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## Exactly solvable points and symmetry protected topological phases of quantum spins on a zig-zag lattice

Haiyuan Zou,<sup>1</sup> Erhai Zhao,<sup>2</sup> Xi-Wen Guan,<sup>3</sup> and W. Vincent Liu<sup>4, 5, 6</sup>

<sup>1</sup>Tsung-Dao Lee Institute, Shanghai Jiao Tong University, Shanghai 200240, China

<sup>2</sup>Department of Physics and Astronomy & Quantum Materials Center,

George Mason University, Fairfax, Virginia 22030, USA

<sup>3</sup>State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics,

Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan 430071, China

<sup>4</sup>Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA 15260, USA

<sup>5</sup>Wilczek Quantum Center, School of Physics and Astronomy and T.D. Lee Institute,

Shanghai Jiao Tong University, Shanghai 200240, China

<sup>6</sup>Shenzhen Institute for Quantum Science and Engineering and Department of Physics,

Southern University of Science and Technology, Shenzhen 518055, China

A large number of symmetry protected topological (SPT) phases have been hypothesized for strongly interacting spin-1/2 systems in one dimension. Realizing these SPT phases however often demands fine-tunings hard to reach experimentally. And the lack of analytical solutions hinders the understanding of their many-body wavefunctions. Here we show that two kinds of SPT phases naturally arise for ultracold polar molecules confined in a zigzag optical lattice. This system, motivated by recent experiments, is described by a spin model whose exchange couplings can be tuned by an external field to reach parameter regions not studied before for spin chains or ladders. Within the enlarged parameter space, we find the ground state wavefunction can be obtained exactly along a line and at a special point, for these two phases respectively. These exact solutions provide a clear physical picture for the SPT phases and their edge excitations. We further obtain the phase diagram by using infinite time-evolving block decimation, and discuss the phase transitions between the two SPT phases and their experimental signatures.

The ground states of strongly interacting many-body systems of quantum spins can differ from each other by three mechanisms: symmetry breaking, long range entanglement (topological order), or symmetry fractionalization [1]. Symmetry-protected topological (SPT) phases are equivalent classes of states that share the same symmetries but are topologically distinct [2–4]. They only have short-range entanglement, are gapped in the bulk, but have edge/surface states protected by symmetries. Recent years have witnessed significant advancement in our understanding of fermionic and bosonics SPT phases. For example, for one-dimensional (1D) spin systems, a complete classification of possible SPT phases was achieved based on group cohomology [1]. A plethora of SPT phases are shown to be mathematically allowed. When translational symmetry, inversion, time reversal (TR) and  $D_2$  symmetry of spin rotation  $\pi$  are all present, there are in total  $2^{10}$  possible SPT phases in 1D [1].

Only a small fraction of these SPT phases have been identified to arise from realistic spin models that are experimentally accessible. The best known example is the Haldane phase of spin-1 antiferromagnetic Heisenberg chain [5]. For spin-1/2 systems, spin ladders,  $J_1 - J_2$ chains with frustration (for example with antiferromagnetic next-nearest-neighbor interaction  $J_2 > 0$ ) have been extensively studied [6–10], but the parameter space explored was focused on solid state materials such as copper oxides [6]. For example, four SPT phases  $D_{\pm}$ , VCD<sub>±</sub> have been discussed in spin-1/2 chains [11]. And Ref. [12] found four SPT phases  $t_0, t_x, t_y, t_z$  in a spin-1/2 ladder and proposed ways to realize them using coupled quantum electrodynamics cavities. The  $t_0$  and  $t_z$  phase were also shown to exist in narrow regions for a ladder of dipole molecules [13]. In quantum gas experiments, a noninteracting SPT phase was observed with fermionic ytterbium atoms [14], and an interacting bosonic SPT phase was realized using Rydberg atoms [15].

In this paper, we propose and solve a highly tunable 1D spin-1/2 zigzag lattice model describing polar molecules [16–18] (or magnetic atoms [19]) localized in a deep optical lattice. This model has several appealing features as a platform to realize SPT phases. (1) It is inspired by recent experimental realization of spin-1/2XXZ model using polar molecules in optical lattices [16– 18]. (2) The relative magnitude and sign of the exchange interactions are relatively easy to control by tilting the dipole moment using an electric field to reach a large, unexplored parameter space. The frustration resulting from dipole tilting has been recently shown to give rise to possible spin liquid states in 2D [20-23]. (3) The bulk of its phase diagram is occupied by two SPT phases, the singlet-dimer (SD) and even-parity dimer (ED) phase. (4) The exact ground state wave function for each SPT phase is found and their nature is firmly established by exploiting the characteristic of the lattice as a chain of edge sharing triangles. The spin-1/2 edge states of an open chain are also derived. (5) It reveals a novel direct phase transition between the SPT phases.

