DMRG study of the topological Haldane phase in the anisotropic spin-1 $XXZ$ chain

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(Dated: July 25, 2014)

We reexamine the one-dimensional spin-1 $XXZ$ model with on-site uniaxial single-ion anisotropy as to the appearance and characterization of the symmetry-protected topological Haldane phase. By means of large-scale density-matrix renormalization group (DMRG) calculations the central charge can be determined numerically via the von Neumann entropy, from which the ground-state phase diagram of the model can be derived with high precision. The nontrivial gapped Haldane phase shows up in between the trivial gapped even Haldane and Néel phases, appearing at large single-ion and spin–exchange interaction anisotropies, respectively. We furthermore carve out a characteristic degeneracy of the lowest entanglement level in the topological Haldane phase, which is determined using a conventional finite-system DMRG technique with both periodic and open boundary conditions. Defining the spin and neutral gaps in analogy to the single-particle and neutral gaps in the intimately connected extended Bose-Hubbard model, we show that the excitation gaps in the spin model qualitatively behave just as for the bosonic system. We finally compute the dynamical spin structure factor in the three different gapped phases and find significant differences in the intensity maximum which might be used to distinguish these phases experimentally.

PACS numbers: 75.10.Pq, 64.70.Tg, 03.67.-a

I. INTRODUCTION

One-dimensional (1D) quantum spin systems received continued attention as paradigms for strongly correlated systems, because miscellaneous—and even exotic—phases can be realized within simple model Hamiltonians. By way of example the exactly solvable spin-1/2 antiferromagnetic (AFM) Heisenberg chain is known to be gapless, while for integer spin a gap exists between the ground state and the first excited state, as conjectured first by Haldane. Especially for the spin-1 chain the Haldane gap was confirmed experimentally and the dynamical spin structure factor has been observed by inelastic neutron scattering, e.g., on $\text{Ni(C}_2\text{H}_4\text{N}_2)\text{ClO}_4$. Affleck, Lieb, Kennedy and Tasaki (AKLT) proposed a exactly solvable model that offers valuable clues to the physics of the spin-1 Heisenberg chain. The so-called AKLT state (cf. Fig. 1 (a) below) describes the ground state of the Haldane phase successfully. Also for the spin-1 $XXZ$ model the ground-state phase diagram has been determined—even if a single-ion anisotropy is added—e.g., by the Lanczos exact diagonalization (ED) technique based on the level spectroscopy method.

Currently quantum integer-spin chains attract extraordinary interest from a topological point of view. The gapped ground states in the Haldane phase can be classified by the projective representations of the underlying symmetry group. The odd Haldane (OH) phase in odd-integer spin chains with two half-integer edge spins is a symmetry-protected topological (SPT) phase, because the odd-S AKLT state cannot be adiabatically connected to another trivial state without undergoing a phase transition. On the other hand, the even Haldane (EH) state in the even-integer spin systems with integer edge spins is a trivial state, since the even-S AKLT state is adiabatically connected to a trivial state without a bulk phase transition. Interestingly, a hidden SPT phase analogous to the OH phase was discovered in the extended Bose-Hubbard model (EBHM) with longer-range repulsions. This Haldane insulator (HI) phase, embedded between the Mott insulator (MI) and the density wave (DW) phases in the intermediate coupling regime, exhibits the characteristic degeneracy of the entanglement spectrum in the Haldane phase. The excitation gaps at the quantum phase transition lines depend on their universality classes. Beyond that, the dynamical density structure factor $S_{\text{EBHM}}(k,\omega)$ significantly differs in the MI, DW, and HI states.

On the basis of our recent EBHM study in the present work, we investigate the topological properties of the odd Haldane phase in the anisotropic spin-1 $XXZ$ chain which, as we will show, can be taken as an effective model for the EBHM. Using the density matrix renormalization group (DMRG) technique we determine first the phase boundaries by exploiting the central charge. In order to confirm the closing of the excitation gap at the trivial-nontrivial phase transition points, we simulate both the spin and neutral gaps. We furthermore demonstrate the degeneracy of entanglement levels in the OH phase with both periodic and open boundary conditions (for the anisotropic spin-1 $XXZ$ chain it is well known how the edge spins should be treated in the latter case). In order to detect the topological HI phase in the EBHM experimentally, various dynamical quantities have been proposed. Here we will examine the dynamical spin structure factor $S^{zz}(k,\omega)$ for the spin-1 model by means of the dynamical DMRG (DDMRG) technique. We will demonstrate that the intensity maximum in $S^{zz}(k,\omega)$ features a gapped dispersion in the non-trivial Haldane phase as obtained for $S_{\text{EBHM}}(k,\omega)$ in the EBHM. Since this quantity is directly accessible...
by inelastic neutron scattering, significant differences in \( S^z(k, \omega) \) could be used to detect the various gapped phases.

