Vector chiral order in frustrated spin chains

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(Dated: February 2, 2008)

By means of a numerical analysis using a non-Abelian symmetry realization of the density matrix renormalization group, we study the behavior of vector chirality correlations in isotropic frustrated chains of spin $S = 1$ and $S = 1/2$, subject to a strong external magnetic field. It is shown that the field induces a phase with spontaneously broken chiral symmetry, in line with earlier theoretical predictions. We present results on the field dependence of the order parameter and the critical exponents.

PACS numbers: 75.10.Pq, 75.40.Cx, 75.40.Mg

I. INTRODUCTION

The so-called vector chirality in quantum spin chains is defined as the vector product of two adjacent spins along the chain:

$$\kappa_n = \langle S_n \times S_{n+1} \rangle.$$

In a chirally ordered state spins have a tendency to “rotate” in some preferred plane in a certain preferred direction (clockwise or counterclockwise). Chiral phases in quantum spin chains were predicted long ago and have attracted considerable interest recently. After they have been found numerically in frustrated chains with easy-plane anisotropy, as noted by Villain, the chiral order should survive at finite temperature in the presence of three-dimensional interactions without transforming into a usual helical long-range order: at finite temperatures the chirality correlation length is much larger than the spin correlation length, so with decreasing temperature chiral order should set in before spin order does; there are experimental indications that the chiral order may exist in the quasi-one-dimensional anisotropic organic magnet Gd(hfac)$_2$NITiPr. The projection of the vector chirality $\kappa$ on the direction of the applied field could be experimentally detected with the help of polarized neutrons.

In all known cases of numerically confirmed existence of chiral states, the preferred plane for spin rotation is chosen by some anisotropy of the easy-plane type, and the chiral phase disappears in the isotropic limit. Recently, it has been predicted that in isotropic frustrated chains the chiral phase may appear in presence of an external magnetic field, strong enough to close the spectral gap. In such a state, the system approximately decouples into a gapped antisymmetric sector and a gapless symmetric sector, the latter being described by the Tomonaga-Luttinger liquid (TLL). An alternative two-component TLL scenario assumes the existence of the Tomonaga-Luttinger liquid in both sectors and implies absence of the chiral order.

The phase diagrams of the antiferromagnetic zigzag spin chains in applied field have been studied numerically in Ref. for $S = 1/2$, and in Ref. for $S = 1$. However, both works focused only on the magnetization process and did not check the presence of the chiral order. The theoretical analysis of Ref. involves some uncontrolled approximations (mean-field decoupling of the “twist” term) and, to our knowledge, the chiral order in isotropic spin chains has never been directly probed numerically (the only exception being the calculation of short-range correlations in a $S = 1/2$ chain), so the question of the correct scenario remains unsettled.

Several materials are known which realize isotropic zigzag spin chains among them, (N$_3$H$_3$)CuCl$_3$ can be viewed as a promising candidate for experimental studies, since its small exchange constants make it feasible to reach magnetic fields comparable to the gap.

In this paper we present a study of vector chirality correlations in the isotropic $S = 1$ and $S = 1/2$ zigzag chains in the presence of applied magnetic field, using a powerful non-Abelian symmetry realization of the density matrix renormalization group technique, in its matrix product state formulation. It is demonstrated that the chiral order does exist in the high-field phase, both for $S = 1$ and $S = 1/2$, and the behavior of chiral correlations is in a qualitative agreement with the expectations following from the theoretical analysis of Ref. This implies that a chiral one-component Tomonaga-Luttinger liquid scenario is realized.

II. THEORETICAL ESTIMATES

We consider the model of a frustrated antiferromagnetic spin chain, defined by the Hamiltonian:

$$\mathcal{H} = J_1 \sum_n S_n \cdot S_{n+1} + J_2 \sum_n S_n \cdot S_{n+2} - H \sum_n S_n^z$$

where $S_n$ are spin-1 operators at the $n$-th site, $J_1 > 0$ and $J_2 > 0$ are the nearest and next-nearest neighbor exchange constants, respectively, and $H$ is the external magnetic field, assumed to be applied along the $z$ axis.

