Symmetry-protected trivial phases and quantum phase transitions in an anisotropic antiferromagnetic spin-1 biquadratic model

Xi-Hao Chen,1,2 Ian McCulloch,3 Murray T. Batchelor,4,5,1 and Huan-Qiang Zhou1

1Centre for Modern Physics, Chongqing University, Chongqing 400044, The People’s Republic of China
2Research Institute for New Materials and Technology, Chongqing University of Arts and Sciences, Chongqing 400000, The People’s Republic of China
3Department of Physics, The University of Queensland, Brisbane, Australia
4Department of Theoretical Physics, Research School of Physics, The Australian National University, Canberra ACT 2601, Australia
5Mathematical Sciences Institute, The Australian National University, Canberra ACT 2601, Australia

The ground state phase diagram is obtained for an antiferromagnetic spin-1 anisotropic biquadratic model. With the help of symmetry and duality transformations, three symmetry-protected trivial phases and one dimerized symmetry breaking phase are found. Local and nonlocal order parameters are identified to characterize these phases. Quantum phase transitions between the symmetry-protected trivial phases belong to the Gaussian universality class with central charge $c = 1$, and quantum phase transitions from the symmetry-protected trivial phases to the dimerized phase belong to the Ising universality class with central charge $c = 1/2$. In addition, the model admits three characteristic lines of factorized ground states, which are located in the symmetry-protected trivial phases instead of a symmetry breaking phase, in sharp contrast to other known cases.

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Introduction.—Much attention has been focused on critical phenomena in quantum many-body systems, with an aim towards a complete classification of quantum states of matter. In this regard, significant progress has been made for quantum spin systems in one dimension, resulting in the introduction of novel concepts, such as symmetry-protected topological order [1], and symmetry-protected trivial (SPt) order [2].

An intriguing question is how then to demonstrate the powerfulness of these phases. Quantum phase transitions between the symmetry-protected trivial phases belong to the Gaussian universality class with central charge $c = 1$, and quantum phase transitions from the symmetry-protected trivial phases to the dimerized phase belong to the Ising universality class with central charge $c = 1/2$. In addition, the model admits three characteristic lines of factorized ground states, which are located in the symmetry-protected trivial phases instead of a symmetry breaking phase, in sharp contrast to other known cases.

The model is antiferromagnetic, in the sense that it becomes the antiferromagnetic spin-1/2 XYZ model, which itself is an exactly solvable model [7], if $S_{i}^{α}$ are spin-1/2 operators.

The model Hamiltonian (1) reduces to the spin-1 SU(2)-invariant biquadratic model when $J_{x} = J_{y} = J_{z}$. The spin-1 biquadratic model has been extensively investigated. It can be either mapped to the 9-state Potts model [5] or solved directly in terms of Bethe Ansatz or functional relations [6]. It is thus known to be in a dimerized phase with a relatively small spectral gap. The Hamiltonian (1) of the anisotropic generalization of this model commutes with the three operators $\Sigma_{x} = \Sigma_{i}(-1)^{(x_{i}^{2})} - (x_{i}^{2})^{2}$, $\Sigma_{y} = \Sigma_{i}(-1)^{(y_{i}^{2})} - (y_{i}^{2})^{2}$ and $\Sigma_{z} = \Sigma_{i}(-1)^{(z_{i}^{2})} - (z_{i}^{2})^{2}$. In particular, these three commuting operators, combining with $S_{i}^{α}$, generate an SU(3) symmetry when $J_{x} = J_{y} = J_{z}$. It is the staggered nature of the symmetry operators which explains why spontaneous dimerization occurs in the spin-1 SU(2)-invariant biquadratic model [8].

Duality transformations.—Key information about the nature of the phase diagram can be obtained from duality relations among the spin couplings. Here quantum duality is represented by a local unitary transformation $U$ acting on Hamiltonian (1). For convenience and simplicity we define the variables $X = J_{x}/J_{z}$ and $Y = J_{y}/J_{z}$ and consider $H(X, Y)$. In general if $H(X', Y')$ is dual to $H(X, Y)$ there should exist a unitary transformation $U$ satisfying

$$H(X, Y) = k(X, Y) U H(X', Y') U^\dagger.$$  

(2)

The coupling parameters $X'$ and $Y'$ are functions of $X$ and $Y$ with $k(X, Y)$ being positive.

