PHYSICAL REVIEW B **77**, 094404 (2008)

Vector chiral order in frustrated spin chains

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(Received 18 December 2007; published 6 March 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.

DOI: 10.1103/PhysRevB.77.094404 PACS number(s): 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:

$$\boldsymbol{\kappa}_n = \langle \boldsymbol{S}_n \times \boldsymbol{S}_{n+1} \rangle.$$

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[1,2] and have attracted considerable interest recently[3–8] after they have been found numerically in frustrated chains with easy-plane anisotropy.[4,7] As noted by Villain,[1] 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 $Gd(hfac)_3NITiPr$.[9] The projection of the vector chirality $\boldsymbol{\kappa}$ on the direction of the applied field could be experimentally detected with the help of polarized neutrons.[10]

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.[7] Recently, it has been predicted[8] that in isotropic frustrated chains, the chiral phase may appear in the 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[11–13] assumes the existence of the Tomonaga-Luttinger liquid in both sectors and implies the absence of the chiral order.

The phase diagrams of the antiferromagnetic zigzag spin chains in applied field have been studied numerically in Ref. 13 for $S=1/2$ and in Ref. 14 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. 8 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[15]), so the question of the correct scenario remains unsettled.

Several materials are known which realize isotropic zigzag spin chains;[16] among them, $(N_2H_5)CuCl_3$ 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[17] of the density matrix renormalization group (DMRG) technique[18,19] in its matrix product state formulation.[20] 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. 8. 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

$$\mathcal{H} = J_1 \sum_n \boldsymbol{S}_n \cdot \boldsymbol{S}_{n+1} + J_2 \sum_n \boldsymbol{S}_n \cdot \boldsymbol{S}_{n+2} - H \sum_n S_n^z, \qquad (1)$$

where $\boldsymbol{S}_n$ are spin-S operators at the nth 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 the case of $S=1$, at $H=0$, the ground state is always gapped: For small frustration parameter $\alpha \equiv J_2/J_1$, 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 phase where the string order disappears with a finite jump, giving way to a more complicated hidden order.[21] 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

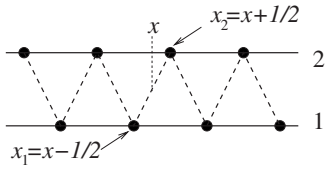

FIG. 1. A zigzag spin chain and the notation adopted in Eq. (3).

$\alpha<\alpha_c\simeq 0.24$,[22,23] and $\alpha>\alpha_c$ corresponds to a gapped dimerized phase.[24]

We are interested in the properties of the partially magnetized state in the field range $H_c<H<H_s$, and we assume that α 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,[25–27] as well as its $S=1$ counterpart.[28–31] Above the first critical field H_{c1}, 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

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

Here, K is the so-called TLL parameter, $v\propto J_2$ is the Fermi velocity, ϕ is the bosonic field (compactified by the condition $\varphi\equiv\varphi+\sqrt{\pi}$), and θ 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[8,30] through the bosonic field φ and its dual θ:

$$S^z_a(x_a)=M+\frac{2}{\sqrt{\pi}}\partial_x\phi_a(x_a)+A_3\sin\{k_Fx_a+\sqrt{4\pi}\phi_a(x_a)\}+(\cdots),$$

$$S^+_a(x_a)=e^{i\pi x/2}e^{i\sqrt{\pi}\theta_a(x_a)}\{A_1+A_2\sin(k_Fx_a+\sqrt{4\pi}\phi_a(x_a))\}+(\cdots). \tag{3}$$

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), $k_F=\pi M$ for $S=1$, and $k_F=\pi(1+M)/2$ for $S=1/2$, 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.[30]

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,[29,32] while for $S=1/2$, it is available from the exact Bethe ansatz solution.[25]

For $S=1$, the most important feature[28,29,32] is that generally the TLL parameter $K>1$ at $H>H_{c1}$ nonmonotonically 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 $H=H_{s1}$. In contrast to that, for $S=1/2$, the TLL parameter $K<1$ and is a monotonically increasing function of the applied field.[25,26]

