Spin-*S* Kitaev model: Classical ground states, order from disorder, and exact correlation functions

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In the first part of this paper, we study the spin-*S* Kitaev model using spin-wave theory. We discover a remarkable geometry of the minimum-energy surface in the *N*-spin space. The classical ground states, called Cartesian or CN-ground states, whose number grows exponentially with the number of spins *N*, form a set of points in the *N*-spin space. These points are connected by a network of *flat valleys* in the *N*-spin space giving rise to a continuous family of classical ground states. Further, the CN-ground states have a correspondence with *dimer coverings* and with *self-avoiding walks* on a honeycomb lattice. The zero-point energy of our spin-wave theory picks out a subset from a continuous family of classically degenerate states as the quantum ground states; the number of these states also grows exponentially with *N*. In the second part, we present some exact results. For arbitrary spin *S*, we show that localized Z_2 flux excitations are present by constructing plaquette operators with eigenvalues ± 1, which commute with the Hamiltonian. This set of commuting plaquette operators leads to an exact vanishing of the spin-spin correlation functions beyond nearest-neighbor separation found earlier for the spin-1/2 model [G. Baskaran *et al.*, Phys. Rev. Lett. **98**, 247201 (2007)]. We introduce a generalized Jordan-Wigner transformation for the case of general spin *S* and find a complete set of commuting link operators similar to the spin-1/2 model, thereby making the Z_2 gauge structure more manifest. The Jordan-Wigner construction also leads, in a natural fashion, to Majorana fermion operators for half-odd-integer spin cases and hard-core boson operators for integer spin cases strongly suggesting the presence of Majorana fermion and boson excitations in the respective low-energy sectors. Finally, we present a modified Kitaev Hamiltonian, which is exactly solvable for all half-odd-integer spins; it is equivalent to an exponentially large number of copies of spin-1/2 Kitaev Hamiltonians.

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I. INTRODUCTION

Frustrated quantum spin systems have become a new paradigm in condensed-matter science. More and more systems are joining this family. A richness is emerging in terms of novel ground states and excitations. They not only enrich the basic science of strongly correlated electron systems, but also have started playing a key role in an unexpected corner, namely, quantum computers. Kitaev has suggested that excitations of frustrated quantum spin systems have a special robustness arising from their nontrivial topological property, which makes them suitable elements of a topological quantum computer. An exactly solvable two-dimensional frustrated spin-1/2 model introduced by Kitaev[1,2] exemplifies this.

The spin-1/2 Kitaev model is interesting in its own right as a condensed-matter spin model.[3–9] In fact a similar model, called the *compass model*, although not exactly solvable, was introduced by Kugel and Khomskii in the late 1970s (Ref. 10) to understand the magnetic properties of transition-metal oxides, which have orbital degeneracies. Recently an optical lattice realization of the spin-1/2 Kitaev model has been discussed.[11]

The spin-*S* Kitaev model for $S>1/2$ is not exactly solvable. It is a challenging question if the Z_2 gauge structure and the presence of low-energy Majorana fermions, discovered by Kitaev for the spin-1/2 case, survive for arbitrary spin *S*. Are there differences between half-odd-integer and integer spins? In the present paper we approach the problem on two fronts. First we find exact classical ground states and perform a spin-wave analysis. The structure of the ground-state manifold in the *N*-spin space is rich; an exponentially large number of isolated points are connected by flat valleys. We will call the ground state corresponding to these isolated points as Cartesian or CN-ground states as any given spin points along one of the three Cartesian directions. We also find the phenomenon of order from disorder in our spin-wave analysis. We discover a nice connection between finding the CN-ground states and the dimer covering problem on the honeycomb lattice. In our spin-wave analysis we find an equal number of finite-frequency and zero-frequency spin-wave modes, which live on self-avoiding walks (SAWs) that are uniquely connected to the dimer covering.

On the other front, we get some useful and exact results for the spin-*S* Kitaev model, which prove the survival of the Z_2 gauge structure. There are also good indications that the low-energy Majorana fermion excitations survive for half-odd-integer spins. Specifically we find plaquette operators (with eigenvalues ± 1) which commute with the Hamiltonian. This set of commuting plaquette operators leads to a vanishing of the spin-spin correlation functions beyond nearest-neighbor separation found earlier for the spin-1/2 model.[6] We also discover a Jordan-Wigner transformation for arbitrary *S*, which leads to new bond operators (with eigenvalues ± 1) which commute with the Hamiltonian. This makes the Z_2 gauge structure manifest. The Jordan-Wigner construction leads, in a natural fashion, to Majorana fermion operators for the case of half-odd-integer spins and to hard-

core boson operators for the integer spin case strongly suggesting the presence of Majorana fermions and bosons in the respective low-energy sectors.