In case of $S = 1$, at $H = 0$ the ground state is always gapped: for small frustration parameter $\alpha = J_2/J_1$ one remains in the Haldane phase characterized by the long-range string order, while for $\alpha > \alpha_c \approx 0.75$ there...
is a first-order transition into another gapped state, the so-called "double-Haldane" (DH) phase where the string order disappears with a finite jump, giving way to a more complicated hidden order. When the applied field exceeds the critical value \( H = H_c \) (\( H_c \) is obviously equal to the gap at \( H = 0 \), the system acquires finite magnetization. There is another special field value, the saturation field \( H_s \) above which the spins are fully polarized. In the \( S = 1/2 \) case, the ground state at \( H = 0 \) is gapless for \( \alpha < \alpha_c \approx 0.24 \), and \( \alpha > \alpha_c \) corresponds to a gapped dimerized phase.

We are interested in the properties of the partially magnetized state in the field range \( H_c < H < H_s \), and we assume that \( \alpha \) is large enough to make the system gapped at \( H = 0 \). In the limit \( \alpha \gg 1 \) the system may be viewed as two weakly coupled chains. A single \( S = 1/2 \) chain in external field has been extensively studied,22,23,24 as well as its \( S = 1 \) counterpart.25,26,27,28 Above the first critical field \( H_{1,2} \), the low-energy physics of a single chain is well described in terms of the effective Tomonaga-Luttinger liquid (TLL) theory, described by the Hamiltonian

\[
\mathcal{H}_{\text{TLL}}[\theta, \varphi] = \frac{v}{2} \int dx \left\{ \frac{1}{K} (\partial_x \phi)^2 + K (\partial_x \theta)^2 \right\}. \tag{2}
\]

Here \( K \) is the so-called TLL parameter, \( v \propto J_2 \) is the Fermi velocity, \( \phi \) is the bosonic field (compactified by the condition \( \varphi \equiv \varphi + \sqrt{\pi} \)), and \( \theta \) is its dual satisfying the commutation relations \([\phi(x), \theta(y)] = i \Theta(y-x), \) where \( \Theta(x) \) is the Heaviside function.

In the continuum limit, the lattice spin operators both for \( S = 1/2 \) and \( S = 1 \) can be represented\(^{22,27} \) through the bosonic field \( \varphi \) and its dual \( \theta \):

\[
S^z_a(x_a) = M + \frac{2}{v} \partial_x \phi_a(x_a) + A_3 \sin \left\{ \pi M x_a + \sqrt{4\pi} \phi_a(x_a) \right\} + \cdots \tag{3}
\]

\[
S^+_a(x_a) = e^{i\pi/2} e^{\sqrt{4\pi} \theta_a(x_a)} \left\{ A_1 \right\} + A_2 \sin \left\{ \pi M x_a + \sqrt{4\pi} \phi_a(x_a) \right\} + \cdots,
\]

Here \( a = 1, 2 \) labels the two chains, the space coordinate \( x \) is defined along the zigzag path as shown in Fig. 1, the lattice sites correspond to \( x_{1,2} = x \mp \frac{1}{2} \). \( M \) is the ground state magnetization per spin in units of saturation (which corresponds to the filling factor in the TLL model), and \( A_i \) are nonuniversal amplitudes. In the case of \( S = 1 \) the dots denote additional operators which correspond to massive fields connected to the high-energy \( S^z = 0, -1 \) magnon branches of the Haldane chain.\(^{22} \)

The theory parameters \( M, K, \) and \( v \) should be understood as functions of the field \( H \); for \( S = 1 \) their behavior can be extracted from the comparison of the TLL theory predictions with the numerical results\(^{26,29} \) while for \( S = 1/2 \) it is available from the exact Bethe ansatz solution.\(^{22} \)

For \( S = 1 \) the most important feature\(^{25,26,29} \) is that generally the TLL parameter \( K > 1 \) at \( H > H_{c1} \), non-monotonically depends on \( H \) and tends to the free fermion value \( K = 1 \) both at the first critical field \( H = H_{c1} \) and at the saturation field \( H = H_{c1} \). In contrast to that, for \( S = 1/2 \) the TLL parameter \( K < 1 \) and is a monotonically increasing function of the applied field.\(^{22,23} \)