This paper is organized as follows. In the next section we establish the anisotropic spin-1 XXZ model and the corresponding EBHM. The physical quantities of interests are introduced in Sec. [III] Large-scale (dynamical) DMRG results for the anisotropic spin-1 XXZ chain will be presented and discussed in Sec. [IV] Section [IV] contains a brief summary and our main conclusions.

II. MODEL HAMILTONIANS

In this section we introduce the anisotropic spin-1 XXZ model and get back to its established ground-state properties. We then define the extended Bose-Hubbard model and point out the correspondences with an effective spin-1 XXZ model.

A. Spin-1 XXZ model with single-ion anisotropy

The Hamiltonian of the 1D spin-1 XXZ model with on-site anisotropy is given by

\[
\hat{H} = J \sum_j \left[ S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + J_z S_j^z S_{j+1}^z \right] + D \sum_j (S_j^z)^2, 
\]

(1)

where \( S_j \) denotes a spin-1 operator. The parameter \( D \) represents the uniaxial single-ion anisotropy. The ground-state phase diagram of the model [11] exhibits various gapful and gapless phases, namely, following the conventional notations, the Haldane phase, the large-\( D \) phase, two XY phases, the ferromagnetic phase, and the Néel phase. According to this different types of phase transitions occur between these phases: (i) a gapful-gapful Gaussian phase transition takes place between the large-\( D \) phase and the Haldane phase with the central charge \( c = 1 \), (ii) the Haldane-Néel transition appears to be of the Ising universality class with \( c = 1/2 \), and (iii) a gapless-gapfull Berezinskii-Kosterlitz-Thouless (BKT) transition emerges between the XY phase and the Haldane or large-\( D \) phase. In what follows we set \( J = 1 \) and restrict ourselves to the parameter region where \( J_z > 0 \) and \( D > 0 \). Following the notation by Kjäll et al. [22], we use the termini EH, OH and AFM phases instead of the large-\( D \), Haldane, and Néel phases, respectively. The lattice inversion symmetry, which projects the SPT state of the Haldane phase, can be broken by adding a perturbation to the Hamiltonian [11]:

\[
\delta \hat{H} = g \sum_j \left[ S_j^z (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) + S_{j+1}^z (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) + \text{H.c.} \right].
\]

(2)

Any finite \( g \) immediately lifts the characteristic degeneracy of the lowest entanglement level in the Haldane phase. As we will see later, thereby the EH-OH quantum phase transition also disappears.

B. Extended Bose-Hubbard model

In 2006, E. Dalla Torre et al. [12] discovered the so-called Haldane-insulator (HI) phase in the 1D extended Bose-Hubbard model with longer-range repulsions. The HI phase features the properties of the OH phase in the spin-1 model [11]. The EBHM Hamiltonian reads

\[
\hat{H}_{\text{EBHM}} = -t \sum_j (\hat{b}_j^\dagger \hat{b}_{j+1} + \text{h.c.}) + U \sum_j \hat{n}_j (\hat{n}_j - 1)/2 + V \sum_j \hat{n}_j \hat{n}_{j+1},
\]

(3)

where \( \hat{b}_j^\dagger (\hat{b}_j) \) creates (annihilates) a boson at lattice site \( j \), and \( \hat{n}_j = \hat{b}_j^\dagger \hat{b}_j \) is the corresponding boson number operator. The nearest-neighbor boson transfer amplitude is given by \( t \) and \( U \) (\( V \)) parametrizes the on-site (nearest-neighbor) particle repulsion. Assuming that the site occupation is restricted to \( n_j = 0, 1 \) or 2, with \( S_j^z = n_j - 1 \) for a mean boson filling factor \( \rho = N/L = 1 \), the system can be mapped onto an effective spin-1 Hamiltonian,

\[
\hat{H}_{\text{eff}}^{\text{EBHM}} = \hat{H} + \hat{H}' ,
\]