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^zS^z) part of the zigzag exchange, apart from producing terms of the type $(\partial_x\varphi_1)(\partial_x\varphi_2)$ which lead to a splitting of the TLL parameter values for the symmetric and antisymmetric sectors,

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

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

yields another contribution proportional to $\cos[\sqrt{8\pi}\varphi_- -k_F]$. 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 $S=\frac{1}{2}$ chain, $K<1$, and this operator is a relevant perturbation. Thus, as pointed out in Ref. 8, for $S=1$ the leading contribution to the interaction is given by the "twist term" produced by the transversal part of the zigzag exchange. For the $S=1/2$, the twist term competes with a relevant operator and can only win if $K_-(H)$ is above a certain critical value K_c; 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. 33) type. A characteristic feature of the even-odd phase[13] is the $\Delta S^z=2$ step in the magnetization curve $S^z_{\rm tot}(H)$. The even-odd phase has been also observed[34] 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 $S=1/2$:

$$\mathcal{H}_{\rm eff}=\sum_{\sigma=\pm}\mathcal{H}_{TL}[\varphi_\sigma,\theta_\sigma]+\mathcal{H}_{\rm int},$$

$$\mathcal{H}_{\rm int}=g\int dx\sin(\sqrt{2\pi}\theta_-)(\partial_x\theta_+). \tag{5}$$

Mean-field decoupling of the twist term in the spirit of Ref. 3 then leads to the conclusion[8] that both $\langle\partial_x\theta_+\rangle$ 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 $H\to H_c,H_s$. Formulas (4) indicate that the system becomes unstable against phase separation[35] as soon as $v<2K/(\pi\alpha)$.

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

$$\kappa^z(x) = \sin(\sqrt{2\pi}\theta_-)\left\{A_1^2 - \frac{(\pi A_1)^2}{4}(\partial_x\theta_+)^2 + \frac{A_2^2}{2}\cos(\sqrt{8\pi}\varphi_+ + 2k_F x)\right\} + (\cdots), \tag{6}$$

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

$$\langle\kappa^z(x)\kappa^z(0)\rangle \to \kappa_0^2\left(1 + \frac{C_1}{x^4} + \frac{C_2\cos(2k_F x)}{x^{4K_+}}\right), \quad x \gg \xi, \tag{7}$$

where ξ 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 $\tilde{\xi}$, which is determined by the high-lying excitation branches that are neglected in the bosonization formulas (3); 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 Eq. (4), is renormalized to smaller values when the zigzag coupling is switched on, so the two decaying contributions in Eq. (7) may be competing with each other. In the $S=1/2$ chain, the oscillating contribution always has the slowest decay since $K_+<K<1$.

In a similar way, one can obtain the transversal chirality component

$$\kappa^+(x) = 2A_1 M \sin(\sqrt{\pi/2}\theta_-)\exp\left\{\frac{i\pi x}{2} + i\sqrt{\frac{\pi}{2}}\theta_+\right\} + (\cdots). \tag{8}$$

It is easy to see that the leading term in $\kappa^+(x)$ is simply proportional to $S_1^+ - S_2^+$. The leading contribution to the corresponding asymptotic correlator is slowly decaying,

$$\langle\kappa^+(x)\kappa^-(0)\rangle \propto A_1^2\frac{M^2}{x^{1/(4K_+)}}\exp\{iQx\}, \quad x \gg \xi, \tag{9}$$

and incommensurate, with the wave vector given by

$$Q = \frac{\pi}{2} + \sqrt{\frac{\pi}{2}}\langle\partial_x\theta_+\rangle.$$

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[8] allows mapping the system to an effective model of two bosonic species with repulsive interaction, which, condense driven by the magnetic field, play 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, and the other condensate is depleted. So, one deals, in fact, with the one-component pseudocondensate 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:

$$\langle\kappa^z(x)\kappa^z(0)\rangle \to \kappa_0^2 - \frac{C}{x^2}, \tag{10}$$

