dimerized configurations would have the same energy, therefore they resonate and the real ground state is a state which has low-energy bonds at

both ends and a moving "domain wall" somewhere in-between [16]. In this case the ground state cannot be considered as a real vacuum, since it contains already one quasi-particle. This fact would make it extremely difficult to draw conclusions from results on chains with odd L, therefore we have not studied such chains.)

The longest chain we could reasonably study had $L = 48$ sites. The computed value of the gap is believed to be precise to at least five digits, when the maximum number of block states kept during the renormalization was $m = 160$.

Figure 4 shows the scaled value of the gap from the ground state to the lowest $S_T = 2$ state in the $-.75\pi < \theta < -.68\pi$ interval. This gap vanishes exactly even in finite systems at $\theta_F = -3\pi/4$ due to the extra $SU(3)$ symmetry, and is extremely small near this point. Above θ_F, however, the scaled gap increases, indicating the opening of the mass gap in the whole studied interval. In order to analyze quantitatively the opening of this singlet-quintuplet gap, we studied the finite lattice approximants of the Callan-Symanzik β-function [18,8]

$$\beta_{L_1,L_2}(\theta) = \frac{\ln[L_2\Delta(\theta, L_2)/L_1\Delta(\theta, L_1)]}{\ln(L_2/L_1)\frac{1}{2}\frac{\partial}{\partial\theta}\ln[\Delta(\theta, L_1)\Delta(\theta, L_2)]} \ . \tag{4}$$

$\beta_{L_1,L_2}(\theta)$ depends rather weakly on L_1 and L_2 (see the inset of Fig. 4). This allowed us to determine the opening of the gap at the edge of the ferromagnetic regime rather convincingly. The β-function increases above $\theta_F = -3\pi/4$ with a power law

$$\beta(\theta) = -\frac{1}{c\sigma}(\theta - \theta_F)^{1+\sigma} \ , \qquad \theta > \theta_F \ , \tag{5}$$

giving a straight line on the log-log plot, like in a Kosterlitz-Thouless transition. The best fit was obtained with $c = 3.9\pm0.4$, $\sigma = .51\pm0.03$. This means that the gap opens exponentially as

$$\Delta(\theta) = \text{const} \cdot \exp[-c(\theta - \theta_F)^{-\sigma}] \ , \qquad \theta > \theta_F \ . \tag{6}$$

This is in agreement with Chubukov's result, which suggested an exponentially slow opening of the gap [5]. Note that although this form resembles that of the Kosterlitz-Thouless transition, we think that the phase transition here is not really a KT transition but a first

order one because the transition from the ferromagnetic to this state is due to the crossing of the $S_T = L$ and $S_T = 0$ levels, which are the ground states on the two sides, respectively.

For $\theta > \theta_{\mathrm{F}}$, for the chain lengths we could use, there did not appear any sign of further level crossings. We did not find any level that would soften at a $\theta_c \neq \theta_{\mathrm{F}}$, ie. we did not find any trace of an additional phase transition. It should be noted, however, that the DMRG method gives precise energies only for those states that are targeted from the very beginning of the iteration. The procedure can easily miss a level, thus leading to false conclusion, if its energy comes down into the interesting energy range for long system sizes only, and hence it is not targeted at the beginning of the algorithm.

IV. STUDY OF THE DIMERIZATION ORDER PARAMETER

An alternative way to study phase transitions is by analyzing order parameters and correlation functions. They require the knowledge of the ground-state wave function only.

Even though both the dimerized phase and the nondimerized quantum nematic phase are disordered, an order parameter can be defined in the dimerized phase by using the fact that the translational invariance is spontaneously broken. The dimerization order parameter is usually defined as

$$D \equiv |\langle \boldsymbol{S}_{i-1} \cdot \boldsymbol{S}_i - \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}\rangle| \, . \tag{7}$$

In Ref. [11] Xian pointed out that for the pure biquadratic model a more proper definition would be the bond-strength oscillation in the ground state. Following this suggestion we define the dimerization order parameter as

$$D = |\langle h_{i-1,i} - h_{i,i+1}\rangle| \, , \tag{8}$$

where $h_{i,j}$ is the local Hamiltonian of Eq. (1), and the expectation value is taken in the ground state of an infinite chain whose ends are subject to open boundary condition.