(4)

with the replacements \( J \to -t, JJ_z \to V \) and \( D \to U/2 \) in Eq. [1]. \( \hat{H}' \) contains further terms which breaks the particle-hole symmetry of \( \hat{H} \) (see Eq. (A1) of Ref. [14] for the explicit form of \( \hat{H}' \)). The EBHM exhibits three insulating phases, where the nontrivial HI phase appears in between the MI and DW phases for intermediate-couplings. The MI, HI and DW phases of the EBHM correspond to the EH, OH, and AFM phases of the spin-1 model [11], respectively.

III. PHYSICAL QUANTITIES OF INTEREST

In this section we assert the quantities that can be used to characterize the different phases and phase transitions in the spin-1 model [11] and accordingly in the EBHM. We furthermore explain how the quantities can be simulated using the DMRG technique.

A. Entanglement spectrum, von Neumann entropy and central charge

After Li and Haldane’s proposal [23] to characterize topological phases by the entanglement spectrum this has become one of the most powerful tools to investigate the SPT state. Dividing a system with \( L \) sites into two sub-blocks and considering the reduced density matrix
the formation about the criticality of the system. Adding up Fig. 1 (c), just as for the HI phase in the EBHM.

\[ \lambda \]

The entanglement analysis provides also valuable information about the criticality of the system. Adding up the \( \lambda \_\alpha \) during the simulation, we have direct access to the von Neumann entropy \( S_L(\ell) = - \text{Tr}[\rho_\ell \ln \rho_\ell] \). From conformal field theory\(^{23}\), it follows that in the case of a periodic system the von Neumann entropy takes the form

\[ S_L(\ell) = c \frac{\lambda}{3} \ln \left[ \frac{L}{\pi} \sin \left( \frac{\pi \ell}{L} \right) \right] + s_1, \tag{6} \]

where \( s_1 \) is a non-universal constant. Since the most precise data of \( S_L(\ell) \) are obtained when the length \( \ell \) of the sub-block equals half the system size \( L \), the relation\(^{23}\)

\[ c^* (L) = \frac{3 [S_L(L/2) - S_L(L/2)]}{\ln [\cos(\pi/L)]}, \tag{7} \]

is much better suited for determining the central charge than directly using the above expression for \( S_L(\ell) \).

For the EBHM the phase boundaries can be assigned very effectively using the (numerically determined) central charge \( c^* \), because the system becomes critical only at the MI-HI (HI-DW) transition points where \( c = 1 \) \((c = 1/2)\), and there \( c^* \) shows pronounced peaks.\(^{13}\) Hence we adopt this method for the spin-1 model\(^{14}\) as well to pinpoint the EH-OH and OH-AFM transition points.

### B. Excitation gaps

Monitoring various excitation gaps for the EBHM, significant features have been found at the MI-HI and HI-DW transition points.\(^{12,14}\) For example, the single-particle gap,

\[ \Delta_e = E_0(N + 1) + E_0(N - 1) - 2E_0(N), \tag{8} \]

is finite in all three insulating phases, except for the MI-HI transition point. By contrast, the neutral gap,

\[ \Delta_n = E_1(N) - E_0(N), \tag{9} \]

closes at both the MI-HI and HI-DW transition. In Eqs. \( 8 \) and \( 8 \), \( E_0(N) \) and \( E_1(N) \) denote the energies of the ground state and first excited state of the \( N \)-particle system for the EBHM, respectively.

Since adding (removing) a particle in the EBHM corresponds to raising (lowering) the spin \( S^z \)-projection in a pseudo-spin model, we consider for the spin-1 \( XXZ \) model the spin gap,

\[ \Delta_s = E_0(1) - E_0(0), \tag{10} \]

which likewise might be finite in all three phases, except for the EH-OH transition point. As for the EBHM, the neutral gap in the spin-1 model\(^{14}\) can be defined as

\[ \Delta_n = E_1(0) - E_0(0), \tag{11} \]

where \( E_0(M) \) and \( E_1(M) \) denote the ground-state and first excited energies within the subspace \( M = \sum_j S_j^z \), respectively. By analogy to the behaviour of the neutral gap in the EBHM, \( \Delta_n \) should vanish at the EH-OH and OH-AFM transition points for the spin-1 chain model.
C. Dynamical spin structure factor