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:

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

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

$$Q' = \pm[\pi - \arccos(1/4\alpha)], \tag{12}$$

and the amplitude $C' \propto (H_s - H)^{1/2-1/(4K')}$. As the field approaches the saturation point, $H \to H_s$, 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 Eq. (1) 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,[18] we refer the reader to 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[17,20] is the use of the non-Abelian symmetry SU(2) instead of the Abelian U(1). While the magnetic field H breaks SU(2) symmetry, the fact that the Zeeman energy term commutes with the rest of the Hamiltonian makes it possible 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_{tot}. The advantage of the method lies in a drastic reduction of the number of states m 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 ground state of the zigzag chain, the effective improvement in the number of states is a factor of ~ 3 (for $S=1/2$) or ~ 4 (for $S=1$), leading to a reduction in the computational effort by factors of ~ 27 and ~ 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 us 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

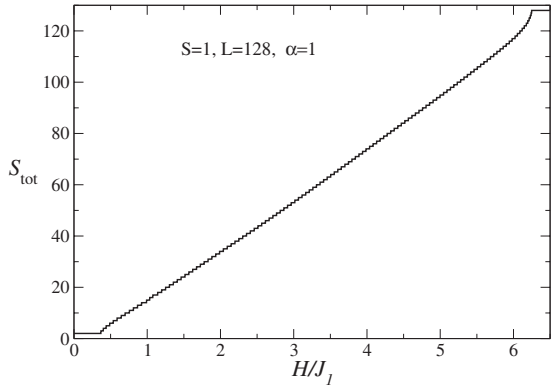

FIG. 2. Numerically calculated magnetization curve $S^z_{tot}(H)$ for a $S=1$ zigzag chain of length $L=128$ with frustration parameter $\alpha=J_2/J_1=1$.

calculate is the rotationally invariant scalar product,

$$F(n-n') = \langle \boldsymbol{\kappa}(n) \cdot \boldsymbol{\kappa}(n') \rangle, \tag{13}$$

which is a mixture of the longitudinal and transversal contributions.[37] 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 η_z 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 $m\simeq 400$ to $m\simeq 2000$, depending on L and S_{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 plateaus, 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 (13) in the ground states of a large number of sectors with certain total spin quantum number S_{tot}. When computing $F(n-n')$, it was averaged over the starting and final positions n and n', and care was taken to stay in the bulk, away from the ends of the chain. The DMRG data for the correlator have been fitted to the power-law form

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

suggested by Eqs. (7) and (9). The introduction of a finite phase shift δ is necessary due to the open boundary conditions. Typical fits are presented in Fig. 3. From those fits, we have extracted the behavior of the chirality order parameter κ_0^2 and the exponent η as functions of the chain magnetization $M=S_{tot}/L$, shown, respectively, in Figs. 4 and 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 Eq. (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 is shown in Fig. 6: The scaling $A\propto M^2$ suggested by Eq. (9) is indeed observed for small M, and strong deviations appear for $M>0.3$.