In case of finite chains, let us denote the energy difference of neighboring bonds in the middle of the open chain with length L by

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$$D(L) = \left| \langle h_{L/2,L/2+1} - h_{L/2+1,L/2+2} \rangle \right| . \tag{9}$$

The (infinite volume) dimerization order parameter is then

$$D = \lim_{L \to \infty} D(L). \tag{10}$$

$D(L)$ is shown in Fig. 5 in the range $\theta_{\mathrm{F}} \leq \theta \leq 0$. It is finite also for $\theta \geq -\pi/4$, where no dimerization is expected. It vanishes at the VBS point $\theta = \arctan 1/3$ [17] only, where the ground state has a simple form and $D(L) \equiv 0$ for all L.

The finiteness of $D(L)$ can be understood by observing that the bond strength is generally not uniform in an open chain near the ends but alternate between strong and weak bonds, even if in the thermodynamic limit the system is not dimerized [16]. As we move towards the middle of the chain this oscillation gradually decreases. In a noncritical model this decay is exponential. In leading order $D(L)$ is expected to vary as

$$D(L) = D + c \exp(-L/\xi) , \tag{11}$$

where c is a constant and ξ is a kind of a correlation length. When the model has a nondimerized thermodynamic limit, $D = 0$.

In case of critical behavior, however, $D(L)$ scales to zero as a power law, ie.

$$D(L) = cL^{-\alpha} , \tag{12}$$

where α is a relevant surface exponent. Using this property, a systematic scaling analysis of our data for $D(L)$ allows to determine D for various values of θ.

As a first test we computed $D(L)$ at $\theta = -.5\pi$, where the exact result for D is available. Fitting the values of D, c and ξ of Eq. (11) to the last three points, $L = 40, 44$ and 48, we got $D = 1.1288$ which is quite close to Xian's [11] exact value $D_{\mathrm{exact}} = 1.1243$, when it is properly rescaled according to our definition of D. Our value for the correlation length is $\xi = 19.93$, which compares well with the exact value for bulk correlation length $\xi_{\mathrm{exact}} = 21.0728$ [4].

Figures 6 and 7 show a log-log plot of $D(L)$ vs L for various values of θ near $\theta = -\pi/4$ and θ_{F}, respectively. The transition between the dimerized phase and the Haldane phase is

easily spotted: for $\theta < -\pi/4$ the curves have an upward curvature indicating a finite value for D, while for $\theta > -\pi/4$ the curvature is in the opposite direction implying $D = 0$. At the critical point, where the asymptotic scaling is expected to be of the form of Eq. (12), the points should lie on a straight line. From this analysis we obtain $\theta = (-.25 \pm .01)\pi$ for the transition point, as expected.

In contrast to this behavior, all the curves have a slight upward curvature for $\theta_{\mathrm{F}} < \theta < -.68\pi$, although this curvature is almost zero in the close vicinity of θ_{F}. This implies a very small but finite dimerization in this region as well. Our results are, however, more uncertain in this region than near $\theta = -\pi/4$. Since $D(L)$ is small, the relative accuracy of the method is not very satisfactory, even when $m = 160$ basis states are kept during the renormalization. There is also a possibility that we are not yet in the asymptotic regime. Nevertheless, these results seem to indicate that most likely D remains finite down to θ_{F}. Like the gap, its value becomes exponentially small near the transition point.

Finally in Fig. 8 we present the two-point correlation function $\langle S_0^z S_l^z \rangle$ for three different values of θ. Well inside the dimerized region the correlation function alternates in sign strongly. It is positive for even l, and negative for odd l. For smaller values of θ, however, this behavior changes drastically. At $\theta = -.68\pi$ already all correlations are found to be negative and this property remains valid down to θ_{F}. There appears to be no sign of period doubling, just as it was proposed for the nondimerized quantum nematic phase. Although we do not fully understand the reason of this change, we think that the presence of dimerization should not necessarily mean an alternation in the sign of the correlation function, and thus the observed behavior cannot be viewed as a direct evidence for the appearance of a nondimerized regime.

V. CONCLUSIONS

In the present paper we studied the ground-state phase diagram of the bilinear-biquadratic spin-1 chain near the ferromagnetic instability, where Chubukov proposed the

existence of a nondimerized quantum nematic phase. We considered four independent quantities. First we looked at the degeneracy of the ground state, ie. whether the ground state is unique or doubly degenerate. Then we determined the opening of the gap. Finally we studied the behavior of the dimerization order parameter and the ground-state correlation function. We did not find any real evidence in any of these quantities for the existence of the hypothesized nondimerized quantum nematic phase.

Our results are in better agreement with the assumption that the dimerization appears exactly at the point where ferromagnetism becomes unstable, ie. at $\theta_{\mathrm{F}} = -3\pi/4$. The gap opening is well described by a Kosterlitz-Thouless-like form, although the transition is expected to be of first order.

