Exact dimerized phase in anisotropic XYZ model for quasi-one-dimensional magnets

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We report the exact dimer phase, in which the ground states are described by product of singlet dimer, in the extended XYZ model by direct generalizing the isotropic Majumdar-Ghosh model to the fully anisotropic regime. This model also supports three different ferromagnetic (FM) phases, denoted as x-FM, y-FM and z-FM. The boundaries between the dimer phase and FM phases are infinite-fold degenerate. The breaking of this infinite-fold degeneracy by either translational symmetry or Z2 symmetry lead to dimer phase and FM phases, respectively. Moreover, the boundaries between the three FM phases are critical with central charge c = 1. We characterize the properties of these boundaries using entanglement entropy, excitation gap and long-range spin-spin correlations. These results are relevant to a large number of quasi-one-dimensional magnets, in which anisotropy is necessary to isolate a single chain out from the bulk material. We discuss the possible experimental signatures in true materials with magnetic field along different directions, and show that the anisotropy may resolve the long-standing disagreements between theory and experiments.

The spin models for magnetism phases are basic topics in modern physics. In these models, only a few of them, most of which focused on one dimension, can be solved exactly and understood completely. In general, we may categorize these models into two groups. In the first group, the models can be solved exactly using some mathematical techniques based on their symmetries[1], with typical examples such as transverse Ising, XX and XXZ models[2–4]. Some of them may even be mapped to the Hubbard model [5–9]. Thus, their whole spectra and thermodynamic properties can be obtained exactly. In some of these models, the excitations can be totally different from that in three dimensional bulk. Recently, the spinon excitations in these models have been direct measured in experiments[10–12] by neutron diffraction. These solvable models also play essential role in the understanding of the non-equilibrium dynamics, phase transitions and entanglement in many-body systems[9, 13–16].

In the other group, which is relevant to the research in this work, only the ground states (GSs) of the Hamiltonian can be obtained. For example, in the most representing Majumdar-Ghosh (MG) model[17–22], the GSs can be expressed exactly as product of singlet dimer (see Eq. 2). Soon after, this idea was generalized to the Affleck-Kennedy-Lieb-Tasaki (AKLT) model[23–26] for the searching of symmetry protected topological (SPT) phases with non-Abelian excitations. In experiments, this dimer phase is relevant to a large number of quasi-one-dimensional magnets, such as CuGeO3[27–29], NaV2O5[30, 31], TIOCl[32–34], TTFCuBDT[35], MEM(TCNO)2[36, 37], BCPTTF2PF6[38], CuCrO4[39], SrCu2O3[40], SrCu2(BO3)2[41], Cu3(MoO4(OH))2[42], etc. To date, most of these candidates are explained by isotropic spin models, while in experiments, strong anisotropy is always necessary to isolate a single chain out from the three dimensional bulk. It was found that the isotropic models are insufficient to understand all results in experiments[29, 43, 44].

We aim to extend the realm of exact dimerized phase to the fully anisotropic regime. Our model harbors not only the exact dimer phase, but also three gapped ferromagnetic (FM) phases, denoted as x-FM, y-FM and z-FM, according to their symmetry breaking directions, and we determine their phase boundaries. We find that the

FIG. 1. (Color online). Phase diagram for the fully anisotropic XYZ model. We have assumed \( x = \cos(\theta) \) and \( y = \sin(\theta) \). The phase boundaries between dimer phase and FM phases are infinite-fold degenerate, while the boundaries between the FM phases are critical and gapless with central charge \( c = 1 \). The black dots are boundaries determined by order parameters (see Eq. 7), with accuracy better than \( 3.0 \times 10^{-4} \). In dimer phase, the deep red regimes cannot be explained by mixing of two anisotropic dimer models. The classical limits are denoted as \( H(1, 0, 0) \), \( H(0, 1, 0) \) and \( H(0, 0, 1) \) and the dashed lines are conditions for exact FM states.
boundaries between dimer and FM phases are infinite-fold degenerate, while the boundaries between the FM phases are critical with central charge \( c = 1 \). Thus these two phases represent two different ways for spontaneous symmetry breaking, either by translational or \( \mathbb{Z}_2 \) symmetry breaking, from the infinite-fold degenerate boundaries. We finally discuss the relevant of our results to quasi-one-dimensional magnets and present evidences to distinguish these phases in experiments.

