Oddness in the spin-S Kitaev honeycomb model

1. **Anisotropy as a diagnostic test for distinct tensor-network wave functions of integer- and half-integer-spin Kitaev quantum spin liquids**
   Authors: Hyun-Yong Lee, Takafumi Suzuki, Yong Baek Kim, and Naoki Kawashima
   Phys. Rev. B 104, 024417 (2021)

2. **$\mathbb{Z}_2$ Spin Liquids in the Higher Spin-S Kitaev Honeycomb Model: An Exact Deconfined $\mathbb{Z}_2$ Gauge Structure in a Nonintegrable Model**
   Authors: Han Ma
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The $S = 1/2$ Kitaev honeycomb model [1]

$$\mathcal{H} = J \sum_{\langle j,k \rangle} J_\mu S_j^\mu S_k^\mu, \tag{1}$$

where $\mu = x, y, z$ depending on the direction of the nearest-neighbor bond between sites j and k on the honeycomb lattice, is a fascinating example of exactly solvable quantum many-body systems, demonstrating the existence of nontrivial quantum spin liquids as the ground state of the Hamiltonian with only the nearest-neighbor bilinear spin-spin interaction. Furthermore, possible experimental realization of the "Kitaev spin liquid" is one of the most active topics in quantum magnetism in recent years [2, 3]. Given these circumstances, it is natural to study Kitaev honeycomb model with $S \geq 1$, which also has several material candidates [4, 5]. Unfortunately, the Kitaev honeycomb model is exactly solvable only for $S = 1/2$. Nevertheless, thanks to numerous works, in particular the earlier work [6] and the highlighted papers, we now have some insights including the important difference between half-integer and integer spin S.

First let us quickly review why the $S = 1/2$ Kitaev honeycomb model is exactly solvable. Kitaev introduced a representation of a single $S = 1/2$ spin in terms of 4 Majorana fermions $\gamma^{0,x,y,z}$, so that each of the spin operator is written as a bilinear of Majorana fermions as $S^\mu = \frac{i}{2}\gamma^0\gamma^\mu$, where $\mu = x, y, z$. The Hilbert space of 4 Majorana fermions, or equivalently 2 complex fermions, is 4-dimensional. Nevertheless, by imposing a parity condition $\gamma^0\gamma^x\gamma^y\gamma^z = 1$, the dimension of the "physical subspace" is reduced to 2, matching the Hilbert space of $S = 1/2$. The bilinear spin-spin interaction $S_j^\mu S_k^\mu$ is thus written as a 4-fermion term $-\gamma_j^0\gamma_j^\mu\gamma_k^\mu\gamma_k^0/4$. The Hamiltonian, given as a sum of these 4-fermion terms, is apparently not exactly solvable. However, $u_{jk} = \gamma_j^\mu\gamma_k^\mu = \pm 1$ can be regarded as a $\mathbb{Z}_2$ gauge field. Furthermore, since u_{jk} commute with each other and with the Hamiltonian, we can diagonalize the Hamiltonian within each sector corresponding to a fixed configuration of the $\mathbb{Z}_2$ gauge field u_{jk}. In fact, each sector is characterized by the $\mathbb{Z}_2$ gauge flux W_p through each plaquette p, which is the product of u_{jk} along the plaquette p. Thus the Hamiltonian is reduced to a sum of fermion bilinears, which is exactly solvable.

Interestingly, some of the features of the $S = 1/2$ Kitaev honeycomb model are inherited by the Kitaev honeycomb model with $S \geq 1$. That is, the $\mathbb{Z}_2$ gauge flux W_p, defined as the product of $e^{i\pi S^\mu}$ on the plaquette p, commutes with each other and with the Hamiltonian [6]. On the other hand, tensor-network wavefunctions, which may be regarded as variational ground states of the Kitaev honeycomb model, imply that the phase diagram for $S = 1$ Kitaev honeycomb model is rather different from $S = 1/2$ [7]. That is, at the isotropic point $J_x = J_y = J_z$, the ground state of the $S = 1$ model is a gapped $\mathbb{Z}_2$ spin liquid, unlike the gapless spin liquid at the isotropic point of the $S = 1/2$ model. Moreover, in the anisotropic limit $J_x, J_y \to 0$, the ground state of the $S = 1$ model is trivial. Furthermore, as shown in the highlighted paper 1, the tensor-network picture suggests that the spin-S Kitaev honeycomb model may be classified into two classes: half-integer S and integer S.