The model. Our model, illustrated in Fig. 1, is a spin

1/2 XXZ model on the one-dimensional zigzag chain,

$$H = \sum_{i,j} J_{i,j} [S_i^x S_j^x + S_i^y S_j^y + \eta S_i^z S_j^z].$$
(1)

Here i, j are the site indices, and  $\eta$  is the exchange anisotropy. The exchange coupling is restricted to nearest neighbors (n.n.) and next nearest neighbors (n.n.n.),

$$J_{2i,2i+1} = J_1, \quad J_{2i-1,2i} = J'_1, \quad J_{i,i+2} = J_2.$$
 (2)

So the n.n. exchange alternates between  $J_1$  and  $J'_1$  (see Fig. 1). In the special case of  $\eta = 1$ , the model reduces to the  $J_1$ - $J_2$ -type Heisenberg model with bond alternation  $(J_1 \neq J'_1)$ . In the literature, the XXZ chain or  $J_1$ - $J_2$ Heisenberg chain have been extensively studied [6, 24]. It is known that when  $J_2 > 0$  (assuming  $\eta > 0$ ), the system is frustrated. The model has a rich phase diagram on the plane spanned by the two independent parameters:  $\eta$  and  $J_1/J_2$  [6]. With a small bond alternation  $\delta =$  $|J_1 - J'_1| \ll |J_1|, |J'_1|$ , there are four SPT phases [11, 25]. The parameter space of this model, e.g. for  $J_2 < 0$ and strong bond alteration  $\delta \sim |J_1|, |J'_1|$ , have not been explored [26].

The model Eq. (1) naturally arises for polar molecules such as KRb and NaK localized in deep optical lattices [16–18]. Here the spin 1/2 refers to two chosen rotational states of the molecules, and the exchange interaction  $J_{i,j}$ is dictated by the dipolar interaction between the two dipoles, which depends on their relative position  $\mathbf{r}_{ij} =$  $\mathbf{r}_i - \mathbf{r}_j$  as well as  $\hat{d}$ , the direction of the dipoles controlled by external electric field [20, 21]. Explicitly,  $J_{i,j} = J[1 - 3(\hat{r}_{ij}\cdot\hat{d})^2]/r_{ij}^3$  where J > 0 sets the overall exchange scale. For the zigzag lattice, we assume the external field is in plane, and makes an angle  $\theta$  with the y-axis (Fig. 1). We further assume the lattice spacing is large and neglect longer range interaction beyond n.n.n.. It follows that

$$J_{1} = J[1 - 3\cos^{2}(\theta + \gamma)],$$
  

$$J'_{1} = J[1 - 3\cos^{2}(\theta - \gamma)],$$
  

$$J_{2} = J[1 - 3\sin^{2}\theta]/8\sin^{3}\gamma.$$
(3)

In general, the zig-zag angle  $\gamma$  can be tuned. Here we keep  $\gamma = 30^{\circ}$  fixed, so the zigzag lattice consists of a chain of identical, equilateral triangles. Note that itinerant dipoles [27] and atoms [28, 29] on the zig-zag lattice have been studied. Here we focus on spin models of localized dipoles. The anisotropy  $\eta$  can be tuned by varying the strength of the electric field [16, 20].

Tuning the exchange couplings. By titling electric field (and the dipole moment  $\hat{d}$ ), one sweeps through the parameter space of H and gain access to nontrivial SPT phases. It is sufficient to consider  $\theta \in [0, 90^{\circ}]$ . The resulting exchange coupling  $J_1, J'_1, J_2$  are shown in Fig. 1(b). As  $\theta$  is varied, the system goes through a few points studied before in the literature. For example, at  $\theta = 0^{\circ}$ ,  $J_1 = J'_1 = -1.25J_2$ , the ground state was shown to