Simulating the dynamical spin structure factor by DDMRG is of particular importance since it might be directly compared with inelastic neutron scattering experiments, e.g., on Ni(C₂H₈N₂)₂NO₂ClO₄. Its \( z \)-component is defined by

\[
S^{zz}(k, \omega) = \sum_{n} |\langle \psi_{n} | S_{z}^{\dagger} | \psi_{0} \rangle|^{2} \delta(\omega - \omega_{n}).
\]

(12)

where \(|\psi_{0}\rangle\) and \(|\psi_{n}\rangle\) denote the ground state and \(n\)th excited state, respectively. The corresponding excitation energy is \(\omega_{n} = E_{n} - E_{0}\). For \(D = 0\), i.e., for the isotropic Heisenberg or XXZ fix points of \(H\), \(S^{zz}(k, \omega)\) was extensively studied by ED and time-dependent DMRG techniques. That is, the behavior of \(S^{zz}(k, \omega)\) in the Haldane phase is well known, albeit numerical results for the EH and AFM states are rare. Taking the relation \(S_{z} = n_{j} - \rho\) for the pseudospin in the effective model \(H_{\text{EBHM}}\) into account, one expects that the spin structure factor \(S^{zz}(k, \omega)\) corresponds to the dynamical density structure factor \(S_{\text{EBHM}}(k, \omega)\) in the EBHM, which exhibits different behavior in the three insulating phases \(27\).

IV. NUMERICAL RESULTS

In this section we present our numerical (D)DMRG results for the spin-1 XXZ model with and without single-ion anisotropy. We first determine the phase boundaries and then analyze the behavior of the excitation gaps at the transitions between the nontrivial and trivial phases. Furthermore we discuss the entanglement spectra of odd Haldane phase. Finally we simulate the dynamical spin structure factor and compare it with the dynamical density response in the EBHM.

In the numerics we keep up to \(m = 3200\) density-matrix states for the static DMRG runs, so that the discarded weight is typically smaller than \(1 \times 10^{-10}\). For the DDMRG simulations we take \(m = 800\) examining the ground state along the first five DMRG sweeps and then use \(m = 400\) states computing dynamical properties.

A. Phase boundaries

1. OH-AFM transition

Let us first discuss the spin-1 model \(H\) with \(D = 0\). In this case it is known that a BKT transition occurs at \(J_{z} = 0\) between the \(XY\) and OH phases. At \(J_{z} > 0\), solely an OH-AFM transition takes place, where \(c = 1/2\) is expected.

Figure 2 shows the central charge \(c^*(L)\), computed from Eq. 7. If \(J_{z}/J\) is raised at fixed system size, the maximum in \(c^*(L)\) sharpens at the OH-AFM transition point \(J_{z,c1}/J\), and we deduce \(c^* \approx 0.5\). The other critical point \(J_{z,c2}/J \approx 1.185\) with \(c^* \approx 0.503\) approximates the recent infinite-system DMRG result \(J_{z,c2}/J = 1.186 \pm 0.003\) very well already for \(L = 32\). The agreement becomes perfect if we increase the system size: \(J_{z,c2}/J \approx 1.186\) with \(c^* \approx 0.500\) for \(L = 128\). Note that \(c^*(L)\) stays equal to one in a relatively wide region (from \(J_{z}/J = 0\) to \(J_{z}/J \approx 0.3\) for \(L = 128\)), indicating the BKT transition between the \(XY\) and the OH phases at \(J_{z}/J = 0\) with \(c = 1\).

2. EH-OH transition

We now turn to the case \(D > 0\). In previous works \(27,28,30\) a Gaussian transition between the EH and OH phases has been found by employing the level spectroscopy technique to ED results obtained for small systems. Applying the twisted boundary conditions, \(S_{L+1}^{zz} = -S_{L}^{zz} + S_{L}^{yy}\), \(S_{L+1}^{yy} = -S_{L}^{yy}\), and \(S_{L+1}^{zz} = S_{L}^{zz}\) within DMRG, the two lowest energy levels can be simulated accurately for much larger system sizes than accessible to ED. Figure 3(a) demonstrates that the two lowest energies assigned to the EH and OH states cross at \(J_{z,c1}/J \approx 1.6945\) by increasing \(J_{z}/J\) at fixed \(D/J = 1.5\) for \(L = 32\) (and twisted boundary conditions). The critical points \(J_{z,c1}/J(L)\) strongly depend on the system size and can be extrapolated linearly to the thermodynamic limit as indicated by Fig. 3(b). For \(L \to \infty\) we obtain \(J_{z,c1}/J \approx 1.6938\).