The common feature of the Kitaev honeycomb model for all S and the difference between half-integer and integer S were further elucidated in the highlighted paper 2, where Kitaev's Majorana fermion representation is generalized to general spin quantum number S. That is, we can introduce $2S$ flavors of Majorana fermions $\gamma_a^{0,x,y,z}$ $(a = 1, 2, \ldots, 2S)$ at each site, to represent spin operators as $S^\mu = \frac{i}{2}\sum_{a=1}^{2S}\gamma_a^0\gamma_a^\mu$, with the constraints $\gamma_a^0\gamma_a^x\gamma_a^y\gamma_a^z = 1$ for $a = 1, 2, \ldots, 2S$ and $\sum_\mu\left(\sum_a\gamma^0\gamma_a^\mu\right)^2 = -4S(S+1)$. The $\mathbb{Z}_2$ gauge structure becomes manifest by introducing "giant parton" operators

$$\Gamma^\alpha \equiv i^{S(2S-1)}\prod_{a=1}^{2S}\gamma_a^\alpha. \tag{2}$$

In terms of the giant partons, the $\mathbb{Z}_2$ gauge field on each link is given as $u_{jk} = \Gamma_j^\mu\Gamma_k^\mu$, from which the $\mathbb{Z}_2$ flux W_p can be constructed. Similarly to the $S = 1/2$ case, u_{jk} on any link commute with each other, and also with the Hamiltonian. Therefore we can again fix the gauge field configuration first. However, this does not reduce the Hamiltonian to fermion bilinears for $S \geq 1$, resulting in the loss of the exact solvability.

We can also construct a "string operator" by the product of the giant parton operators along a path. The string operator contains the product of the $\mathbb{Z}_2$ gauge field along the path and the $\mathbb{Z}_2$-charged operator Γ^0 at the ends of the path. Since the gauge field part of the string operator commutes with the Hamiltonian, creation of two $\mathbb{Z}_2$ charged excitation by application of the string operator costs only a constant energy coming from the ends which does not grow with the length of the string. This seems to imply a deconfinement of the $\mathbb{Z}_2$ charge, signaling a nontrivial spin liquid phase. However, a trivial phase is also possible if Γ^0 condenses. Here, the crucial difference between half-integer and integer S arises: being a product of $2S$ Majorana fermions, the giant parton operator Γ^0 is fermionic when S is a half-integer while Γ^0 is bosonic when S is an integer. Therefore, the trivial phase due to the condensation of Γ^0 seems only possible for an integer S. This is indeed consistent with the observation in the highlighted paper 1.

The observed even-odd effect certainly reminds us of the now established "Haldane conjecture" [8]. Although initially it appeared rather mysterious and was believed by few, now it is understood as a manifestation of a more general principle, *filling-enforced* or *Lieb-Schultz-Mattis (LSM)* type constraint [9, 10, 11, 12]. It is tempting to consider the difference between half-integer and integer S in the Kitaev honeycomb model as a consequence of the LSM-type constraint. Although the Kitaev honeycomb model lacks the continuous SU(2) or even U(1) symmetry, recent developments have shown that the discrete dihedral group symmetry, which is present in the Kitaev honeycomb model, can lead to a LSM-type constraint [13, 14, 15, 16]. Indeed, as shown in the highlighted paper 1, in the anisotropic limit $J_z \gg J_x, J_y$, the effective model of the Kitaev honeycomb model with a half-integer S is reduced to a $S = 1/2$ model on a square lattice, which must have a nontrivial ground state because of the LSM constraint. However, except for the anisotropic limit, there is no known LSM-type constraint for the Kitaev honeycomb model even when S is a half-integer. This is essentially because the unit cell (or the fundamental domain) of the honeycomb lattice contains two sites, so that the "total spin" of the fundamental domain is integer. Thus the observed difference between half-integer and integer S in the Kitaev honeycomb model is still a mystery from a general viewpoint.

It is an interesting question if there is a universal mechanism similar to the LSM-type constraint which excludes a trivial ground state of the Kitaev honeycomb model with a half-integer S. Or, is it actually possible to realize a trivial ground state of the Kitaev honeycomb model (or its deformation respecting all the symmetries) with a half-integer S, going beyond the validity of Ma's argument? I would like to note that, although it is allowed by LSM constraints, it was rather challenging to realize a trivial ground state on the honeycomb lattice at "half filling" in the presence of the U(1) symmetry. Eventually, however, it turned out that a trivial ground state is indeed possible, as demonstrated in Ref. [17]. Therefore, in order to rule out a trivial ground state on the honeycomb lattice for half-integer S, probably we have to impose an extra symmetry or a condition which is satisfied by the Kitaev honeycomb model. In any case, it would be interesting to continue investigation of the Kitaev honeycomb and related models with general spin quantum number S, with the perspectives provided by the highlighted papers.

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