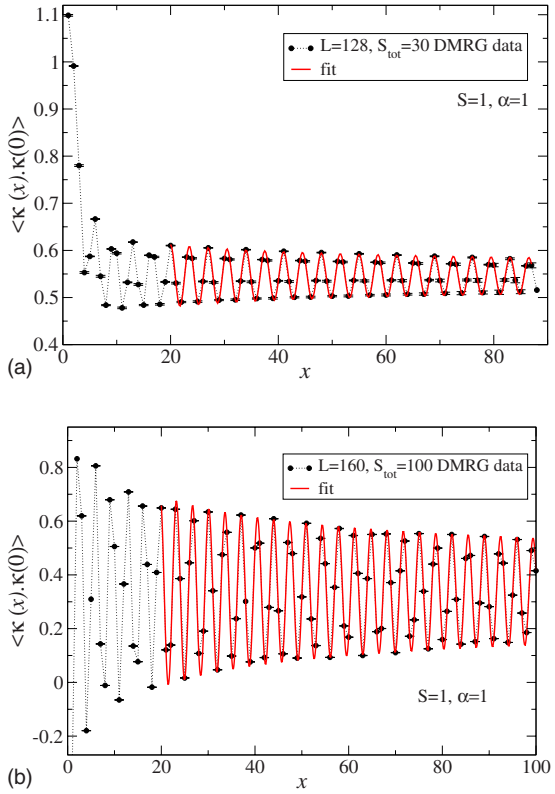

FIG. 3. (Color online) Typical DMRG results for the chirality correlator (13) and results of fitting it to form (14). The error bars (Ref. 36) (here, smaller than the symbol size) indicate the variance of $F(x=n-n')$ calculated from averaging over the initial and final points n and n'.

One can see that for the bulk of M values, the order parameter κ_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 $M\to 1$ [see Fig. 4(b)]: The $\kappa_0^2(M)$ dependence at finite L shows κ_0 vanishing at some $M=M_c\neq 1$. The finite-size scaling of M_c [see the inset of Fig. 4(b)] shows that there is no trend to convergence even for $L=192$, although there is a sizeable increase in M_c toward 1 with increasing the size L. From the theoretical analysis, one expects $M_c\to 1$ for $L\to\infty$; however, studying this limit numerically can be quite difficult, since for $M\to 1$, 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.

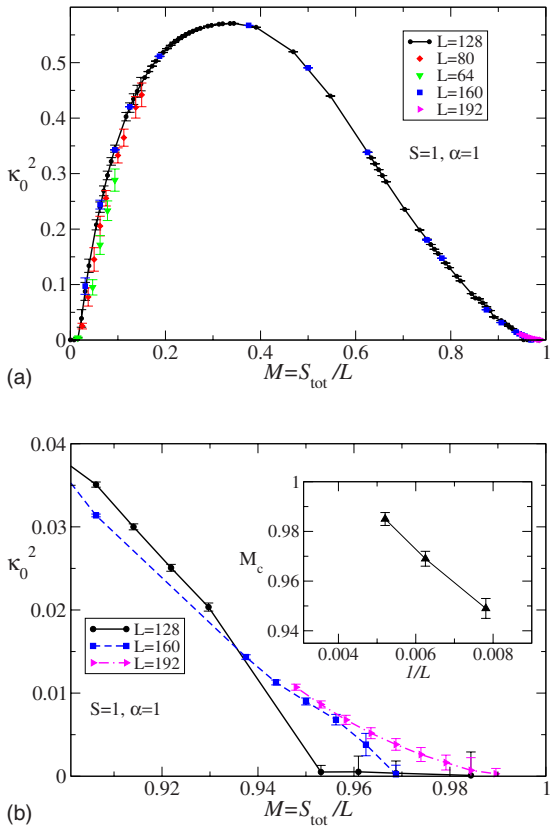

FIG. 4. (Color online) (a) The square chirality order parameter κ_0^2 as a function of magnetization $M=S_{\mathrm{tot}}/L$ for a $S=1$ zigzag chain with $\alpha=1$, extracted from fits of chirality correlation functions; (b) zoom in of the same picture in the vicinity of $M=1$, where finite-size effects become important. The inset shows the L scaling of the point M_c where the long-range chirality order disappears in a finite system of size L.

The quality of fits deteriorates for very large S_{tot}, since the overall scale of the chirality correlations goes to zero as $M\rightarrow 1$. The fits become less reliable for small S_{tot} as well for