For the description of weakly coupled chains it is convenient to introduce the symmetric and antisymmetric combinations of the bosonic fields

\[
\phi_\pm = (\phi_1 \pm \phi_2)/\sqrt{2}, \quad \theta_\pm = (\theta_1 \pm \theta_2)/\sqrt{2}.
\]

The longitudinal \( (S^z S^z) \) part of the zigzag exchange, apart from producing terms of the type \( (\partial_x \phi_1)(\partial_x \phi_2) \) which lead to a splitting of the TLL parameter values for the symmetric and antisymmetric sectors,

\[
K_\pm \approx K \left[ 1 \pm 2K/(\pi v\alpha) \right]^{1/2},
\]

\[
v_\pm \approx v \left[ 1 \pm 2K/(\pi v\alpha) \right]^{1/2}, \tag{4}
\]

yields another contribution proportional to \( \cos \sqrt{8\pi \varphi_\pm - \pi M} \). The scaling dimension of this latter perturbation is \( 2K_- \). In the case of \( S = 1 \) it is irrelevant since \( K > 1 \) and so can be neglected; in contrast to that, for \( S = 1/2 \) the twist term competes with a relevant operator and can only win if \( K_+ \) (\( H \)) is above a certain critical value \( K_{c1} \); for \( K < K_c \) the so-called “even-odd” phase is realized, whose dominant correlations are of the spin-nematic (or XY2 in the nomenclature of Ref. 30) type.

A characteristic feature of the “even-odd” phase\(^{13} \) are the \( \Delta S^z = 2 \) steps in the magnetization curve \( S^z_{\text{tot}}(H) \). The “even-odd” phase has been also observed\(^{21} \) in zigzag chains with ferromagnetic nearest-neighbor exchange.

In the chirally ordered phase the twist term is the most relevant perturbation, so one obtains the same effective Hamiltonian for \( S = 1 \) as well as for \( S = 1/2 \):

\[
\mathcal{H}_{\text{eff}} = \sum_{\sigma=\pm} \mathcal{H}_{\text{TLL}}[\varphi_\sigma, \theta_\sigma] + \mathcal{H}_{\text{int}}
\]

\[
\mathcal{H}_{\text{int}} = g \int dx \sin (\sqrt{2\pi} \theta_-) (\partial_x \theta_-) \tag{5}
\]

Mean-field decoupling of the twist term in the spirit of Ref. 3 then leads to the conclusion\(^{13} \) that both \( (\partial_x \theta_+) \) and \( \langle \sin (\sqrt{2\pi} \theta_-) \rangle \) become nonzero, and the antisymmetric sector becomes gapped.
One should mention that the above description makes sense only when we are far enough from the critical fields $H_c$ or $H_s$: the theory is applicable only up to the energies of the order of the bandwidth $v$, and $v \to 0$ if $H \to H_c, H_s$. The formulae indicate that the system becomes unstable against phase separation as soon as $v < 2K/(\pi \alpha)$.

The components of the chirality operator $\kappa$ can be expressed through bosonic fields. The longitudinal part of the chirality can be obtained in the following form:

$$\kappa^z(x) = \sin \left(2\sqrt{2}\pi \theta_+\right) \left\{ A_1^2 - \frac{(\pi A_1)^2}{4} (\partial_x \theta_+)^2 \right\} + \frac{A_2^2}{2} \cos \left( \sqrt{8\pi \varphi} + 2\pi M x \right) + \cdots,$$

where dots denote massive fields (the most important contribution of that sort is proportional to $(-1)^c \cos (\sqrt{2\pi \theta_-} (\partial_x \theta_+) )$ and operators with higher scaling dimensions. The leading contribution to the long-distance correlator is thus given by

$$\langle \kappa^z(x) \kappa^z(0) \rangle \to \kappa^2_0 \left(1 + \frac{C_1}{x^4} + \frac{C_2 \cos(2\pi M x)}{x^{4K+}} \right), \quad x \gg \xi,$$