Alternatively, the EH-OH transition points can be extracted from the central charge \(c^*(L)\) if compared with the field theoretical prediction, \(c = 1\). This is demonstrated in Fig. 3(c). Here the maxima of \(c^*(L)\) show almost no system-size dependence. They are located at the EH-OH transition point, in perfect agreement with the ones via level spectroscopy in the panels (a) and (b).
Note that also the OH-AFM transition can be reliably determined from the pronounced peak at \(J_{z,c}/J \approx 2.138\).

### B. Characterization of the topological phase

In the following subsection we analyze the signatures of the topological OH phase and of the transition between the trivial and nontrivial topological states for the model (1) in close analogy to the EBHM(1). To this end, we simulate the excitation gaps and the entanglement spectra.

#### 1. Excitation gaps

So far the excitation gaps of (1) have been studied mostly at the isotropic Heisenberg point with respect to the magnitude of the Haldane gap. At the trivial-nontrivial phase transition points the excitation gaps should close, as demonstrated, e.g., for the EBHM. Here we compute the spin and neutral excitation gaps as defined in Sec. III B instead of calculating the simple first excitation gap. Thereby, we adopt PBC instead of OBC within DMRG, avoiding the use of edge spins, which have to be adapted according to the considered parameter region.

Figure 4 (a) shows first the excitation gaps at \(D = 0\). Upon increasing \(J_z/J\) the gaps open exponentially, reflecting the BKT transition at \(J_z/J = 0\). \(\Delta_n\) and \(\Delta_s\) cross each other exactly at the Heisenberg point, \(J_z/J = 1\), where \(\Delta_n(L) = \Delta_s(L)\) (see the discussion about the system-size dependence of the excitation gaps and the magnitude of the Haldane gap for the spin-1 Heisenberg model in the Appendix). At the OH-AFM transition \((J_{z,c}/J \approx 1.186)\), \(\Delta_n\) closes linearly because the transition belongs to the Ising universality class, while \(\Delta_s\) remains finite.

For \(D/J = 1.5\) [see Fig. 4 (b)], the EH-OH transition occurs at \(J_{z,c}/J \sim 1.6938\), where both spin and neutral gaps vanish. Increasing \(J_z/J\) above \(J_{z,c}/J\), only \(\Delta_n\) closes at the Ising transition point \(J_{z,c}/J\), just as in the case of \(D/J = 0\) [compare panels (a) and (b)]. If we turn on the perturbation \(\delta \hat{H}\) [see Eq. (2)], which breaks the lattice-inversion symmetry explicitly, the EH-OH transition disappears, so that \(\Delta_s\) stays finite for \(g/J = 0.1\) as shown in Fig. 4 (b).

Comparing the behavior of the excitation gaps with those of the EBHM, one sees that the spin (neutral) gap in the spin-1 model takes the role of the single-particle (neutral) gap in the EBHM.
2. Entanglement spectra

Let us now analyze the entanglement properties of the topological states for intermediate single-ion anisotropy \((D/J = 1.5)\), where both the EH-OH and OH-AFM transitions exist. Here Pollmann et al. [10] showed that the SPT state in the OH phase has a twofold degenerate lowest entanglement level for the quantum spin chain model. The infinite-time evolving block decimation procedure used by those authors, gives the entanglement spectra data directly in the thermodynamic limit. In the following we show that simulating the model \(\mathcal{H}\) for a finite system by conventional DMRG, this characteristic degeneracy of the OH phase can also be obtained, but the degree of the degeneracy depends on the boundary conditions.