For Hamiltonian (1) there are two symmetry transformations and four duality transformations, as presented in Table I. These symmetry and duality transformations imply six self-dual lines defined by $X = \pm 1$, $Y = \pm 1$ and $Y/X = \pm 1$. 

$$H(X, Y) = k(X, Y) U H(X', Y') U^\dagger.$$  

(2)
**Ground state phase diagram.**—To obtain the phase diagram we consider the self-dual lines \( J_x/J_z = 1 \), \( J_x/J_y = 1 \) and \( J_z/J_y = 1 \), which delineate the six regions shown in Fig. 1(a). Because of the various symmetries and dualities, we only need to focus on one of these six regions, with the whole phase diagram following by mapping with the help of the duality transformations. We thus define region I as the principal regime. To determine the phase boundary in region I, we examine order parameters based on numerical simulations in terms of the infinite Time-Evolving Block Decimation (iTEBD) algorithm \[9\] and the infinite Density Matrix Renormalization Group (iDMRG) algorithm \[10\]. In both algorithms, ground state wave functions are represented in terms of infinite Matrix Product States (iMPS). We will also make use of the von Neumann entropy. Fig. 1(b) shows the ground state phase diagram determined in this way, as discussed in detail below.

**Factorized states.**—When \( J_y = 0 \) the system is in a factorized ground state. The wave function of this factorized state can be written as a simple product of the vector \( \frac{1}{\sqrt{2}} (1, 0, -1) \). The corresponding factorized energies are given by \( e = (J_y^2 + J_z^2) \). Similarly, the system is also in a factorized state when \( J_y = 0 \) or \( J_z = 0 \), respectively, as follows from the duality transformations. The wave functions can then be written as products of the vector \( \frac{1}{\sqrt{2}} (1, 0, 1) \) or \( (0, 1, 0) \) with energies \( e = -(J_y^2 + J_z^2) \) or \( e = -(J_y^2 + J_z^2) \), respectively. These three factorized states are dual to each other. Note that, if we choose \( J_z \) as an energy scale, then \( J_y = 0 \) is equivalent to saying that both \( J_x \) and \( J_y \) approach infinity with a fixed ratio \( J_x/J_y \). We also note that when \( J_x = J_y = 0 \), the model has \( 2^N \) degeneracies with entanglement varying between 0 and \( \infty \), consistent with previous results for systems with largely degenerate ground states \[11\].

**Symmetry-protected trivial phases.**—Spontaneous symmetry breaking (SSB) occurring in quantum many-body systems implies the existence of local order which can be characterized by local order parameters. Significantly, there exist other concepts of order in quantum many-body systems which are beyond Landau theory due to the absence of any SSB. Examples are the three SPt phases mentioned above, which cannot be successfully characterized by local order parameters. Fortunately appropriate non-local order parameters can be used to characterize such order, which may be regarded as a natural extension of the SPt order introduced in Ref. \[2\]. Indeed, distinct non-local order parameters can successfully distinguish various symmetry-protected phases and are also effective for symmetry-protected gapped phases with partial symmetry breaking \[12, 13\].

For a given ground state wave function \( |\psi\rangle \) of an infinite-size spin chain represented by the iMPS, the site-centered non-local order parameters can be written based on reversing an odd-sized segment of the chain and then calculating the resulting overlap \[2, 14\]. This can be defined in terms of the inversion operator

\[
O^L_\alpha = \frac{\langle \psi | I_1(L) \Sigma^\alpha (1,L) | \psi \rangle}{tr(\Sigma^\alpha (1,L))},
\]

where \( O^L_\alpha \) is the inversion on the segment from 1 to \( L \) with internal symmetry operations \( \Sigma^\alpha (1,L) \) acting on the physical indices. Here \( \Sigma^\alpha (1,L) = \exp(i\pi S^\alpha) \), with \( S^\alpha \) a spin-1 matrix and \( \alpha = x, y, \) or \( z \). The segment length \( L \) is odd. \( \lambda_A \) and \( \lambda_B \) are Schmidt decomposition coefficients.