FIG. 1. (a) Dipolar molecules localized on a zigzag chain. The dipoles point to the **d** direction controlled by external electric field, forming an angle  $\theta$  with the vertical direction. The exchange couplings  $J_1$ ,  $J'_1$  and  $J_2$  are defined in Eq. (2), (b) The variation of the exchange couplings as functions of  $\theta$  ( $\gamma = 30^{\circ}$ ). (c) This highly tunable model contains a few limits, some of which studied before in the literature. (I) a  $J_1 - J_2$  chain [6]; (II) a coupled antiferromagnetic ladder [7]; (III) a bond alternating chain [8]; (V) a ferromagnetic ladder [10]; (VI) weakly coupled ferromagnetic chains. The solid line and dashed line stand for positive (antiferromagnetic) and negative (ferromagnetic) coupling respectively. The point (IV), where  $J'_1 = 2J_2 < 0$  and  $J_1 > 0$ , is exactly solvable. Here the thick dashed line indicates  $|J'_1| > |J_2|$ .

be the so-called Haldane dimer phase [6]. At  $\theta \sim 25^{\circ}$ ,  $J_1 = 0$ , the zigzag chain reduces to a ladder of ferromagnetically coupled antiferromagnetic chains, known to be connected to the spin-1 Haldane chain [7]. At  $\theta \sim 35^{\circ}$ , where  $J_2 = 0$ , the system turns into a spin chain with alternating ferro- and antiferro-exchange [8]. At  $\theta \sim 85^{\circ}$ ,  $J'_1 = 0$ , it reduces to a ladder system of two ferromagnetic chains with antiferromagnetic coupling and a ground state called the rung singlet phase [10]. These ground states seem unrelated: they bear distinct names and are obtained using different methods for various models.

A main result of our work is that all the aforementioned points (Fig. 1c) belong to a single phase that extends to all  $\theta \in [0^{\circ}, 90^{\circ})$  and  $\eta = 1$ , and are adiabatically connected to each other before touching the Tomonaga-Luttinger liquid (TLL) limit at  $\theta = 90^{\circ}$ . Our model H thus unifies these known topological phases in one-dimensional spin 1/2 systems. Furthermore, we will show that the ground state wave function can be obtained exactly for a special point (IV in Fig. 1c) at  $\theta \sim 50.9^{\circ}$ , where  $J'_1 = 2J_2 < 0$  and  $J_1 > 0$ . We prove that it is a pure product state of singlet dimers. Via continuity, the ground state of our model for  $\eta = 1$ , including its topological character, can then be understood from this exact ground state. We will also show that as for  $\eta < 1$ , a different SPT phase arises, and it also has an exactly solvable point.

Phase diagram. To orientate the discussion, first we summarize the phase diagram of H on the  $\theta$ - $\eta$  plane in Fig. 2, obtained from infinite time-evolving block decimation (iTEBD) numerical calculations [30]. Here both the singlet dimer (SD) and even-parity dimer (ED) phase are gapped SPT phases, while the TLL phase is gapless. For a very narrow region,  $\theta < 0.5^{\circ}$ , there is also a gapless chiral phase consistent with previous study [25]. The chiral phase is not our main focus here and discussed further in the supplementary material [31]. The suppression of the chiral phase is due to the alternating n.n. coupling which breaks the translational symmetry  $S_i \rightarrow S_{i+1}$ . In large  $\theta$  region, the arc-shaped phase boundary between the SD and TLL phase on the  $\theta$ - $\eta$  plane is consistent with the prediction from effective field theory [31].



FIG. 2. The phase diagram of H in the  $\theta - \eta$  plane obtained from iTEBD. The insets depict the singlet dimer (SD) and even-parity dimer (ED) phases. The thick solid lines in the SD case indicate a singlet  $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$  and the thick dashed lines in the ED case stand for an even-parity bond  $(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$ . The oval stand for the effective spin-1's defined in Eq. 4. The dashed line at  $\theta \sim 50.9^{\circ}, \eta \in [0.747, 1]$ and a point at  $\eta = 0, \theta \sim 42.4^{\circ}$  are exactly solvable, and their singlet/even-parity product state are shown. A chiral phase (Ch) exists in a small  $\theta$  regime, and the Tomonaga-Luttinger liquid (TLL) phase occupies the large  $\theta$  region. The error bars are due to the finite step size in scanning  $\theta$  or  $\eta$ .