where $\xi$ is the largest correlation length determined by the gap in the antisymmetric sector. (For $S = 1$ there is also another, much smaller, characteristic correlation length $\xi$ which is determined by the high-lying excitation branches that are neglected in the bosonization formulae; it roughly corresponds to the correlation length of the Haldane chain at zero field, typically a few lattice constants.) For $S = 1$, although $K > 1$ for $H_c < H < H_s$, the parameter $K_+$, according to [4], is renormalized to smaller values when the zigzag coupling is switched on, so the two decaying contributions in (7) may be competing with each other. In $S = 1/2$ chain the oscillating contribution always has the slowest decay since $K_+ < K < 1$.

In a similar way one can obtain the transversal chirality component

$$\kappa^x(x) = 2A_1 M \sin \left( \sqrt{\pi/2} \theta_- \right) \times \exp \left\{ \frac{i\pi x}{2} + i \sqrt{\frac{\pi}{2}} \theta_+ \right\} + \cdots.$$

It is easy to see that the leading term in $\kappa^x(x)$ is simply proportional to $S^+ - S^z$. The leading contribution to the corresponding asymptotic correlator is slowly decaying

$$\langle \kappa^+(x) \kappa^-(0) \rangle \propto A_1^2 \frac{M^2}{x^{2/(4K+1)}} \exp \{ iQx \}, \quad x \gg \xi,$$

and incommensurately, with the wave vector given by

$$Q = \frac{\pi}{2} + \sqrt{\frac{\pi}{2}} (\partial_x \theta_+).$$

The above expressions (7) and (9) are expected to be valid in the limit $\alpha \gg 1$, and for $H$ not very close to the critical fields $H_c, H_s$ (in the vicinity of the critical field the bosonization approach becomes hardly applicable since the effective bandwidth goes to zero). Close to the saturation field $H_s$, a large-$S$ analysis allows mapping the system to an effective model of two bosonic parameters.
species with repulsive interaction, which condense driven by the magnetic field playing the role of the chemical potential. The repulsion turns out to be strong enough to satisfy the phase separation condition, so only one of the species condenses, the other condensate is depleted, so one deals in fact with the one-component pseudo-condensate whose physics is again described by a (one-component) TLL. The asymptotic form of the longitudinal chirality correlator for $H$ close to $H_s$, has been presented in Ref. [8]

$$\langle \kappa^z(x)\kappa^z(0) \rangle \rightarrow \kappa_0^2 \frac{C}{x^2}, \quad (10)$$

with $\kappa_0^2 \propto (H_s - H)$. The leading contribution to the transversal chirality is proportional to the bosonic field itself, so its correlator takes the following asymptotic form:

$$\langle \kappa^+(x)\kappa^-(0) \rangle \rightarrow \frac{C'}{x^{1/(2K')}} e^{iQ'x}, \quad (11)$$

Here $K'$ is another TLL parameter, the characteristic wave vector $Q'$ is given by the expression for the pitch of the classical helical state:

$$Q' = \pm \left( \pi - \arccos(1/4\alpha) \right), \quad (12)$$

and the amplitude $C' \propto (H_s - H)^{1/2 - 1/(4K')}$. As the field approaches the saturation point, $H \rightarrow H_s$, the value of $K'$ tends to 1, so the amplitude $C'$ vanishes.

### III. RESULTS OF NUMERICAL ANALYSIS

We have studied the $S = 1$ and $S = 1/2$ zigzag chain model given by (11) using the DMRG method in its matrix product state formulation, making full use of the non-Abelian $SU(2)$ symmetry.