The main difficulty we had to face in our numerical work was the extreme smallness of the gaps and order parameters in the region where the nondimerized quantum nematic phase was proposed to exist. Due to the restrictions in the numerical calculations and the uncertainties in the extrapolation procedure, our conclusion cannot be definitive. We cannot exclude the possibility that the phase proposed by Chubukov does appear in a very narrow region, say $-.75\pi \leq \theta \lesssim -.74\pi$. To resolve this question satisfactorily calculations on even longer chains would be needed.

VI. ACKNOWLEDGMENTS

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FIGURES

FIG. 1. Ground-state phase diagram of the bilinear-biquadratic spin-1 model. (a) Semiclassical phases without quantum fluctuations ($d \geq 2$). (b) Quantum phases ($d = 1$).

FIG. 2. Scaled gap, $L(E_\pi - E_{\text{GS}})$, between the lowest $k = \pi$ level, and the ground state having momentum $k = 0$, as a function of θ for chains with $L = 8, 10, \ldots, 16$ sites. Arrows indicate to the crossing point of curves belonging to chain lengths L and $L + 2$. Inset shows the L^{-2} scaling behavior of the crossing points.

FIG. 3. Typical dimerized valence bond configurations with (a) strong and (b) weak bonds at the ends.

FIG. 4. Scaled gap $(L - 1)(E_1 - E_{\text{GS}})$ vs θ, to the lowest excited state for chains with $L = 16, 24, \cdots, 48$ sites. Inset shows the Callan-Symanzik β-function computed from pairs of chains with length (L_1, L_2) on a log-log scale.

FIG. 5. Dimerization order parameter $D(L)$ vs θ for chains with $L = 16, 24, \cdots, 48$ sites. The cross shows Xian's exact value for D at $\theta = -\pi/2$.

FIG. 6. Log-log plot of the dimerization order parameter $D(L)$ vs the chain length L for different values of θ near $\theta = -\pi/4$. Dotted lines are guides to the eye. They are straight lines fitted to the last two points.

FIG. 7. Log-log plot of the dimerization order parameter $D(L)$ vs the chain length L for different values of θ near $\theta_{\text{F}} = -3\pi/4$. Dotted lines are guides to the eye. They are straight lines fitted to the last two points.

FIG. 8. Ground-state correlation function $\langle S_0^z S_l^z \rangle$ measured in a chain with $L = 48$ sites as a function of the separation l for different values of θ.