This definition respects two-site translation invariance due to the fact that it can work on non-SSB and SSB wave functions directly. In the absence of SSB, \( O^L_\alpha \) gives a \( \pm 1 \) value. Conversely, \( O^L_\alpha \) gives a 0 value for SSB. Fig. 2 shows the...
graphical representation of non-local order parameters in the MPS framework. Each SPt phase can then be characterized by the values \(O_L^x, O_L^y, O_L^z\) of the non-local order parameters. When \(L\) approaches the thermodynamic limit, the non-local order parameters \((O_L^x, O_L^y, O_L^z)\) obtain the exact values \((K_x, K_y, K_z)\). We denote these three \(\mathbb{Z}_2\) combined symmetry operations by \(K = (K_x, K_y, K_z)\).

We employ the definition of non-local order parameters \([3]\) on the three sample lines, (i) \(J_x/J_z = 0.4\), (ii) \(J_x/J_z = 0.6\) and (iii) \(J_y/J_z = 0.988\), as indicated in the phase diagram Fig. 1(b). First consider lines (i) and (ii). In Fig. 3, we plot \(O_L^x, O_L^y\) and \(O_L^z\) as functions of \(J_x/J_z\) for fixed \(J_y/J_z = 0.4\) and fixed \(J_x/J_z = 0.6\) with truncation dimension \(\chi = 100\). Quantum phase transition (QPT) points are located at \(J_x'/J_z = 0.4\) and \(J_x'/J_z = 0.6\), respectively. Increasing the inversion block size \(L\) from \(L = 101\) to \(L = 201\), \(O_L^z\) reaches the saturation value \(-1\) most efficiently when \(J_y/J_z\) is away from the QPT point \(J_y'/J_z\). In contrast, \(O_L^x\) saturates much slower in the vicinity of \(J_y'/J_z\). The values of \(O_L^x\) and \(O_L^y\) behave similarly.

In this way the SPt phase on the right hand side of QPT points \(J_y'/J_z\) is characterized by \(K = (1, -1, -1)\), which corresponds to the SPt phase above (PA) diagonal phase boundaries. Similarly, the phase on the left hand side of QPT points \(J_y'/J_z\) is characterized by \(K = (-1, 1, -1)\), which corresponds to the SPt phases below (PB) diagonal phase boundaries. Based on the dual regions in Fig. 1(a), the SPt PA phase is in region I and the SPt PB phase is in region VI. These two phases are thus dual to each other, separated by the self-dual line \(J_y = J_x\). The values \(K = (1, -1, -1)\) of the non-local order parameters in region I and \(K = (-1, 1, -1)\) in region VI foretell their duality. Based on duality, one knows, e.g., that the non-local order parameters of the SPt phase in region III and IV can be written as \(K = (-1, 1, -1)\).

Turning to line (iii) in Fig. 1(b) we plot \(O_L^x, O_L^y\) and \(O_L^z\) as a function of \(J_x/J_z\) for fixed \(J_y/J_z = 0.988\) with truncation dimension \(\chi = 100\) in Fig. 4. Here two QPT points are located at \(J_x'/J_z = 0.9799\) and \(J_x'/J_z = 1.003\) at \(\chi = 100\). The SPt phase on the left hand side of \(J_x'/J_z\) corresponding to PA is characterized by \(K = (1, -1, -1)\). The SPt phase on the right hand side of \(J_y'/J_z\) corresponding to PB is characterized by \(K = (-1, 1, -1)\). We note that the saturation rate of \(O_L^x, O_L^y\) and \(O_L^z\) at \(J_x'/J_z = 0.9799\) and \(J_x'/J_z = 1.003\) is much slower than the rate at \(J_x'/J_z = 0.4\) and \(0.6\).

