Quantum criticality in dimerised anisotropic spin-1 chains

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Abstract Applying the (infinite) density-matrix renormalisation group technique, we explore the effect of an explicit dimerisation on the ground-state phase diagram of the spin-1 XXZ chain with single-ion anisotropy $D$. We demonstrate that the Haldane phase between large-$D$ and antiferromagnetic phases survives up to a critical dimerisation only. As a further new characteristic the dimerisation induces a direct continuous Ising quantum phase transition between the large-$D$ and antiferromagnetic phases with central charge $c = 1/2$, which terminates at a critical end-point where $c = 7/10$. Calculating the critical exponents of the order parameter, neutral gap and spin-spin-correlation function, we find $\beta = 1/8 (1/24)$, $\nu = 1 (5/9)$, and $\eta = 1/4 (3/20)$, respectively, which proves the Ising (tricritical Ising) universality class in accordance with field-theoretical predictions.

1 Introduction

In the last decade, quantum integer-spin chains have received revived attention from a topological point of view. In contrast to the gapless ground state in the spin-1/2 antiferromagnetic (AFM) Heisenberg chain, for integer spins there exists a finite gap between the ground state and the first excited state, as conjectured first by Haldane [1]. In the spin-1 Heisenberg chain, this so-called Haldane phase is a representative of symmetry-protected-topological (SPT) phases [2,3], which is protected by lattice inversion, time-reversal, and dihedral ($Z_2 \times Z_2$) symmetries. The Haldane phase has attracted much attention also from an experimental point of view and the Haldane gap was confirmed, e.g., in a Ni-compound Ni(C$_2$H$_4$N$_2$)$_2$NO$_2$(ClO$_4$)$_2$ [4,5], which possesses a small single-ion anisotropy [6].

A natural extension of the spin-1 XXZ chain with a single-ion anisotropy is an alternating strength of the spin exchange interaction, for example, caused by a bond dimerisation, as realised in a compound again with Ni$^{2+}$ ions [Ni(333-tet)(µ-N$_3$)$_n$](ClO$_4$)$_n$ [7]. We expect that such a bond dimerisation will substantially influence the ground-state properties of the spin model, just as in case of the half-filled extended Hubbard model where it opens an energy gap in the spin-density-wave regime and leads to new types of quantum phase transitions [8].

At present the most reliable method for an exact numerical treatment of one-dimensional (strongly correlated) electron, boson and spin systems seems to be the density-matrix renormalization group (DMRG) technique, which is based on a matrix-product state (MPS) approximation of the ground state [9,10]. Here, we employ an infinite DMRG (iDMRG) variant that uses an infinite MPS representation and thus—working in the thermodynamic limit—avoids any boundary and finite-size effects [11].

2 Model and ground-state phase diagram

The Hamiltonian of a dimerised spin-1 AFM spin chain with single-ion anisotropy $D$ reads

\[ \hat{H} = J \sum_j (1 + \delta(-1)^j)(\hat{S}_j \cdot \hat{S}_{j+1}) + D \sum_j (\hat{S}_j^z)^2, \]

(1)

where $(\hat{S}_j \cdot \hat{S}_{j+1}) = \hat{S}_j^x \hat{S}_{j+1}^x + \hat{S}_j^y \hat{S}_{j+1}^y + \Delta \hat{S}_j^z \hat{S}_{j+1}^z$. For vanishing dimerisation $\delta$ and not too large $\Delta$ and $D/J$, the ground-state phase diagram of the model (1) develops a nontrivial topological Haldane phase between topologically trivial large-$D$ (LD) and AFM phases (see Fig. 1a). The phase transitions from Haldane to the LD and AFM phases belong to the Gaussian and Ising universality classes, respectively, while the LD$\leftrightarrow$AFM transition is of first order.

A finite dimerisation strongly affects the phase boundary between the dimerised LD (D-LD) and AFM (D-AFM) phases: Now, at sufficiently large $\Delta$ and $D/J$, a new direct Ising transition appears with $c = 1/2$, which terminates at a tricritical Ising point where $c =$
Fig. 1 IDMRG ground-state phase diagram of the spin-1 XXZ chain (1) with dimerisation $\delta = 0$ (a), 0.1 (b) and 0.5 (c). The phase boundaries are determined by means of the methods described in our previous work [12,13].

Fig. 2 Absolute value of the AFM order parameter $|\langle m_{AFM} \rangle|$ (upper row) in the vicinity of the D-LD$\rightleftharpoons$D-AFM Ising (a) and tricritical Ising (c) transition for $\delta = 0.1$ at fixed $D/J = 3$ and $D/J = 3.64$, respectively. Symbols are iDMRG data obtained with bond dimension $\chi = 800$, dashed lines display the fitting function with critical exponents $\beta = 1/8$ (a) and 1/24 (c). Here the relative error of the exponents is less than 7% and might be reduced further increasing the bond dimension $\chi$. The corresponding log-log plots (b) and (d) in the lower row demonstrate that these power-laws apply with high precision close to the critical points. Here, $\Delta_c \simeq 3.303$ and $\Delta_{ce} \simeq 3.900$.

7/10 [13]. Beyond this critical end-point, in the very strong-coupling regime, the quantum phase transition becomes first order (see Fig. 1b). Increasing dimerisation further, the dimerised Haldane phase (D-H) disappears at about $\delta \gtrsim 0.26$, if we limit ourselves to the case $J, D > 0$. Figure 1c shows a situation, where only D-LD and D-AFM phases appear, for $\delta = 0.5$.