The iTEBD method is based on the matrix product state representation of many-body wave functions in the thermodynamic limit. The Schmidt rank  $\chi$  characterizes the entanglement of the system and it serves as the only adjustable parameter for precision control. Our calculation employs a unit cell of four sites and random complex initial states. Several quantities are computed to characterize the phases and detect possible phase transitions. The first is the string order parameter [32] defined as

$$O_n^z = -\lim_{r \to \infty} \langle (\hat{S}_n^z + \hat{S}_{n+1}^z) e^{i\pi \sum_k \hat{S}_k^z} (\hat{S}_{2r+n}^z + \hat{S}_{2r+n+1}^z) \rangle,$$
(4)

where the k sum is restricted to  $n + 2 \le k \le 2r + n - 1$ . The motivation behind this definition is that the two neighboring spins  $\hat{S}_n^z + \hat{S}_{n+1}^z$  may form an effective spin-1 degree of freedom (represented by an oval in Fig. 2). A finite  $O^z$  detects hidden long range order. The SD (ED) phase is associated with a finite  $O_n^z$  value for even (odd) site, say n = 2 (n = 1). A clear ED-to-SD phase transition is observed in Fig. 3(b) as  $\eta$  is varied.

We also compute the von Neumann entanglement entropy by cutting a  $J'_1$  bond,  $S^{vN} = -\sum_{\chi} \lambda_{\chi}^2 \ln \lambda_{\chi}^2$ , where  $\lambda_{\chi}$  is a set of normalized Schmidt coefficients with Schmidt rank  $\chi$ . As shown in Fig. 3(a) for  $\eta = 1$ , both  $S^{\rm vN}$  and  $O_2^z$  are finite and continuous while  $O_1^z$  remains zero as  $\theta$  is tuned. Together with other physical quantities [31], these results show that the ground state remains in a single SD phase for all  $\theta < 90^{\circ}$ . Interestingly, at  $\theta = 50.9^{\circ}$ ,  $S^{vN}$  vanishes, hinting a pure product state. We will show below that this is an exact solvable point. On the other hand, as  $\eta$  is varied for fixed  $\theta = 40^{\circ}$ ,  $S^{vN}$ develops a sharp peak in Fig. 3(b). The peak position coincides with the jump in  $O_n^z$  and unambiguously identifies a phase transition from ED to SD. The variation of the string order parameters near the transition depends on the value of  $\theta$ . For large  $\theta$ , the transition appears to be first order, but it slowly changes to a continuous transition as  $\theta$  decreases. We find that the central charge  $c \sim 2$  at  $\theta = 10^{\circ}, 20^{\circ}, 30^{\circ}$ , which suggests that the SPT phase transition has stronger interacting behavior than the Gaussian type phase transition [31].

*Exact solutions.* Now we elucidate the nature of the SD and ED phase by two types of solvable points on the  $\eta - \theta$  plane. At  $\theta \sim 50.9^{\circ}$ , the relation  $J'_1 = 2J_2 < 0$ is satisfied with  $J_1 > 0$ . Along this line (vertical dashed line in Fig. 2) of fixed  $\theta$ , the ground state of H can be solved exactly for  $\eta \geq \eta_c = (|J_1'| - J_1)/J_1 \approx 0.747$ . The procedure of constructing the exact ground state wave function follows the spirit of the Majumdar-Ghosh (MG) point for the antiferromagnetic Heisenberg chain: when  $J_1 = J'_1 = 2J_2$ , its ground state is a direct product of singlet dimers with two-fold degeneracy [33]. The MG exact solution has been extended to the more general case of  $J_1 \neq J'_1, J'_1 = 2J_2$  with exchange anisotropy  $\eta$  for all J > 0 by Shastry and Sutherland [34], and to cases with ferromagnetic exchange by Kanter (for a different model where not all n.n.n. interactions are included) [9]. We find that the technique can be applied to the zigzag Hamiltonian H here and the ground state is also a direct product of singlet dimers on  $J_1$  bonds.