**Model.** We consider the following spin-1/2 model directly generalized from the isotropic MG model,

\[
H(x, y, z) = J \sum_i h_{i,i+1} + \alpha h_{i,i+2},
\]

where \( \alpha = \frac{1}{2} \) (MG point), \( J > 0 \) and \( h_{i,j} = x s_i^x s_j^x + y s_i^y s_j^y + z s_i^z s_j^z \), with \( x, y, z \in \mathbb{R} \). Hereafter, if unspecified, we let \( J = 1 \). The case when \( x = y = z > 0 \) corresponds to the well-known MG model, which supports exact dimer phase[17, 18]. Anisotropy can be introduced to this model by letting \( x = y > 0 \), in which when \( z > -x/2 \) the GSs are also exact dimerized[45, 46]. Mathematically, the two exact dimer states can be written as,

\[
|\varphi_0\rangle = \prod_{2n} |2n, 2n + 1\rangle, \quad |\varphi_1\rangle = \prod_{2n} |2n - 1, 2n\rangle,
\]

where \( |i, i + 1\rangle = \frac{1}{\sqrt{2}} (|\uparrow_{i+1}\rangle - |\downarrow_{i+1}\rangle) \) represents the singlet dimer between neighboring sites. These two states have the same energy. There are several ways to extend this model to more intriguing conditions, for example, in the presence of some proper long-range interactions[15, 16]. Abelian excitations\[19\] to integer spins, it may support SPT phases with non-Abelian excitations[48–51].

**Phase boundary for dimer phase.** Our determined phase diagram for the dimer phase is presented in Fig. 1. This regime has the advantage to be determined exactly with even a small lattice sites with periodic boundary condition, provided that the wave functions are in form of Eq. 2. We consider the simplest case with \( L = 4 \):

\[
H_4 = h_{12} + h_{23} + h_{34} + h_{41} + \alpha (h_{13} + h_{24} + h_{31} + h_{42}).
\]

Their eigenvalues are listed below:

- \( E_{1-3} = -x/2 \), \( E_{4-6} = -y/2 \), \( E_{7-9} = -z/2 \),
- \( E_{10} = 3x/2 \), \( E_{11} = 3y/2 \), \( E_{12} = 3z/2 \),
- \( E_{13-14} = (x + y + z)/2 \pm \sqrt{x^2 + y^2 + z^2 - xy - yz - zx} \),
- \( E_{15-16} = -(x + y + z)/2 \).

The last two states with twofold degeneracy correspond to the exact dimer phase with eigenvectors in form of Eq. 2. To ensure the dimerized states has lowest energy, we require \( E_{15-16}^{\text{dimer}} < E_i \) for \( i = 1 \) – 14, which yields

\[ x + y + z > 0, \quad xy + yz + zx > 0. \]

This is the major phase boundary determined for the dimer phase (see boundaries in Fig. 1). From the first equation, we may always assume that \( x + y > 0 \), then these two equations give rise to \( z > -xy/(x + y) \). The same analysis can be performed for \( L = 6 \), which can also be solved exactly and give the same phase boundary. By this result, the GS energy for the dimer phase in a length \( L \) system \( (L \text{ is an even number}) \)

\[
F_q^{\text{dimer}} = -(x + y + z)L/8.
\]

This result naturally includes the previous known results in the MG model with \( x = y = z > 0 \)[47] and extended XXZ model with \( x = y > 0 \) and \( z > -x/2 \)[45, 46].

Eq. 4 can lead to an interesting conclusion, that is, at most one parameter is allowed to be negative for the exact dimerized phase, which can be reached as following. Let \( y \) and \( z \) to be negative values, then \( x > |y| + |z| \). However, the second condition in Eq. 4 means \( \frac{1}{x} > \frac{1}{|y|} + \frac{1}{|z|} \). The multiply of these two inequalities yields obvious contradiction, \( x(1/x) > (|y| + |z|)(1/|y| + 1/|z|) \). Nevertheless, in the presence of two negative parameters, we may compute \( -H \), which may support dimerized state in its GSs. In this case the highest levels can be dimerized with two negative parameters.