The plan of the paper is as follows. In Sec. II, we consider a one-dimensional version of the Kitaev model and study spin-wave theory in the large S limit. We find that although there is a continuous family of classical ground states parameterized by an angle, the zero-point energy of the spin waves picks out a discrete set of values of the angle as the quantum ground states; these correspond to dimer coverings on alternate bonds of the model. In Sec. III, we study the two-dimensional Kitaev model using spin-wave theory. We first present a general argument to find the classical ground-state energy. We then identify a discrete and infinite number of classical ground states; these have an interesting correspondence with SAWs and dimer coverings of the honeycomb lattice. The spin-wave spectrum is found to contain *one-dimensional* finite-frequency spin-wave modes and an equal number of zero-frequency modes living on the SAWs. The zero-point energy of the spin waves again picks out a special class of self-avoiding walks as the quantum ground states. The number of classical and quantum ground states both grow exponentially with the number of sites, although the latter number grows slower than the former. In Sec. IV, we construct, for any value of the spin S, an infinite set of Z_2 operators, which commute with each other and with the Hamiltonian. We use these operators to show that in any eigenstate of the Hamiltonian, the spin-spin correlations vanish unless the two spins are nearest neighbors; even for nearest neighbors, only certain components of the correlations are nonzero. Finally, we use a Jordan-Wigner-type transformation to construct a set of operators, which act like Majorana fermions (hard-core bosons) for half-odd-integer (integer) values of S, respectively. The Z_2 operators defined earlier can be written as products of the Majorana fermion (hard-core boson) operators. In Sec. V, we present a modified Kitaev Hamiltonian whose energy spectrum can be found for any value of half-odd-integer spin; this model is equivalent to an exponentially large number of copies of the spin-1/2 Kitaev Hamiltonian. Some directions for future work are pointed out in Sec. VI.

II. ONE-DIMENSIONAL KITAEV MODEL

In this section, we will discuss a one-dimensional spin-S model, which is obtained by considering a single row of the Kitaev model in two dimensions. We illustrate the order from disorder phenomenon explicitly. The model is a spin S chain governed by the Hamiltonian

$$H_1 = \frac{J}{S}\sum_{i=-\infty}^{\infty}(S_{i,1}^x S_{i,2}^x + S_{i,2}^y S_{i+1,1}^y). \tag{1}$$

We assume that $J>0$. (If $J<0$, we can change its sign by performing a unitary rotation, which flips the signs of $S_{i,1}^x$, $S_{i,1}^z$, $S_{i,2}^y$, and $S_{i,2}^z$ for all values of i.) In Eq. (1), the unit cells are labeled by i, and each unit cell has two spins labeled as 1 and 2. A factor of $1/S$ has been introduced in Eq. (1) so that the ground-state energy is proportional to S in the limit $S\to\infty$.

Let us introduce two vectors in the x-y plane,

$$\hat{\mathbf{n}} = \cos\theta\hat{\mathbf{x}} + \sin\theta\hat{\mathbf{y}}$$

$$\text{and } \hat{\mathbf{e}} = -\sin\theta\hat{\mathbf{x}} + \cos\theta\hat{\mathbf{y}}. \tag{2}$$

Then a classical ground state of the Hamiltonian in Eq. (1) is given by the configuration

$$\mathbf{S}_{i,1}^{\mathrm{cl}} = S\hat{\mathbf{n}} \text{ and } \mathbf{S}_{i,2}^{\mathrm{cl}} = -S\hat{\mathbf{n}}. \tag{3}$$

The classical energy of this state is $E^{\mathrm{cl}}=-JSN/2$, where N is the number of sites (the number of unit cells is $N/2$). Thus the classical ground states form a continuous family parametrized by an angle θ, which lies in the range $[0,2\pi]$. We will now perform a spin-wave analysis and show that this picks out four values of θ as having the lowest zero-point energy; these correspond to Cartesian ground states.