Figure 5 presents the entanglement spectrum \(\xi_\alpha\) for the anisotropic spin-1 \(XXZ\) model \(\mathcal{H}\) with \(D/J = 1.5\). For a small system \((L = 64)\) with PBC \([\text{panel (a)}]\) the lowest entanglement level is fourfold degenerate only deep inside the OH phase. This reflects the possession of the two edges for the sub-block \(L/2\). Increasing the system size this degeneracy is observed for a larger region of the OH phase, as demonstrated by panel \(b\) for \(L = 128\), but close to the EH-OH transition point the lowest entanglement level is still non-degenerate. To overcome this drawback we apply OBC with half-spin edges \([\text{cf. Fig. 1 (b)}]\). The same procedure has been used to estimate the magnitude of the Haldane gap at the isotropic Heisenberg point. Figure 5 (c) gives \(\xi_\alpha\) for \(L = 128\) and OBC, pointing out the twofold degeneracy of the lowest level in the nontrivial phase and its non-degeneracy anywhere else. The degeneracy is clearly caused by the single edge spin of sub-block \(L/2\).

Figure 6 (a) \[(c)\] exemplifies that the fourfold \[twofold\] degeneracy with PBC \[OBC\] indeed dissolves for any finite \(g\). Thereby, the gap between the lowest levels becomes larger as \(g\) increases, see panel \(c\) \[panel \(d\)\] for PBC \[OBC\]. Obviously inversion symmetry protects the Haldane phase.
FIG. 7. (Color online) DMRG ground-state phase diagram of the 1D spin-1 XXZ model with single-ion anisotropy. Shown are the even Haldane (EH), odd Haldane (OH), and antiferromagnetic (AFM) phases. The EH-OH (squares) and OH-AFM (circles) transition points are determined from the central charge $c = 1$ and $c = 1/2$, respectively, which was extracted from the von Neumann entropy via Eq. (7). The EH-OH transition points (line) were confirmed by a careful finite-size scaling of the two low-lying energy levels with twisted boundary conditions. The dashed (dotted) line denotes the MI-HI (HI-DW) transition in the EBHM with $n_b = 2$ bosons per site (taken from Ref. 13).

C. Ground-state phase diagram

Figure 7 displays the DMRG ground-state phase diagram of the spin-1 XXZ model with single-ion anisotropy. The phase boundaries have been derived from central charge $c^*$ as explained above. The non-trivial OH phase appears in between the trivial EH and AFM phases, just as the topological HI phase develops between the MI and DW phases in the EBHM. Therefore we have included in Fig. 7 the phase boundaries of the MI-HI and HI-DW transitions for the EBHM with $n_b = 2$ (taken from Ref. 13). Qualitatively, the phase diagram of the spin-1 model looks quite similar to those of the EBHM, except for the existence of the SF phase in the EBHM (not shown). Quantitatively, the topological phase of the EBHM captures a larger region in parameter space than the OH phase however. This might be caused by the particle-hole symmetry breaking term $\mathcal{H}'$ in Eq. (4).

D. Dynamical structure factor

Let us finally discuss the spin dynamical properties of the spin-1 XXZ model. Figure 8 reveals our DDMRG results for $S_{zz}^z(k, \omega)$, obtained in the three different phases of the spin-1 model for fixed anisotropy $D/J = 1.5$. In the EH phase, at $J_z/J = 1$, most of the spectral weight is concentrated in the momentum range $\pi/2 < k < \pi$ [see Fig. 8(a)]. The excitation gap appears at $k \approx 0$. The dispersion of the maximum in $S_{zz}^z(k, \omega)$ behaves cosine-like for small-to-intermediate momenta, and is flattened close to the Brillouin zone boundary (above $k \geq 3\pi/4$). Deep in the Haldane phase, the situation changes drastically [see Fig. 8(b) for $J_z/J = 1.9$]. Now the dispersion of the maximum in $S_{zz}^z(k, \omega)$ takes a sine-like form. Again there are finite excitation gaps at $k = 0$ (Haldane gap) and $\pi$. This resembles the behaviour found at the isotropic Heisenberg point. Here the spectral weight exclusively concentrates at $k \approx \pi$ and finite but small $\omega \ll J$. In the AFM phase [see Fig. 8(c) with $J_z/J = 3$], the dispersion becomes flattened with a large excitation gap that opens at $k = \pi$ however. That is, the dynamical spin structure factor shows a distinct behavior in each phase of the spin-1 model with single-ion anisotropy. Interestingly, the results obtained in the EH, OH, and AFM phases are similar to those for the MI, HI, and DW phases of the 1D EBHM. This corroborates that the spin-1 model can be taken as an effective model for the EBHM with $n_b = 2$.