For a full description of the DMRG technique, we refer the reader to the review Ref. [19]. As discussed in Ref. [20], the formulation in terms of matrix product states is very convenient but for the calculation of ground states does not lead to substantially better results. The decisive point is the use of the non-Abelian symmetry $SU(2)$ instead of the Abelian $U(1)$. While the magnetic field breaks $SU(2)$ symmetry, the fact that the Zeeman energy term commutes with the rest of the Hamiltonian allows it to take the influence of the magnetic field into account by calculating the ground state of the model in a sector with the given total spin $S_{\text{tot}}$. The advantage of the method lies in a drastic reduction of the number of states which is necessary to describe the system, because non-Abelian symmetry allows one to calculate using representatives of groups of states of the same total spin: essentially, one treats the multiplet of states of the same total spin as a single representative state. Comparing to the Abelian version of the method which only uses the $U(1)$ symmetry, the improvement in efficiency can be several orders of magnitude, depending on the problem. For the zero-field groundstate of the zigzag chain, the effective improvement in the number of states is a factor $\sim 3$ (for $S = 1/2$) or $\sim 4$ (for $S = 1$), leading to a reduction in the computational effort by a factor $\sim 27$ and $\sim 64$ respectively. The relative efficiency decreases as the magnetic field is increased, but even for rather high fields the improvement is appreciable.

A slight disadvantage is that the non-Abelian method allows to compute only reduced matrix elements (in the sense of the Wigner–Eckart theorem). In our case, since the chirality is a vector, the correlator that is by far the easiest to calculate is the rotationally invariant scalar product,

$$F(n - n') = \langle \kappa(n) \cdot \kappa(n') \rangle, \quad (13)$$

which is a mixture of the longitudinal and transversal contributions. This obviously makes the analysis of the numerical data more difficult: in our case, from the theoretical analysis it follows that the longitudinal chirality correlations $\langle \kappa^z(x)\kappa^z(0) \rangle$ decay to their asymptotic value much faster than the transversal ones. Thus it turns out...
to be practically impossible to extract the characteristic decay exponent $\eta$ for the longitudinal chirality correlations from the $F(x)$ data, and one can only try to estimate the exponent $\eta = \eta_{xy}$ of the transversal chirality correlations.

### A. $S = 1$ zigzag chain

We have studied spin-1 zigzag chains with the frustration parameter $\alpha = 1$, for several chain lengths $L$ ranging from 64 to 192. For our calculation, even within the $SU(2)$ method we needed a relatively large number of representative states (from $m \approx 400$ to $m \approx 2000$, depending on $L$ and $S_{\text{tot}}$) to reach good convergence. In the $U(1)$ formulation, this corresponds to an $m$ of up to 8000, making an Abelian calculation much more difficult.

As one can see from the numerically calculated magnetization curve shown in Fig. 2 at $\alpha = 1$ the $S^z(H)$ dependence is featureless and shows neither plateaux, nor cusps, nor $\Delta S^z = 2$ steps characteristic for even-odd phase, in accordance with the results of Ref. 14.

We have computed the chirality correlator in the ground states of a large number of sectors with certain total spin quantum number $S_{\text{tot}}$. When computing $F(n-n')$, it was averaged over the starting and final positions $n, n'$, and care was taken to stay in the bulk, away from the ends of the chain. The DMRG data for the correlator has been fitted to the power-law form

$$F(x) = \kappa_0^2 + \frac{A \cos[q(x + \delta)]}{x^\eta}$$  \hspace{1cm} (14)

suggested by (7), (9). The introduction of a finite phase shift $\delta$ is necessary due to the open boundary conditions. Typical fits are presented in Fig. 4. From those fits we have extracted the behavior of the chirality order parameter $\kappa_0^2$ and the exponent $\eta$ as functions of the chain magnetization $M = S_{\text{tot}}/L$, shown respectively in Fig. 4b and Fig. 5. The fitted wave vector $q$ only weakly depends on the magnetization: as $M$ changes from 0 to 1, $q$ varies from 1.79 to 1.83, which favorably compares to the classical value $Q' \approx 1.82$ obtained from (12) at $\alpha = 1$. The phase shift $\delta(\alpha = 1) \approx 1 \pm 0.05$ is also practically independent of $M$. The behavior of the oscillation amplitude $A$ is shown in Fig. 6: the scaling $A \propto M^2$ suggested by (9) is indeed observed for small $M$, and strong deviations appear for $M > 0.3$.