Dimerized phase.—We now concentrate on the dimerized phase in the vicinity of the isotropic point \(J_x = J_y = J_z\), for which local order exists. With fixed \(J_y/J_z = 0.988\), SSB occurs when control parameter \(J_x/J_z\) crosses the points \(J_x'/J_z = 0.9799\) and \(J_x'/J_z = 1.003\). To characterize the local order in the region between these two points, we consider dimerized local order parameter \((S_i S_{i+1} - S_{i+1} S_i)\) \([4]\). Unfortunately, this definition only fits the system with \(SU(2)\) symmetry. However, a systematic method based on tensor network representations to derive local order parameters has been established \([5]\). Following this method, we analyse the combined dimerized local order parameters \(D = (D_x, D_y, D_z)\), with \(D_\alpha = \langle S_i^\alpha S_{i+1}^\alpha - S_{i+1}^\alpha S_i^\alpha \rangle\). Fig. 4 shows plots of these dimerized local order parameters as a function of control parameter \(J_x/J_z\) with truncation dimension \(\chi = 100\) for fixed \(J_y/J_z = 0.988\). The dimerized local order \(D\) is clearly evident between \(J_x'/J_z = 0.9799\) and \(J_x'/J_z = 1.003\). Fig. 4 clearly demonstrates the complementarity between the local and non-local order parameters.

von Neumann entropy and central charge.—To examine the nature of the QPT between SPt and dimerized phases we first discuss the definition of von Neumann entropy, as a mea-

![FIG. 2: Graphical representation of non-local order parameters in the MPS picture. \(\Gamma_x\) and \(\Gamma_y\) are three-index tensors; \(A_x\) and \(A_y\) are Schmidt decomposition coefficients. These four tensors with a two-site translation invariance form the ground state wave function \(|\phi\rangle\) of the infinite-size spin chain.](image)

![FIG. 3: Non-local order parameters \(O_L^z\) as a function of coupling \(J_x/J_z\) with truncation dimension \(\chi = 100\) for fixed \(J_y/J_z = 0.4\) (top) and \(0.6\) (bottom). The parameter \(L\) shown is the inversion block size. QPT points are identified as \(J_x'/J_z = 0.4\) and \(0.6\). For each panel the symmetry parameter values \(K = (-1, 1, -1)\) for the left side and \(K = (1, -1, -1)\) for the right side of the QPT point. The data sets correspond to the lines (i) and (ii) in Fig. 1(b).](image)
measure of bipartition entanglement. Consider the state $|\psi\rangle$ being composed of two semi-infinite chains $L(-\infty,\ldots,i)$ and $R(i+1,\ldots,\infty)$, connected by the Schmidt decomposition coefficient $\lambda_{\alpha}$. This implies $|\psi\rangle$ can be expressed as $|\psi\rangle = \sum_{\alpha=1}^{D} \lambda_{\alpha}|\phi_{\alpha}^{L}\rangle|\phi_{\alpha}^{R}\rangle$, where $|\phi_{\alpha}^{L}\rangle$ and $|\phi_{\alpha}^{R}\rangle$ are the Schmidt bases of the two semi-infinite chains $L$ and $R$. Consequently, the von Neumann entropy can be defined as \[ S = -\sum_{\alpha=1}^{D} \lambda_{\alpha}^{2} \log \lambda_{\alpha}^{2}. \] (4)

At a critical point in a 1D system, the semi-logarithmic scaling of the von Neumann entropy versus truncation dimension $\chi$ follows from conformal invariance, with scaling ruled by the central charge of the underlying conformal field theory. In addition, the correlation length $\xi$ of the iMPS exhibits a power scaling with truncation dimension $\chi$. These two scaling relations can be written as \[ S_{\chi} \propto \frac{c}{6} \log \chi, \quad \xi_{\chi} \propto \xi_{0} \chi^{\kappa}. \] (5)

Here $c$ denotes the central charge and $\kappa$ is a finite entanglement scaling exponent. For a given $\chi$, the correlation length $\xi_{\chi}$ can be obtained by the largest and the second largest eigenvalues $D_{0}(\chi)$ and $D_{1}(\chi)$ of the transfer matrix, with $\xi_{\chi} = 1/\log|D_{0}(\chi)/D_{1}(\chi)|$. By making use of the relations (5) one can obtain numerical estimates for the central charge on the phase boundary between SPt phases and between SPt and dimerized phases.