The spin-wave spectrum around the ground state given in Eq. (3) can be found by using the Holstein-Primakoff (HP) transformation from spins to simple harmonic-oscillator raising and lowering operators.[12–14] To obtain a HP Hamiltonian, which is quadratic in bosons, we expand the fields as

$$\mathbf{S}_{i,1} = S\hat{\mathbf{n}}\left(1 - \frac{p_{i,1}^2 + q_{i,1}^2}{2S}\right) + \sqrt{S}(\hat{\mathbf{e}}q_{i,1} + \hat{\mathbf{z}}p_{i,1}),$$

$$\mathbf{S}_{i,2} = -S\hat{\mathbf{n}}\left(1 - \frac{p_{i,2}^2 + q_{i,2}^2}{2S}\right) + \sqrt{S}(-\hat{\mathbf{e}}q_{i,2} + \hat{\mathbf{z}}p_{i,2}), \tag{4}$$

where $[q_{i,a},p_{j,b}]=i\delta_{ij}\delta_{ab}$. The spin-wave Hamiltonian is then given by

$$\begin{aligned} H_{1,sw} &= J\sum_i (p_{i,1}^2 + q_{i,1}^2 + p_{i,2}^2 + q_{i,2}^2 \\ &\quad - \cos^2\theta q_{i,1}q_{i,2} - \sin^2\theta q_{i,2}q_{i+1,1}) \\ &= J\sum_{k=0}^{\pi} (p_{-k,1} \quad p_{-k,2})\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} p_{k,1} \\ p_{k,2} \end{pmatrix} \\ &\quad + (q_{-k,1} \quad q_{-k,2})\begin{pmatrix} 1 & f(k) \\ f^*(k) & 1 \end{pmatrix}\begin{pmatrix} q_{k,1} \\ q_{k,2} \end{pmatrix}, \end{aligned}$$

$$\text{where } f(k) \equiv -\cos^2\theta - \sin^2\theta e^{ik}, \tag{5}$$

and k goes in steps of $4\pi/N$. The spin-wave energies are

$$\epsilon_{k+} = J\sqrt{1+|f(k)|}$$

$$\text{and } \epsilon_{k-} = J\sqrt{1-|f(k)|}, \tag{6}$$

where $|f(k)|=\sqrt{1-\sin^2(2\theta)\sin^2(k/2)}$. The zero-point energy is

$$E_{1,sw} = J\sum_{k=0}^{\pi}[\sqrt{1+|f(k)|} + \sqrt{1-|f(k)|}]. \tag{7}$$

We see that for each value of k, the spin-wave energies have the same values for θ and $\pi/2-\theta$. Now,

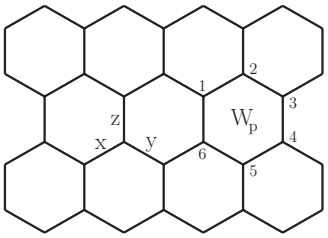

FIG. 1. Schematic picture of the Kitaev model on a honeycomb lattice indicating the three kinds of bonds, x, y, and z. A hexagon with sites marked 1–6 is shown; the corresponding plaquette operator W_p is defined in Eqs. (16) and (18).

$$\frac{\partial}{\partial|f|}(\sqrt{1+|f|}+\sqrt{1-|f|})=\frac{1}{2}\left(\frac{1}{\sqrt{1+|f|}}-\frac{1}{\sqrt{1-|f|}}\right)<0. \tag{8}$$

Thus the total spin-wave energy $\epsilon_{k+}+\epsilon_{k-}$ increases monotonically as $|f|$ decreases, i.e., as θ increases from 0 to $\pi/4$ or decreases from $\pi/2$ to $\pi/4$. Thus the zero-point energy is minimum at $\theta=0,\pi/2,\pi$, and $3\pi/2$, thereby picking out four points from the continuous family of classical ground states. These four points correspond to all the spins pointing along the $\pm\hat{\mathbf{x}}$ or $\pm\hat{\mathbf{y}}$ directions.

Interestingly, the ground states chosen by the *order from disorder* phenomenon have two degenerate and nondispersing spin-wave branches with frequencies, $\epsilon_{k+}=\epsilon_{k-}=J$. It is easy to show that all these modes are localized on nearest-neighbor bonds that have zero interaction energy.