One can see that for the bulk of $M$ values the order parameter $\kappa_0^2$ has practically reached convergence already at $L = 128$, so there is no need to perform the finite-size scaling. The only region where finite-size effects remain strong is $M \rightarrow 1$ (see Fig. 4b): the $\kappa_0^2(M)$ dependence at finite $L$ shows $\kappa_0$ vanishing at some $M = M_c \neq 1$. The finite-size scaling of $M_c$ (see the inset of Fig. 4b) shows that there is no trend to convergence even for $L = 192$, although there is a sizeable increase in $M_c$ towards 1 with increasing the size $L$. From the theoretical analysis one expects $M_c \rightarrow 1$ for $L \rightarrow \infty$, however, studying this limit numerically can be quite difficult: since for $M \rightarrow 1$ one is very close to the fully polarized state, the actual number of particles in the problem is the number of magnons $L(1-M)$, which has to be large enough to observe a phase transition.

The quality of fits deteriorates for very large $S_{\text{tot}}$, since the overall scale of the chirality correlations goes to zero as $M \rightarrow 1$. The fits become less reliable for small $S_{\text{tot}}$, as well, for the following reason: with (14) one attempts to fit just the oscillating (transversal) part of the chirality correlator. For small $S_{\text{tot}}$ the amplitude of the oscillating part is small, while the gap in the antisymmetric sector is small, so the oscillations appear on top of the exponential decay characterized by two very different correlation

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**FIG. 5:** (Color online) Behavior of the transversal chirality correlations exponent $\eta$ for a $S = 1$ chain with $\alpha = 1$ as a function of magnetization $M = S_{\text{tot}}/L$, extracted from fits of the correlation function (13) to the functional form (14). The error bars shown correspond to the uncertainties of the fit.

**FIG. 6:** (Color online) Behavior of the oscillations amplitude $A$ as a function of the magnetization $M = S_{\text{tot}}/L$ for a $S = 1$ chain with $\alpha = 1$. One can see that the scaling $A \propto M^2$ suggested by (9) is only applicable for small $M$.  

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FIG. 7: Typical DMRG results for the chirality correlator \( \langle \kappa(x)\kappa(0) \rangle \) of a \( S = 1/2 \) zigzag chain with \( \alpha = 1 \). The error bars have the same meaning as in Fig. 3a (Color online) A point in the chiral phase. The solid line shows a fit to (14); (b) a correlator in the nonchiral "even-odd" phase.

FIG. 8: (Color online) Behavior of the square chirality \( \kappa_0^2 \) as the function of magnetization \( M = 2S_{tot}/L \) for a \( S = 1/2 \) zigzag chain with \( \alpha = 1 \), extracted from fits of chiral correlation functions.

FIG. 9: (Color online) Behavior of the transversal chirality correlations exponent \( \eta \) for a \( S = 1/2 \) chain with \( \alpha = 1 \) as the function of magnetization \( M = 2S_{tot}/L \), extracted from fits of the correlation function (13) to the functional form (14). The error bars shown correspond to the uncertainties of the fit.

The chosen value of \( \alpha = 1 \) is rather small and does not allow a direct comparison of the chirality correlation functions with the theoretical predictions. However, for \( \alpha \gg 1 \) it should vary from approximately 0.25 to 0.5; the error bars in Fig. 5 are in fact only of indicative nature since they only show uncertainties of the fit to the fixed fit parameter which would result from adding subleading contributions to the main correlation length \( \tilde{\xi} \).

The other hand, the chirality correlators become more and more "polluted" by the exponentially decaying contributions with ever larger correlation length \( \xi \).

B. \( S = 1/2 \) zigzag chain

We have also computed the chirality correlation function (13) for \( S = 1/2 \) zigzag chains of length \( L = 168, 256 \), with frustration parameter \( \alpha = 1 \). Typically, 300 to 400 representative \( SU(2) \) states were kept in the calculation. The magnetization curve for a \( S = 1/2 \) zigzag chain with \( \alpha = 1 \) has been presented in Fig. 3a of Ref. 13. According to the phase diagram obtained in Ref.
at $\alpha = 1$ the $S = 1/2$ chain exhibits several phases with varying the applied field $H$. Some of those phases, namely, the “even-odd” phase and the plateau phase, obviously do not possess any chiral order. “Suspect” with respect to chirality are only two regions marked “TL2” in Ref. [13] and identified as a two-component Tomonaga-Luttinger liquid phase. Indeed, we observe a finite value of vector chiral order in both TL2 regions (although not in the entire high-field TL2 piece, see below).