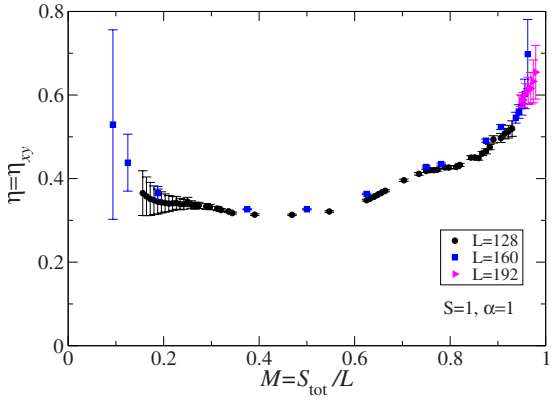

FIG. 5. (Color online) Behavior of the transversal chirality correlation exponent η for a $S=1$ chain with $\alpha=1$ as a function of magnetization $M=S_{\mathrm{tot}}/L$, extracted from fits of the correlation function (13) to the functional form (14). The error bars shown correspond to the uncertainties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

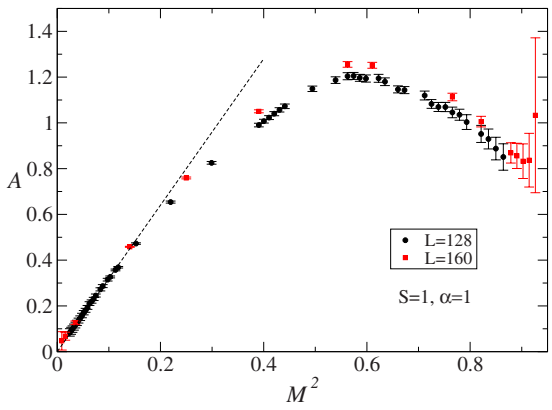

FIG. 6. (Color online) Behavior of the oscillation amplitude A as a function of the magnetization $M=S_{\mathrm{tot}}/L$ for a $S=1$ chain with $\alpha=1$. One can see that the scaling $A\propto M^2$ suggested by Eq. (9) is only applicable for small M.

the following reason: With Eq. (14), one attempts to fit just the oscillating (transversal) part of the chirality correlator. For small S_{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 lengths $\tilde{\xi}$ (for $\alpha=1$, one has $\tilde{\xi}\approx 7$) and $\xi\gg\tilde{\xi}$. It thus becomes a numerically ill-posed problem to filter out the power-law decaying oscillating part on top of such a background.

The extracted critical exponent slowly changes with M and lies in the range $\eta\sim 0.3$–0.6, which qualitatively agrees with the theoretical estimates predicting that for $\alpha\gg 1$, it should vary from approximately 0.25 to 0.5; the error bars shown in Fig. 5 are, in fact, only of indicative nature since they only show uncertainties of the fit to the fixed fit function and do not take into account the variations of the fit parameters which would result from adding subleading (e.g., exponentially decaying) contributions to Eq. (14).

The chosen value of $\alpha=1$ is rather small and does not allow a direct comparison of η with the theoretical value $(4K_+)^{-1}$: If one naively tries to extract the velocity parameter v assuming that K_+ is given by Eq. (4) and using the data of Ref. 32 for the $K(M)$ dependence, the obtained values of v fall below the phase separation threshold $v_c=2K/(\pi\alpha)$. We have refrained from studying chains with $\alpha\gg 1$ since, on the one hand, increasing α causes a dramatic increase in numerical effort and, on the other hand, the chirality correlators become more and more "polluted" by the exponentially decaying contributions with ever larger correlation length ξ.

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, 300–400 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. 3(a) of Ref. 13. According to the phase diagram obtained in Ref. 13, at $\alpha=1$, the $S=1/2$ chain ex-