Finally, let us briefly discuss the case in which the couplings are not equal on all the bonds. Suppose that the xx couplings have a strength J_x and the yy couplings have a strength J_y. If $J_x>J_y$, we find that the classical ground states are given by states in which the spins 1 and 2 in each unit-cell point in the $+\hat{\mathbf{x}}$, $-\hat{\mathbf{x}}$ or $-\hat{\mathbf{x}}$, $+\hat{\mathbf{x}}$ directions. The classical ground-state degeneracy is therefore $2^{N/2}$. We find that this degeneracy is not broken by the zero-point energy of the spin waves.

III. TWO-DIMENSIONAL KITAEV MODEL

We will now consider the spin-S Kitaev model in two dimensions. This is a model on a honeycomb lattice with the Hamiltonian

$$H_2=\frac{J}{S}\sum_{j+l=\text{even}}(S^x_{j,l}S^x_{j+1,l}+S^y_{j-1,l}S^y_{j,l}+S^z_{j,l}S^z_{j,l+1}), \tag{9}$$

where j and l denote the column and row indices of the honeycomb lattice, respectively. We again assume, without loss of generality, that $J>0$. Note that each spin is coupled to three other spins through xx, yy, and zz couplings; we will denote the corresponding bonds as x, y, and z bonds, respectively. (We present a schematic picture of the model in Fig. 1.) We will first assume that the couplings on the three kinds of bonds are equal. Note that the honeycomb lattice is bipartite with sites belonging to the two sublattices A and B having $j+l$ as even and odd, respectively. If the total number of sites N is even, each sublattice has $N/2$ sites.

We first present a general argument to obtain the classical ground-state energy of the Hamiltonian in Eq. (9). We consider the spins at different sites $\mathbf{S_n}$ to be classical (commuting) vectors and introduce a Lagrange multiplier $\lambda_\mathbf{n}$ at each site to enforce the relation $\mathbf{S}^2_\mathbf{n}=S^2$; we do this by adding a term

$$H_\lambda=-\frac{J}{2S}\sum_\mathbf{n}\lambda_\mathbf{n}(\mathbf{S}^2_\mathbf{n}-S^2) \tag{10}$$

to Eq. (9). Extremizing the sum of Eqs. (9) and (10) leads to the equations

$$S^a_{\mathbf{n}+\mathbf{m}}=\lambda_\mathbf{n}S^a_\mathbf{n},$$

$$S^a_\mathbf{n}=\lambda_{\mathbf{n}+\mathbf{m}}S^a_{\mathbf{n}+\mathbf{m}}, \tag{11}$$

for any two neighboring sites $\mathbf{n}$ and $\mathbf{n}+\mathbf{m}$, which are coupled by an a bond ($a=x,y,z$). Substituting Eq. (11) in Eq. (9) and using the relation $\mathbf{S}^2_\mathbf{n}=S^2$, we find that the energy of such a state can be written in two ways, which must be equal to each other, namely,

$$E_\text{cl}=JS\sum_{\mathbf{n}\in A}\lambda_\mathbf{n}=JS\sum_{\mathbf{n}\in B}\lambda_\mathbf{n}. \tag{12}$$

Now, in any classical ground state, we can assume that for each site $\mathbf{n}$, the spin on at least one of its three neighbors must point in such a direction that $S^a_\mathbf{n}S^a_{\mathbf{n}+\mathbf{m}}\neq 0$. For such a pair, Eq. (11) implies that $\lambda_\mathbf{n}\lambda_{\mathbf{n}+\mathbf{m}}=1$; note that $\mathbf{n}$ and $\mathbf{n}+\mathbf{m}$ necessarily belong to different sublattices. Extending this argument to all pairs of neighboring sites, we conclude that $\lambda_\mathbf{n}$ for all sites $\mathbf{n}$ belonging to sublattice A must have the same value denoted as λ_A, while $\lambda_\mathbf{n}$ for all sites $\mathbf{n}$ belonging to sublattice B must have the same value denoted as λ_B, where $\lambda_A\lambda_B=1$. Equation (12) then implies that $E_\text{cl}=(JSN/2)\lambda_A=(JSN/2)\lambda_B$. The condition $\lambda_A\lambda_B=1$ then implies that the minimum energy will be attained if $\lambda_A=\lambda_B=-1$. Thus the classical ground state is equal to $-JSN/2$ corresponding to $\lambda_\mathbf{n}=-1$ at all sites.