A typical example of the correlator in the chiral phase is shown in Fig. 7a; for a comparison, we also show a correlator in the “even-odd” phase which is nonchiral. The maximal magnitude of chirality in $S = 1/2$ chain is roughly one order of magnitude smaller than in the $S = 1$ case. To analyse the chirality correlators, we had to use relatively large chain lengths, because the gaps are smaller than in the $S = 1$ case, and the results for small $L$ are polluted by slow exponentially decaying contributions.

We have employed the same fitting procedure as described above for the $S = 1$ chain, and analyzed the behavior of the chirality order parameter $\kappa_0^2$ and the critical exponent $\eta$ as functions of the magnetization $M = 2S_{\text{tot}}/L$. The results are shown respectively in Fig. 8 and Fig. 9. For the low-$M$ chiral region, the amplitude of oscillations in the correlation function turns out to be too small to extract the exponent $\eta$ with any reasonable accuracy, so for that region we were only able to extract the order parameter $\kappa_0^2$.

The boundaries of the low-field piece of the chiral phase coincide with the low-field TL2 region of Ref. [13]. Surprisingly, this is not the case for the high-field piece: while its lower boundary reasonably agrees with the transition from “even-odd” phase to TL2, its upper boundary lies at a finite $M = M_c \simeq 0.75$ and not at $M = 1$ as one expects from the theoretical analysis. It is worth mentioning that the magnetization curve of the $S = 1/2$ chain at $\alpha = 1$ (see Fig. 3a of Ref. [13]) seems to exhibit a weak feature around $M \simeq 0.75$, namely a fast growth of the second derivative $d^2 M/dH^2$. At $M \to M_c$, the critical exponent $\eta$ tends to $1/2$, the value which is expected theoretically close to the saturation field.

In contrast to $S = 1$, where the respective boundary exhibited strong finite-size scaling, in the $S = 1/2$ case we have not observed any significant change of $M_c$ with increasing $L$ from 168 to 256, as seen from Fig. [13]. We have found no chiral order for $L = 516$ chain with $S_{\text{tot}} = 205$, which means that even for such a long chain $M_c(L = 516) < 0.787$. On the basis of available data, one can conclude that the $S = 1/2$ chain might possess another nonchiral phase close to the saturation field. The nature of this phase needs further investigation.

IV. SUMMARY

We have studied spin-1 and spin-1/2 isotropic antiferromagnetic zigzag chains in strong magnetic fields by means of the matrix product density matrix renormalization group technique. Existence of a phase with field-induced vector chiral order is established for $S = 1$ as well as for $S = 1/2$, and the behavior of the order parameter and its correlations as functions of the magnetization is analyzed. The chiral phase is gapless and corresponds to a one-component Luttinger liquid, thereby confirming the scenario proposed in Ref. [8].

Acknowledgments

We would like to thank T. Vekua for useful discussions. This work was partly supported by the Deutsche Forschungsgemeinschaft (DFG). A.K.K. was supported by the Heisenberg Program Grant No. KO 2335/1-2 from DFG.