V. SUMMARY

We studied the topological properties of the anisotropic spin-1 XXZ model with single-ion anisotropy in close analogy to a recent investigation of the extended Bose-Hubbard model (EBHM) with the nearest-neighbor repulsion. The focus was on the nontrivial Haldane phase as well. The phase boundaries between trivial phases [even Haldane (EH) and AFM phases] and non-trivial odd Haldane (OH) phase were determined numerically with high precision via the central charge. The ground-state phase diagram resembles those of the restricted EBHM with a maximum number of bosons per site $n_b = 2$, but the topological phase takes a much narrower region in the parameter space. Simulating the spin and neutral gaps, which correspond to the single-particle respectively neutral gaps in the EBHM, we confirmed the closing of the gap at the trivial-nontrivial quantum phase transition as for the EBHM.

The degeneracy of the lowest entanglement level in the OH phase could be observed by finite-system DMRG calculations with both periodic (P) and open (O) boundary conditions (BC). With PBC the lowest level in the entanglement spectrum is fourfold degenerate in the OH phase; notably the system-size dependence of the results is much stronger than for OBC. Adopting half spins ($S = 1/2$) at the open edges, the twofold degeneracy corresponding to
FIG. 8. (Color online). Intensity plots of the dynamical structure factor $S^{zz}(k, \omega)$ in the EH [panel (a)], OH [panel (b)], and AFM [panel (c)] phases. Data are obtained by the DDMRG technique for $L = 64$, using PBC and a Lorenzian broadening $\eta = 0.1t$. Crosses give the maximum value of $S^{zz}(k, \omega)$ at fixed momenta $k = 2\pi j/L$ with $j = 1, \cdots, L/2$.

ACKNOWLEDGEMENT

The authors would like to thank Y. Fuji, F. Lange, S. Nishimoto, and F. Pollmann for valuable discussions. This work was supported by Deutsche Forschungsgemeinschaft through SFB 652, Project B5.

Appendix A: Haldane gap

After Haldane’s conjecture about the finite excitation gaps for integer-spin chains, it was a challenging issue to estimate these (so-called) Haldane gaps numerically (note that even the spin-1 XXZ Heisenberg chain is not integrable). White presented first accurate DMRG results for the Haldane gap subsequently a series of more elaborated DMRG and QMC studies have been performed. However, only OBC have been used within the DMRG framework so far, mainly because of the less computational costs. In this Appendix, we demonstrate—at least for the spin-1 Heisenberg model—that the Haldane gap can also be determined using PBC, and the system-size dependence of the gap is much smaller than those with OBC adopting the half spin edges [cf., Fig. 1 (b)].

| method           | $L$   | $\Delta$          | $T$           | BC   |
|------------------|-------|-------------------|---------------|------|
| QMC[15]          | 128   | 0.41048(6)        | 0.0156250     | PBC  |
| DMRG[12]         | 120   | 0.41050(2)        | 0             | OBC  |
| DMRG (this work)| 96    | 0.4104792(7)      | 0             | PBC  |
| DMRG (this work)| 128   | 0.4104792(5)      | 0             | PBC  |

TABLE I. First excitation gap $\Delta$ in the spin-1 XXZ chain as obtained by QMC and DMRG for a system size $L$, at temperature $T$, using the specified boundary conditions BC.
Figure 9 presents the finite-size extrapolation of the corresponding spin and neutral excitation gaps, as defined in Sec. III B, for both OBC and PBC. The spin and neutral gaps become equal ($\Delta$) only at the Heisenberg point for $D = 0$ [cf., Fig. 3 (a)]. Computing $\Delta$ for systems with up to $L = 512$ sites and OBC, we can extrapolate the results to the thermodynamic limit and obtain $\Delta = 0.41050(3)$ (in agreement with Ref. [32]). On the other hand, the first excitation gaps $\Delta = 0.410479(3)$ obtained with PBC show almost no finite-size dependence; see also the raw data for $L = 96$ and $L = 128$ in Table I. This value is very close to the (low-temperature) QMC result.\textsuperscript{31} Let us emphasize that although the accessible system size is rather limited for PBC, $\Delta$ for PBC is always lower than for OBC. Most notably, the system-size dependence is almost negligible (for enough large $L$). Therefore we conclude that $\Delta = 0.410479(3)$ represents a very good estimate of the Haldane gap.

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