We will now explicitly find a large set of classical ground states. To this end, we observe the following interesting *one to many* correspondence of dimer coverings on a honeycomb lattice with a set of classical ground states of the Kitaev model that *have identical energy*. Consider a covering of the honeycomb lattice with dimers such that every site lies on a dimer. Associate a classical spin configuration to each dimer (bond) as follows. Depending on whether it is an x, y, or z bond, we put the two spins at the ends of the dimer as antiparallel and along the $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, or $\hat{\mathbf{z}}$ direction, respectively, in spin space. This is the reason we call them Cartesian or CN-ground states. All these classical states have an identical energy $-JSN/2$. This follows from the fact that the interaction energy of the two spins of any dimer is $-JS$. Two neighboring spins not belonging to a dimer have zero interaction energy either because they are orthogonal or the corresponding spin components do not appear in the bond-interaction term.

The number of dimer coverings on a honeycomb lattice has an asymptotic form $(1.381)^{N/2}$.[15] Further, the spins of

each dimer can be in two possible antiparallel states; hence we have $2^{N/2}$ classical spin configurations for each dimer covering. This makes the total degeneracy of the CN-ground states to be $(1.662)^N$.

An important question is whether these classical states remain stable under quantum fluctuations. We answer this question in two steps. First we show that the discrete and exponentially large set of degenerate states found above are further connected by flat valleys in the N-spin space. Then we perform a spin-wave analysis and show that to the leading order in $1/S$ there are no negative-energy spin-wave excitations. This ensures local stability of our quantum ground states.

The discrete set of degenerate states obtained from the dimer coverings forms a set of isolated points in the N-spin space, i.e., $\{S^2\}^N$, where S^2 denotes the surface of a sphere in three dimensions. We will now show that there are flat valleys defined by a set of continuous parameter, which connect the discrete points. To see this consider a set of SAWs that completely covers the lattice such that each lattice site appears on one and only one SAW. In each SAW, let alternate bonds form dimers. Each SAW must be either infinitely long or must be a closed loop consisting of an even number of bonds (this is because each bond on the honeycomb lattice goes from a site on sublattice A to a site on sublattice B).

Let us now consider the sites and bonds lying on one particular SAW. To be specific, let us suppose that somewhere in the middle of the SAW, we have some sites and bonds of the form $\ldots 1-x-2-z-3-y-4-x-5\ldots$. A discrete classical ground state is then given by one in which the spins at the sites 1,2,3,4,5 point along $\hat{\mathbf{z}}$, $-\hat{\mathbf{z}}$, $\hat{\mathbf{z}}$, $-\hat{\mathbf{x}}$, $\hat{\mathbf{x}}$; this has an energy of $-2JS$ for the four bonds $xzyx$. Another discrete classical ground state is given by taking the same five spins to point along $\hat{\mathbf{x}}$, $-\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, $-\hat{\mathbf{y}}$, $\hat{\mathbf{y}}$. We now note that a continuous family of classical ground states, which interpolates between the above two discrete states, is given by a configuration in which the five spins point along $\sin\theta\hat{\mathbf{x}}+\cos\theta\hat{\mathbf{z}}$, $-\sin\theta\hat{\mathbf{x}}-\cos\theta\hat{\mathbf{z}}$, $\sin\theta\hat{\mathbf{y}}+\cos\theta\hat{\mathbf{z}}$, $-\cos\theta\hat{\mathbf{x}}-\sin\theta\hat{\mathbf{y}}$, $\cos\theta\hat{\mathbf{x}}+\sin\theta\hat{\mathbf{y}}$, where θ goes from 0 to $\pi/2$; the energy of the four bonds for this configuration is $-2JS$ for all values of θ. This transformation can be extended to all the sites of the SAW.

Thus we have a continuous transformation taking us from one discrete classical ground state of a SAW to another; we will call such a transformation a slide. A slide is parametrized by an angle θ, and it takes us from a discrete classical ground state in which the even-numbered bond energies are minimized to one in which the odd-numbered bond energies are minimized. We now observe that if a slide rotates the spin on a particular site in the $\hat{\mathbf{x}}$-$\hat{\mathbf{y}}$ plane (such as site 4 in the previous paragraph), then that site must be coupled to a site in the neighboring SAW by a z bond; hence the classical interaction energy of that site to its neighboring site on the other SAW remains zero throughout the slide. This is true for any two neighboring sites belonging to different SAWs no matter which plane each of them is rotated during the slides of the two SAWs. Thus, a slide can be carried out on each SAW separately without changing the classical interaction energy between the two SAWs; hence there is a continuous family of classical ground states on each SAW. However, based on the results in Sec. II, we expect that the zero-point energy of the spin waves about such a continuous family of ground states in a SAW will be minimized for a discrete set of values of θ, which corresponds to the spin at each site pointing along one of the six directions $\pm\hat{\mathbf{x}}$, $\pm\hat{\mathbf{y}}$, or $\pm\hat{\mathbf{z}}$. We will therefore consider below only the discrete set of classical ground states described in the previous sentence.