Then, does this boundary contains nontrivial regime that can not be explained by previous models? To this end, we first prove another model for exact dimer phase. For \( z = 0 \) and \( x > 0, y > 0 \), let \( H_{xy} = \)
automatically satisfies the permutation symmetry of $H$. This boundary is numerically verified with extraordinary high accuracy (see Fig. 3). In Eq. 6, we prove that this decoupling only allows solution when $z' > -x'/2$ and $x'' > 0$, $y'' > 0$ and $\beta \in [0, 1]$. From Eq. 4, we find $\beta(2x'' + z'') + (1 - \beta)(x'' + y'') > 0$ and $\beta^2(x'' + 2x'z'') + (1 - \beta)^2x''y'' + \beta(1 - \beta)(x'' + y'') > 0$, which can always be fulfilled for the given condition. Nevertheless, not all dimer state defined by Eq. 4 can be explained in this way. In Eq. 6, one may replace the XXZ model by anisotropic XYZ model and we prove that this decoupling only allows solution when $z \geq -\frac{1}{2}\min(\cos(\theta), \sin(\theta))$ for $\theta \in [0, \pi/2]$, $z \geq -2\cos(\theta)$ for $\theta \in [\pi/2, \pi - \arctan(2)]$, and $z \geq -2\sin(\theta)$ for $\theta \in [3\pi/2 + \arctan(2), 2\pi]$ (see the light red regime in Fig. 1), beyond which it can not be understood by mechanism of Eq. 6, indicating of nontriviality for this phase.

Infinite-fold degeneracy at the boundary by Eq. 4. The boundary in Eq. 4 automatically satisfies the permutation symmetry of $H$. This boundary is numerically verified with extraordinary high accuracy (see Fig. 1). A typical transition from the dimer phase to the z-FM phase is presented in Fig. 2a, which is characterized by dimer order $\Delta_d$ [51, 53] and magnetization $M_z$ [54],

$$\Delta_d = \{s_i \cdot s_{i+1} - s_{i+1} \cdot s_i\}, \quad M_z = \sum_i \langle s_i^z \rangle. \quad (7)$$

In the exact dimer phase, $\Delta_d = 3/4$, and $M_z = 0$, while in the z-FM phase, $M_z - L/2 \propto 1/z^2$ (from second-order perturbation theory), and $\Delta_d = 0$. The boundary determined in these orders is precisely that from Eq. 4, with difference less than $3 \times 10^{-4}$. The similar accuracy has been found for all black dots in Fig. 1. In Fig. 2b, we show that at the phase boundary, all excitation gaps, $\delta E_{n1} = E_n - E_1$, collapse to zero, indicating of infinite-fold degeneracy extended to infinite volume. In the phase boundary, we have three classical points: $H(1, 0, 0)$, $H(0, 1, 0)$ and $H(0, 0, 1)$. Here, $H(0, 0, 1)$ is relevant to the boundary defined in Eq. 4 in the limit of $x = -y$ and $z \to \infty$. Let us consider

$$H(x, 0, 0) = xH(1, 0, 0) \quad \text{for} \quad x > 0,$$

where $\sigma_i = s_i^x + s_{i+1}^x$. This new operator takes three different values; however, the minimal value $-1$ from the product of the operators can not be reached due to the restriction that $|\sigma_i - \sigma_{i+1}| = |s_i^x - s_{i+1}^x| = \{0, 1\}$. Thus $\sigma_i \sigma_{i+1} \geq 0$ and the GS energy is $-L/8$. Let us consider a special case, that is, $\sigma_{2i} = 0$, and $\sigma_{2i+1} = \{1, 0\}$ or $\{-1, 0\}$. All these states have the same GS energy $-L/8$.

This means that the GSs degeneracy is at least the order of $O(2^{L/2})$, which is infinite-fold degenerate in infinite-volume. From this result, the system may undergo two different spontaneous symmetry breaking. When breaking to the dimer phase, the system breaks the translational symmetry with $\Delta_d \neq 0$, while to the FM phase the $Z_2$ symmetry is broken with $M_z \neq 0$ and $\Delta_d = 0$.