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3. A. Villain, Ann. Isr. Phys. Soc. 2, 565 (1978).
4. A. V. Chubukov, Phys. Rev. B 44, R4693 (1991).
5. A. A. Nersesyan, A. O. Gogolin, and F. H. L. Essler, Phys. Rev. Lett. 81, 910 (1998).
6. M. Kaburagi, H. Kawamura, and T. Hikihara, J. Phys. Soc. Jpn. 68, 3185 (1999).
7. A. K. Kolezhuk, Phys. Rev. B 62, R6057 (2000).
8. P. Lecheminant, T. Jolicoeur, and P. Azaria, Phys. Rev. B 63, 174426 (2001).
9. T. Hikihara, M. Kaburagi, and H. Kawamura, Phys. Rev. B 63, 174430 (2001).
10. A. Kolezhuk and T. Vekua, Phys. Rev. B 72, 094424 (2005).
11. M. Affronte, A. Caneschi, C. Cucci, D. Gatteschi, J. C. Lasjaunias, C. Paulsen, M. G. Pini, A. Rettori, and R. Sessoli, Phys. Rev. B 59, 6282 (1999).
12. S. V. Maleyev, V. V. Plakhty, O. P. Smirnov, J. Wosnitza, D. Visser, R. K. Kremer, and J. Kulda, J. Phys.: Condens. Matter 10, 951 (1998); S. V. Maleyev, Phys. Rev. Lett. 75, 4682 (1995).
13. G. Fáth and P. B. Littlewood, Phys. Rev. B 58 R14709, (1998).
14. K. Okunishi, Y. Hieida, and Y. Akutsu, Phys. Rev. B 60, R6953 (1999).
15. K. Okunishi and T. Tonegawa, J. Phys. Soc. Jpn. 72, 479 (2003).
16. F. Heidrich-Meisner, I. A. Sergienko, A. E. Feiguin, and E. R. Dagotto, Phys. Rev. B 75, 064413 (2007).
17. S. Yoshikawa, K. Okunishi, M. Senda, and S. Miyashita, J. Phys. Soc. Jpn. 73, 1798 (2004).
18. M. Hase, H. Kuroe, K. Ozawa, O. Suzuki, H. Kitazawa, G.
Kido, and T. Sekine, Phys. Rev. B 70, 104426 (2004).
17 I. P. McCulloch and M. Gulaci, Europhys. Lett. 57, 852 (2002).
18 S. R. White, Phys. Rev. Lett. 69, 2863 (1992).
19 U. Schollwöck, Rev. Mod. Phys. 77, 259 (2005).
20 I. P. McCulloch, J. Stat. Mech.: Theor. Exp., P10014 (2007).
21 A. Kolezhuk, R. Roth, and U. Schollwöck, Phys. Rev. Lett. 77, 5142 (1996); A. K. Kolezhuk and U. Schollwöck, Phys. Rev. B 65, 100401(R) (2002).
22 N. M. Bogoliubov, A. G. Izergin, and V. E. Korepin, Nucl. Phys. B 275, 687 (1986).
23 I. Affleck and M. Oshikawa, Phys. Rev. B 60, 1038 (1999).
24 F. H. L. Essler, A. Furusaki, and T. Hikihara, Phys. Rev. B 68, 064410 (2003); T. Hikihara and A. Furusaki, ibid. 69, 064427 (2004).
25 R. M. Konik and P. Fendley Phys. Rev. B 66, 144416 (2002).
26 L. Campos Venuti, E. Ercolessi, G. Morandi, P. Pieri, and M. Roncaglia, Int. J. Mod. Phys. B 16, 1363 (2002).
27 Masahiro Sato, J. Stat. Mech. P09001 (2006).
28 A. Friedrich, A. K. Kolezhuk, I. P. McCulloch, and U. Schollwöck, Phys. Rev. B 75, 094414 (2007).
29 G. Fath, Phys. Rev. B 68, 134445 (2003).
30 H. J. Schulz: Phys. Rev. B 34, 6372 (1986).
31 T. Vekua, A. Honecker, H.-J. Mikeska, and F. Heidrich-Meisner, Phys. Rev. B 76, 174420 (2007).
32 M. A. Cazalilla and A. F. Ho, Phys. Rev. Lett. 91, 150403 (2003).
33 In that way, the error bars shown do not reflect the actual error of the DMRG calculation, which is much smaller, but merely reflect the strength of finite-size effects.
34 By splitting the vector operator into components that change the total spin by $\Delta S = 0, \pm 1$, the components of the correlator transverse and longitudinal to the field can be measured using only rotationally invariant scalar operators, which are expressible in terms of reduced matrix elements of irreducible tensors, but in this form they are quite complicated and difficult to construct.