3 Critical exponents

We now provide further evidence for Ising and tricritical Ising criticality at the D-LD$\rightleftharpoons$D-AFM quantum phase transition of the dimerised XXZ chain (1). Approaching a continuous quantum phase transition, the system behaviour is characterised by a set of universal exponents describing the power-law dependencies of the relevant order parameter, correlation functions or excitation gaps on $(g - g_c)$, where $g$ parametrizes the (general) coupling constant of the model under consideration and $g_c$ is its critical value at the transition point. Assuming the Ising (tricritical Ising) universality class, the critical exponents of the order parameter, neutral gap and spin–spin-correlation function should be $\beta = 1/8$ (1/24), $\nu = 1$ (5/9), and $\eta = 1/4$ (3/20) [14], and will be linked with each other by the scaling relation $\frac{\Delta}{\Delta_c} = \beta (g - g_c)^{\eta}$, where $d$ is the spatial dimension. In what follows, this will be proved for the rather complex model (1) performing unbiased iDMRG simula-
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Fig. 3 Closing of the neutral gap (upper row) at the Ising (a) and tricritical Ising (c) transition for the same parameters as in Fig. 2. The log-log plots (lower row) show that the $L \to \infty$ extrapolated DMRG data can be excellently fitted by $|\Delta - \Delta_c|^{\nu}$ with $\nu = 1$ (b) and $|\Delta - \Delta_{ce}|^{\nu}$ with $\nu = 5/9$ (d).

Fig. 4 Decay of the longitudinal spin–spin two-point functions at Ising (a) and tricritical Ising (b) transition points for $\delta = 0.1$. Symbols give iDMRG data; power laws predicted by field theory drawn in by dotted lines.

3.1 Order parameter

The exponent $\beta$ can be extracted from the AFM order parameter:

$$\langle \hat{m}_{\text{AFM}} \rangle = \frac{1}{L} \sum_j (-1)^j \langle \hat{S}_j^z \rangle.$$  \hspace{1cm} (2)

Figure 2 displays $|\langle \hat{m}_{\text{AFM}} \rangle|$ across the Ising and tricritical Ising D-LD=$D$-AFM transitions when the spin anisotropy $\Delta$ is increased at fixed $D/J = 3$ and $D/J = 3.64$, respectively. The corresponding critical couplings are $\Delta_c \approx 3.303$ and $\Delta_{ce} \approx 3.900$. Evidently, the onset of $|\langle \hat{m}_{\text{AFM}} \rangle|$ in the D-AFM phase is much more abrupt for the transition at the critical end point. More importantly, the critical exponents of the order parameter function are verified to be $1/8$ and $1/24$ at the Ising transition with $c = 1/2$ and the tricritical Ising transition with $c = 7/10$, respectively.

3.2 Neutral gap

The neutral gap is defined as

$$\Delta_n(L) = E_1 - E_0,$$ \hspace{1cm} (3)

where $E_0$ ($E_1$) is the energy of the ground state (first excited state) for a system with $L$ sites and vanishing total spin $z$-component, which is directly accessible by DMRG. To determine the neutral gap we use a DMRG representation with infinite boundary conditions [15]. Figure 3a, b shows that the neutral gap closes and opens linearly on passing the Ising transition, i.e., $\nu = 1$. Also for the tricritical Ising point the prediction of perturbed conformal field theory could be confirmed: Our data clearly yield $\nu = 5/9$, see Fig. 3c, d.

3.3 Spin–spin correlation function

Let us finally investigate the critical behaviour of the staggered $z$-$z$ spin correlator $\langle \hat{\tilde{n}}_j^z \hat{\tilde{n}}_{j+\ell}^z \rangle$ with $\hat{\tilde{n}}_j^z = \hat{S}_j^z - \langle \hat{S}_j^z \rangle$. 


\((-1)^j(\hat{S}_j^z - \hat{S}_{j+1}^z)/2\). For this, we determine the exponent \(\eta\) from the spatial decay of the correlations at large distances \(\ell \gg 1\):

\[
\langle \hat{n}_j^z \hat{n}_{j+\ell}^z \rangle \propto \ell^{-\eta}.
\]

(4)

Figure 4 clearly shows that the critical exponents obtained in such a way from the iDMRG results are \(\eta = 1/4\) and 3/20. That means, according to field theory, the transitions belong to the Ising respectively tricritical Ising universality class.

4 Summary

To conclude, we have examined numerically the criticality of the quantum phase transition between the dimerised large-\(D\) and antiferromagnetic phases in the spin-1 XXZ chain with explicit bond dimerisation and proved the Ising (\(c = 1/2\)) and tricritical Ising (\(c = 7/10\)) universality classes. The critical exponents extracted from large-scale (infinite matrix-product-state based) density-matrix renormalisation group simulations corroborate the predictions of bosonisation-based field theory, and consequently fulfil the desired scaling relation. The calculated ground-state phase diagram shows that a symmetry-protected topological Hal-dane phase appears—in between large-\(D\) and antiferromagnetic phases—for not too large bond dimerisation only.

We note that a similar situation evolves in the one-dimensional extended Bose–Hubbard model with bond dimerisation [16].

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