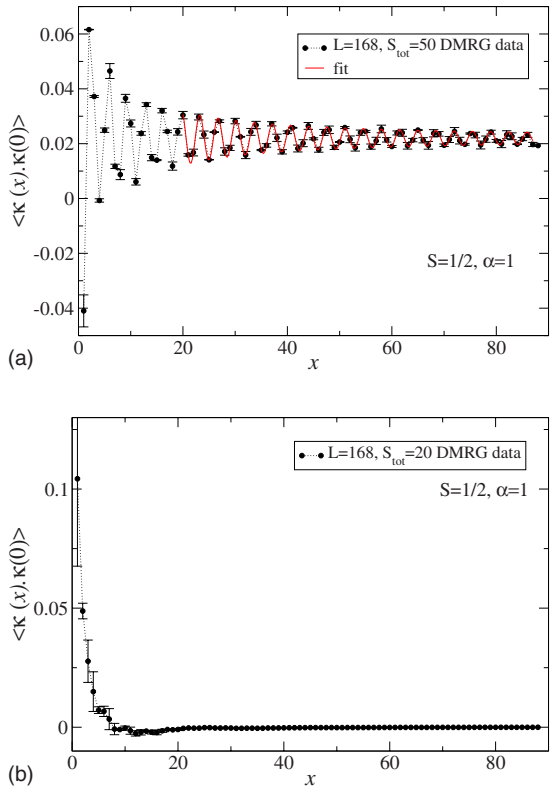

FIG. 7. (Color online) Typical DMRG results for the chirality correlator (13) of a $S=1/2$ zigzag chain with $\alpha=1$. The error bars have the same meaning as in Fig. 3. (a) A point in the chiral phase. The solid line shows a fit to Eq. (14); (b) a correlator in the nonchiral even-odd phase.

hibits several phases with varying 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. 7(a); for a comparison, we also show a correlator in the even-odd phase which is nonchiral. The maximal magnitude of chirality in the $S=1/2$ chain is roughly 1 order of magnitude smaller than in the $S=1$ case. To analyze 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 κ_0^2 and the critical exponent η as functions of the magnetization $M=2S_{\mathrm{tot}}/L$. The results are shown, respectively, in Figs. 8 and 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 η with any reasonable accuracy; so for that region, we were only able to extract the order parameter κ_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. 3(a) of Ref. 13] seems to exhibit a weak feature around $M\simeq 0.75$, namely, a fast growth of the second derivative d^2M/dH^2. At $M\to M_c$, the critical exponent η tends to $1/2$, the value which is expected theoretically close to the saturation field.

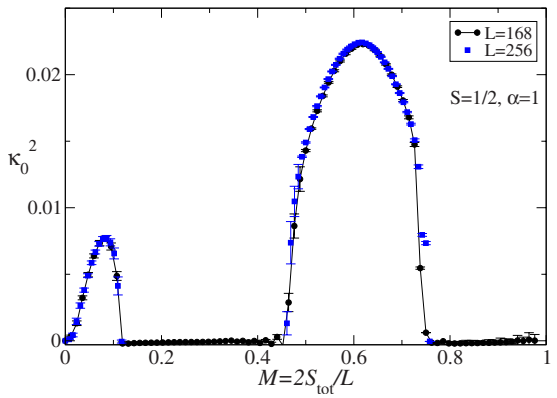

FIG. 8. (Color online) Behavior of the square chirality κ_0^2 as the function of magnetization $M=2S_{\mathrm{tot}}/L$ for a $S=1/2$ zigzag chain with $\alpha=1$, extracted from fits of chiral correlation functions.

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. 8. We have found no chiral order for $L=516$ chain with $S_{\mathrm{tot}}=205$, 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.

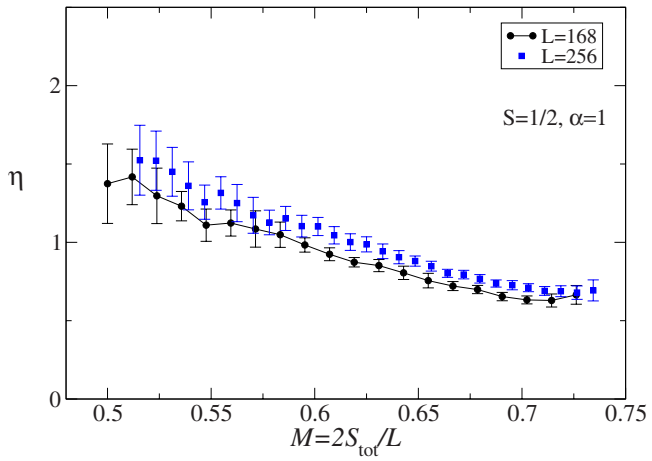

FIG. 9. (Color online) Behavior of the transversal chirality correlation exponent η for a $S=1/2$ chain with $\alpha=1$ as the function of magnetization $M=2S_{\mathrm{tot}}/L$, extracted from fits of the correlation function (13) to the functional form (14). The error bars shown correspond to the uncertainties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