Properties of FM phases. We find three different FM phases, which may polarize along three orthogonal directions. The transitions between them are phase transitions and the boundaries are gapless and critical. The three boundaries for the FM phases are $z = \min(x, y)$ and $z > x = y = -1/\sqrt{2}$. Across this boundary, the polarization of magnetization may change direction. In following, we use some complementary approaches to characterize these phase transitions. In the gapless phase the entanglement entropy (EE) in a finite chain by two partitions can be written as [56–58],

$$S(n) = \frac{3}{\pi} \ln \left( \frac{L}{\pi} \sin \frac{\pi n L}{L} \right) + s_0, \quad (9)$$

where $c$ refers to central charge and $s_0$ is a constant. The results are presented in Fig. 2c. We find the central charge $c = 1$ at the phase boundary (see inset of Fig. 2c). This phase transition may also be characterized by their long-range spin-spin correlations. We only consider the correlation $C_z(r) = \langle s_i^z s_{i+r}^z \rangle$. In the fully gapped z-FM
phase with long-range order, the correlation should approach a constant in the large separation limit. At the boundary, $C_x(r) \propto |r|^{-\eta}$, which is a typical feature of critical phases. In the $x$-FM phase, in which the spontaneous magnetization will polarize along $x$ direction, this correlation should decay exponentially to zero (in this case, $\lim_{|r| \to \infty} C_x(r)$ approaches a constant). The results in Fig. 2d demonstrate all these expected features.

**Exact FM states and dual mapping.** There exist some special lines in the FM phases to support exact FM states\cite{59},

$$|\text{FM}\rangle_{\text{exact}}^{\eta} = |\eta\rangle^\otimes L, \quad (10)$$

where $|\eta\rangle$ is the eigenvector of $s_y$. As shown in Ref. \cite{46}, when $y = x > 0$ and $z < -x/2$, the GSs in an exact FM state spontaneously polarized along $z$ direction. This state can be mapped to the exact FM state along other two directions by dual rotation, $R_x = \prod_i \exp(i\pi s_y)$ for $\eta = x, y$, which induces permutation among the three directions. We find that the other two exact FM states at $z = \max(x, y)$ and $z < x = y = -1/\sqrt{2}$. These lines are presented in Fig. 1 with dashed lines. The arrows mark the evolution of these dual mapping start from $z \to -\infty$. One should be noticed that when $z \to -\infty$, it equals to $-H(0, 0, 1)$, and can be mapped to $-H(1, 0, 0)$ and $-H(0, 1, 0)$ by dual rotation. The GSs of these points should be two-fold degenerate with exact FM states in Eq. 10. This exact two-fold degeneracy can also be proved exactly by considering $-H(0, 0, 1)$ using the method in Eq. 8. In these exact FM states, the corresponding GS energy can be written as $E_{\text{FM}}^{\eta} = -\frac{\delta E}{\delta z} \min\{x, y, z\}$. Notice that the GSs of $-H(1, 1, 1)$ is infinite-fold degenerate, while in $H(1, 1, 1)$ it is exact dimerized.

**Experimental relevant and measurements.** Let us finally discuss the relevant of this research to experiments in quasi-one-dimensional magnets and their experimental signatures. In spin-Peierls compounds, such as CuGeO$_3$\cite{27}, TTF-CuBDT\cite{35} and SrCu$_2$O$_3$\cite{40}, the strong anisotropy in lattice constants (in CuGeO$_3$: $a = 4.81$ Å, $b = 8.40$ Å and $c = 2.94$ Å\cite{27}) is necessary to isolate a single Cu$^{2+}$ chain (or other spin-$\frac{1}{2}$ ions) out from the three-dimensional bulk. For this reason, anisotropy in the effective spin models is inevitable. In experiments, it was found that when the temperature is lower than the spin-Peierls transition temperature $T_{\text{sp}}$, the magnetic susceptibility in all directions will quickly drop to almost zero. Anisotropy in magnetic susceptibility will become significant in FM phase when Zeeman field exceeds a critical value or $T > T_{\text{sp}}$. In experiments, these observations are explained by an isotropic $J_1 - J_2$ model, which may support dimer phase when $\alpha = J_2/J_1 > 0.2411$\cite{60}. This model was also shown to relevant to other anisotropic quasi-one-dimensional magnets such as CuCrO$_2$ with $\alpha = 0.43$\cite{39}, BaV$_2$O$_5$ with $\alpha \approx 0.5$\cite{61}, Cu$_3$(MoO$_4$)(OH)$_4$ with $\alpha = 0.45$\cite{42}, Cu$_6$GeO$_{18}$·$6H_2$O with $\alpha = 0.27$\cite{62}, Cu$_6$Ge$_6$O$_{18}$H$_2$O with $\alpha = 0.29$\cite{62} and Li$_{1.6}$Cu$_{1.4}$O$_2$O$_{0.1}$ with $\alpha = 0.29$\cite{63}. In some of the experiments, strong anisotropy has been reported; especially, some of these parameters may even be negative valued. These results motivate us to think more seriously about the dimerized phase in these compounds.