For this purpose, we choose $J_{y}^{c}/J_{z} = 0.4$ with fixed $J_{z}/J_{z} = 0.4$ and choose $J_{z}/J_{z} = 1$ with varying $J_{y}^{c}/J_{z}$. Fig. 5 shows a corresponding plot of the von Neumann entropy and correlation length as a function of truncation dimension $\chi$ ranging from 75 to 600. Both the von Neumann entropy and correlation length diverge with increasing truncation dimension $\chi$. To extract the central charge, we use the fitting functions $S_{\chi} = \frac{c}{6} \log \chi + a$ and $\log \xi_{\chi} = \kappa \log \chi + b$ and consider two cases. (i) For the case of fixed $J_{z}/J_{z} = 0.4$ with $J_{y}^{c}/J_{z} = 0.4$, shown in purple in Fig. 5 and labeled as Fitting 1, the fitting coefficients are given by $c_{1}k_{1}/6 = 0.20968$, $a_{1} = 0.24527$, $b_{1} = -2.6563$, and $k_{1} = 1.2619$. The central charge is estimated to be $c_{1} = 0.997$. This is consistent with a general argument that a phase transition between SPt phases belongs to the Gaussian universality class $\mathcal{C}$. (ii) For the case of fixed $J_{z}/J_{z} = 1$ with varying $J_{y}^{c}/J_{z}$, shown in red in Fig. 5 and labeled as Fitting 2, the fitting coefficients are given by $c_{2}k_{2}/6 = 0.12929$, $a_{2} = 0.75742$, $b_{2} = -3.2471$, and $k_{2} = 1.4199$. As a result, the central charge is estimated to be $c_{2} = 0.5463$. This indicates that the phase transition falls into the Ising universality class, as anticipated from the fact that a $\mathcal{Z}_{2}$ symmetry is spontaneously broken in the dimerized phase.

Summary.—We have investigated the nature of quantum SPt phases and quantum phase transitions in the spin-1 antiferromagnetic anisotropic biquadratic model (1) by making use of quantum duality and symmetry transformations, along with iTEBD and iDMRG algorithms. The concept of SPt phases, originally defined through the combined operation of the site-centered inversion with the $\pi$-rotation around the $y$-axis in the spin space $\mathcal{C}$, is extended, in order to keep consistency with the duality transformations, which themselves are induced from the symmetric group $\mathcal{S}_{2}$ with respect to $x$, $y$, and $z$. Our results suggest the importance and potential generality of SPt phases in a classification of quantum states of matter.

The ground state phase diagram in Fig. (1b) has been determined by studying the principal regime, which can be mapped to the other five regions of the phase diagram via the quantum duality and symmetry transformations summarized in Table I. The phase boundaries are determined by calculating the non-local and local order parameters of the principal regime. To illustrate our strategy, three sample lines, $J_{z}/J_{z} = 0.4$, $J_{c}/J_{z} = 0.6$ and $J_{c}/J_{z} = 0.988$, are studied in detail. The phase diagram is shown to be composed of
FIG. 5: The scaling of (a) von Neumann entropy $S$ and (b) correlation length $\xi$ with the truncation dimension $\chi$. (i) For fixed $J_x/J_z = 0.4$ with $J_y/J_z = 0.4$, shown in purple and labeled as Fitting 1, the central charge is estimated to be $c_1 = 0.997$. (ii) For fixed $J_x/J_z = 1$ with varying $J_y/J_z$, shown in red and labeled as Fitting 2, the central charge is estimated to be $c_2 = 0.5463$.

The von Neumann entropy and correlation length have been used to estimate the central charge $c = 0.5463$ on the boundary between SP$\tilde{t}$ and dimerized phases. This value is suggestive of the Ising-type universality class. The central charge value $c = 0.997$ is extracted on the phase boundary between SP$\tilde{t}$ phases, corresponding to the Gaussian-type universality class.

We have also identified three characteristic lines of factorized ground states, which are located in the SP$\tilde{t}$ phases instead of a symmetry breaking phase, in sharp contrast to other known cases [21, 22].

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