a,

b,

Fig. 1

Fig. 2

a,

b,
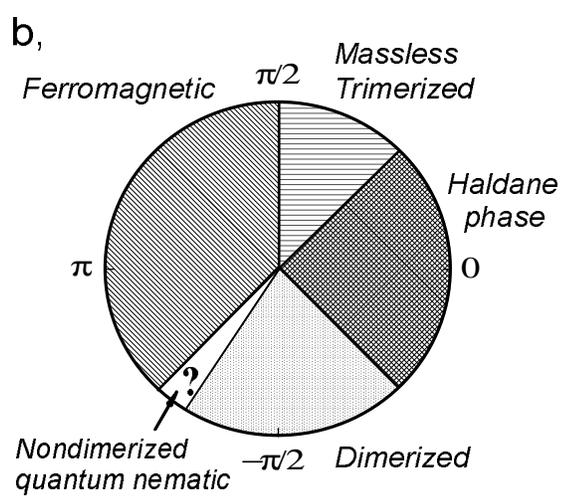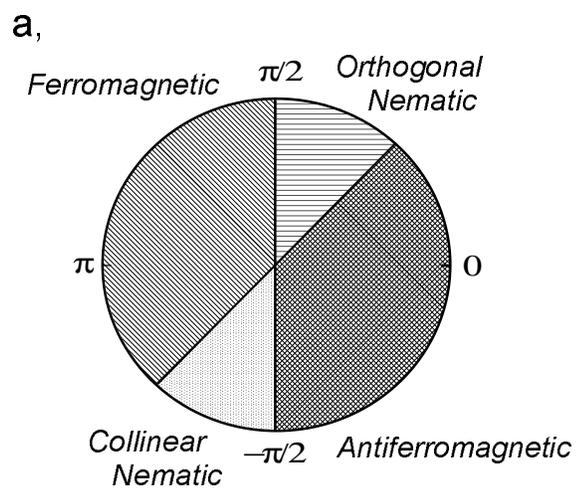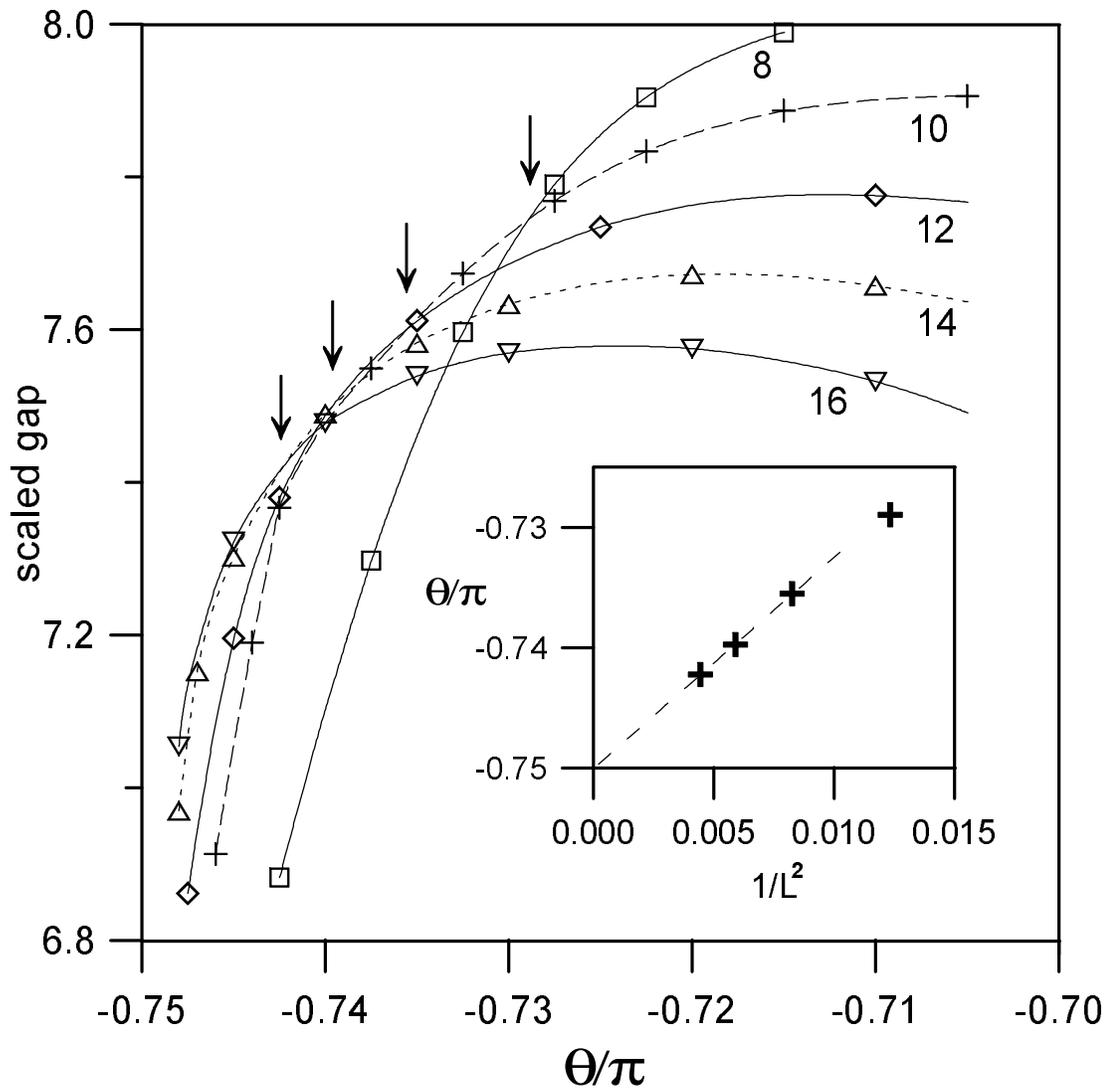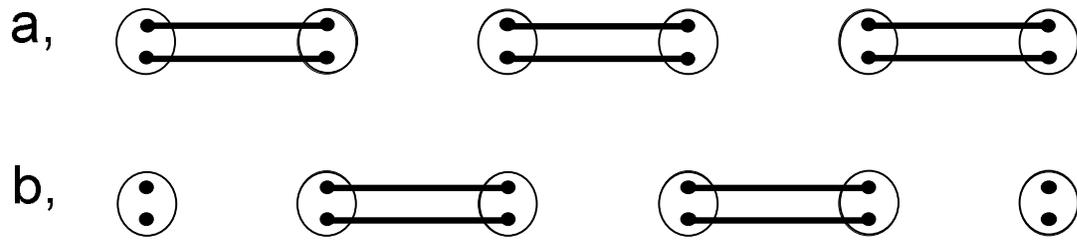
Fig. 3

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