The main steps of the solution are as follows. First,



FIG. 3. Entanglement entropy  $S^{vN}$ , string order parameter  $O_1^z$  and  $O_2^z$  for (a) the Heisenberg limit  $\eta = 1$ , with  $\chi = 300$  and (b) along a line at  $\theta = 40^\circ$ , with  $\chi = 100$ . In (b), there is a phase transition at  $\eta \sim 0.769$  characterized by the peak of  $S^{vN}$  and jumps of string order parameters.

for  $J'_1 = 2J_2 < 0$ , the product state of spin singlet  $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$  on all  $J_1$  bonds, represented by thick solid lines in Fig. 2, for all the  $J_1$  bond can be shown to be an eigenstate of H for any  $\eta \in [0, 1]$  with eigenvalue  $E_{eq} = -M(2+\eta)J_1/4$ , where M is the number of triangles. Second, the total Hamiltonian is decomposed into sum of triangle Hamiltonians,  $H = \sum_{\ell} h_{\ell}$ , where  $h_{\ell}$  is the Hamiltonian for a single triangle labelled by  $\ell$ . The ground state energy  $e_{\ell}$  for  $h_{\ell}$  can be calculated since it only involves three spins. Note that  $Me_{\ell}$  serves as the lower bound of variational ground state energy. We find that for  $\eta \geq 0.747$ ,  $E_{eg} = Me_{\ell}$ , i.e.  $E_{eg}$  saturates the lower bound. Therefore the singlet product state must be the exact ground state. Interestingly, this product state of singlet dimers is smoothly deformed to the Haldane dimer phase at  $\theta = 0$ , which can be understood from emergent spin-1 degree of freedom driven by strong ferromagnetic n.n. couplings [6]. Our model explicitly verifies the connection between these two cases, conjectured earlier using bosonization [6]. Similarly, we find the ground state for the point  $\eta = 0, \theta \sim 42.4^{\circ}$  is the product of spin triplet  $(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$  on all  $J'_1$  bonds, shown by the

thick dashed lines in Fig. 2. Any ground state within the ED phase can be continuously deformed to this triplet product state without closing the gap. Similar to the point  $\eta = 1, \theta \sim 50.9^{\circ}$  shown in Fig. 3(b), the entanglement entropy  $S^{\text{vN}}$  of all the exact solvable cases are zero. Details on the exact solution can be found in [31].

Both exact wave functions feature short range entanglement and preserve the symmetry of the Hamiltonian. Both imply edge states: as the singlet/triplet valence bond is cut open at the edge, free "dangling" spin-1/2 edge excitations are created, similar to the Affleck-Kennedy-Lieb-Tasaki state [35]. Each edge state is twofold degenerate and protected by, e.g., TR symmetry. Despite having the same symmetry, the SD and ED phase are topologically distinct. They cannot be deformed smoothly into each other if TR, inversion and  $D_2$  symmetry of spin rotation  $\pi$  about the x, y, and z axis remain unbroken [1, 11, 36]. Details on all open chain cases can be found in [31]. The SD (ED) phase here is adiabatically connected to the  $D_+$  ( $D_-$ ) phase of  $J_1 - J_2$  model studied in Ref. [11] for  $J_1/J_2 \in (-2.7, -1.5)$  and small bond alteration  $\delta$ . The  $Z_2$  indices  $\alpha, \beta, \gamma, \omega$  of these two SPT phases are tabulated in Ref. [11]. Both SPT phases feature a double degeneracy in the entanglement spectrum [36], and this is confirmed by our iTEBD calcuation.

Experimental signatures. A first step toward realizing Hamiltonian Eq. (1) is to load polar molecules [16] into a deep zigzag lattice [37, 38] with filling close to one. The SPT phases can be detected by measuring the edge excitations or the string order parameter. An open edge can be engineered by a strong local optical potential to terminate the zigzag chain or by creating local vacancies. Such control and probe seem within the reach of recently proposed site-resolved microscopy and spin-resolved detection for polar molecules [39]. Then microwave spectroscopy may resolve edge states as a peak at "forbidden energies" within the bulk gap. Furthermore, local perturbations can be applied to lift the edge degeneracy as outlined in Ref. [13]. Measurements of string order parameters have been achieved in a few systems [40–43].

In summary, we have shown the zig-zag XXZ model inspired by molecular gas experiments provides a promising platform for realizing SPT phases for spin-1/2 systems. It unifies previous results in the Heisenberg limit by revealing the connections between them, and elucidates the nature of two robust SPT phases by finding their exact ground states as product of singlet or triplet dimers. From this perspective, searching for and understanding the myriad of SPT phases could benefit from deforming the Hamiltonian to special anchor points where the ground state wavefunction simplifies, as demonstrated here by exploiting the underlying triangular motif. Other SPT phases in 1D can be potentially represented by such anchor points where their nature is intuitive and apparent from the exact wavefunctions. Finally, tuning the zig-zag angle  $\gamma$  away from 30° opens up a large parameter space of exchange couplings and the possibility of new SPT phases that deserve future investigation.

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