We model the experimental measurements by adding a magnetic field along $\eta$ direction,

$$H' = h \sum_{\tilde{z}} s_\eta^{\tilde{z}}. \quad (11)$$

Since $[H', H] = 0$, the external magnetic field will not immediately destroys the dimer phase. The magnetization $M_\eta$ for the dimer phase along different directions are presented in Fig. 3a. We find that the breakdown of exact dimer phase takes place at roughly $h^c \approx \delta E$ ($\delta E = E_2 - E_1$ is the excitation gap). When $h < h^c$, the magnetization $M_\eta = 0$ along different directions, thus $\chi_\eta = \partial M_\eta/\partial h = 0$. The anisotropy effect will be important in regime when $h > h^c$ or $T > T_{sp}$, which give different susceptibilities along different directions. In FM phases, magnetization $M_\eta \neq 0$ can also be measured. These results are consistent with the experimental observations in literatures\cite{41, 42, 64-66}. This anisotropy effect has been reported even in the first spin-Peierls compound\cite{27}. We show that these features can be used in experiments to distinguish these two different gapped phases. In Fig. 3c, we plot the magnetization away from the MG point. The similar features can also be found in the dimer phase, and the phase transition still takes place at $h^c \approx \delta E$. In experiments, the value of $\alpha$ depends strongly on the lattice constant, thus maybe tuned by temperature or external stress\cite{43}. We plot the boundary for the dimer phase in Fig. 3d, yielding $\alpha_c = 0.4362$ by extrapolation using $\alpha_c(L) = \alpha_c \propto L^{-2}$\cite{55}. We have also confirmed this boundary from the dimer order $\Delta_d$ and the long-range correlation $C_\eta(r)$. This critical value is significantly larger than 0.2411 due to strong anisotropy.

We apply this criteria to estimate the energy gap in CuGeO$_3$\cite{27}, which can not be explained by non of the regular models. In Ref. \cite{29}, $\alpha = 0.5$, $J_{xx} = 48.2$ K, $J_{yy} = 47.2$ K and $J_{zz} = 49.7$ K, we find the energy gap to be $\delta E = 11.8$ K, by letting $J = (J_{xx} + J_{yy} + J_{zz})/3 \approx 48.3$ K. This value is roughly half of that observed in experiments\cite{44}. For another set of parameters, $J = 160$ K and $\alpha = 0.36$ in isotropic model\cite{43}, we estimate $\delta E = 1.6$ K. To obtain these data, we extrapolate the gap width to infinity volume using $\delta E(L) - \delta E \propto L^{-2}$\cite{43}. The XYZ model with exact dimerized GSs can resolve the disagreement between experiments and isotropic models.

**Conclusion.** Motivated by the experiments on the searching of dimerized phase in quasi-one dimensional magnets, in which the anisotropic effect is inevitable, here we explore the exact dimerized phase in an fully anisotropic XYZ model generalized from the MG model. We demonstrate that in a wide range of parameter
regime, the GSs can be expressed by product of exact singlet dimer, breaking of translational symmetry. This model may also supports three different gapped FM phases along different directions. The boundary between dimer phase and FM phases are infinite-fold degenerate, while between the FM phases are gapless, critical with central charge $c = 1$. These results are relevant to a large number of quasi-one-dimensional magnetic materials. Possible experimental signatures are presented to discriminate these phases. These exact results may greatly advance our understanding of exact dimerized phases in solid materials, and may also be simulating for the searching of SPT phases with discrete symmetries[67–70].

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