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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[1] J. Villain, Ann. Isr. Phys. Soc. **2**, 565 (1978).
[2] A. V. Chubukov, Phys. Rev. B **44**, R4693 (1991).
[3] A. A. Nersesyan, A. O. Gogolin, and F. H. L. Eßler, Phys. Rev. Lett. **81**, 910 (1998).
[4] M. Kaburagi, H. Kawamura, and T. Hikihara, J. Phys. Soc. Jpn. **68**, 3185 (1999).
[5] A. K. Kolezhuk, Phys. Rev. B **62**, R6057 (2000).
[6] P. Lecheminant, T. Jolicoeur, and P. Azaria, Phys. Rev. B **63**, 174426 (2001).
[7] T. Hikihara, M. Kaburagi, and H. Kawamura, Phys. Rev. B **63**, 174430 (2001).
[8] A. Kolezhuk and T. Vekua, Phys. Rev. B **72**, 094424 (2005).
[9] 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).
[10] 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).
[11] G. Fáth and P. B. Littlewood, Phys. Rev. B **58**, R14709 (1998).
[12] K. Okunishi, Y. Hieida, and Y. Akutsu, Phys. Rev. B **60**, R6953 (1999).
[13] K. Okunishi and T. Tonegawa, J. Phys. Soc. Jpn. **72**, 479 (2003).
[14] F. Heidrich-Meisner, I. A. Sergienko, A. E. Feiguin, and E. R. Dagotto, Phys. Rev. B **75**, 064413 (2007).
[15] S. Yoshikawa, K. Okunishi, M. Senda, and S. Miyashita, J. Phys. Soc. Jpn. **73**, 1798 (2004).
[16] 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. Gulacsi, 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.: Theory Exp. 2007, P10014.
[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] K. Okamoto and K. Nomura, Phys. Lett. A **169**, 433 (1992).
[23] T. Tonegawa, I. Harada, and M. Kaburagi, J. Phys. Soc. Jpn. **61**, 4665 (1992).
[24] F. D. M. Haldane, Phys. Rev. B **25**, 4925 (1982); **26**, 5257 (1982).
[25] N. M. Bogoliubov, A. G. Izergin, and V. E. Korepin, Nucl. Phys. B **275**, 687 (1986).
[26] I. Affleck and M. Oshikawa, Phys. Rev. B **60**, 1038 (1999).
[27] F. H. L. Essler, A. Furusaki, and T. Hikihara, Phys. Rev. B **68**, 064410 (2003); T. Hikihara and A. Furusaki, *ibid.* **69**, 064427 (2004).
[28] R. M. Konik and P. Fendley, Phys. Rev. B **66**, 144416 (2002).
[29] L. Campos Venuti, E. Ercolessi, G. Morandi, P. Pieri, and M. Roncaglia, Int. J. Mod. Phys. B **16**, 1363 (2002).
[30] Masahiro Sato, J. Stat. Mech.: Theory Exp. 2006, P09001.
[31] A. Friedrich, A. K. Kolezhuk, I. P. McCulloch, and U. Schollwöck, Phys. Rev. B **75**, 094414 (2007).
[32] G. Fath, Phys. Rev. B **68**, 134445 (2003).
[33] H. J. Schulz, Phys. Rev. B **34**, 6372 (1986).
[34] T. Vekua, A. Honecker, H.-J. Mikeska, and F. Heidrich-Meisner, Phys. Rev. B **76**, 174420 (2007).
[35] M. A. Cazalilla and A. F. Ho, Phys. Rev. Lett. **91**, 150403 (2003).
[36] 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.
[37] 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.