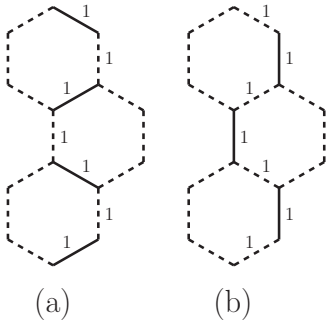

FIG. 2. Pictures of two self-avoiding walks, marked as 1, which are related to each other by a slide. The walk in (a) has only nonvertical dimers, while the walk in (b) has only vertical dimers. The dimers are shown by solid lines.

We have seen that the discrete classical ground states correspond to dimer coverings of the honeycomb lattice. An interesting question to ask is whether all dimer coverings can be continuously connected to each other through the continuous families of classical ground states. We will prove that the answer is yes by showing that any discrete classical ground state can be transformed by a succession of slides to a classical ground state in which all the dimers lie on the z bonds (we will call these vertical dimers). For any dimer covering, the lattice can be covered by SAWs. We now choose these SAWs as follows. If all the dimers are vertical, there is nothing more to be done. If at least one dimer is nonvertical, we consider that dimer; each end of it also belongs to a vertical bond, which is not a dimer (since no point can belong to two dimers). We go to the other end of that vertical bond; that end must belong to a nonvertical dimer. Continuing in this way, we get a SAW that consists of alternating nonvertical dimers and vertical bonds, which are not dimers. We now apply a slide to this SAW; we then get a SAW, all of whose dimers are vertical. (Figure 2 shows an example of two SAWs, which are connected by a slide.) We then repeat the process of taking another nonvertical dimer (which has no points in common with the previous SAW), constructing a new SAW from it using the above procedure, and finally performing a slide, which converts all the dimers to vertical ones. By repeating this until we have SAWs covering all the sites, we reach the state in which all the dimers are vertical. Thus all dimer coverings of the honeycomb lattice are connected through continuous families of classical ground states to the purely vertical dimer covering. Therefore all dimer coverings are also connected to each other through continuous families.

We will now use the HP transformation to compute the spin-wave spectrum about any one of the discrete classical ground states given by a dimer covering. Consider a vertical dimer on which the two spins point along the $\pm\hat{\mathbf{z}}$ direction. Let us consider these two spins separately.

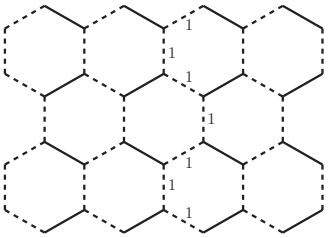

FIG. 3. Picture of a set of self-avoiding walks (dotted lines); one of the walks is marked as 1. The dimers are shown by solid lines.

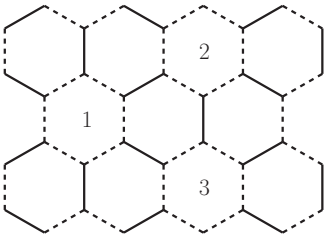

FIG. 4. Picture of a ground state in which the self-avoiding walks (dotted lines) form hexagons; three of these are marked as 1–3. The dimers are shown by solid lines.

(i) For the spin pointing along the $\hat{\mathbf{z}}$ direction, we have $S^z=S-(p^2+q^2)/2$, but (S^x,S^y) can be chosen in four different ways, namely, $\sqrt{S}(q,p)$, $\sqrt{S}(-q,-p)$, $\sqrt{S}(p,-q)$, and $\sqrt{S}(-p,q)$, up to the lowest order in the HP transformation.

(ii) For the spin pointing along the $-\hat{\mathbf{z}}$ direction, we have $S^z=-S+(p^2+q^2)/2$, but (S^x,S^y) can be chosen in four ways, namely, $\sqrt{S}(p,q)$, $\sqrt{S}(-p,-q)$, $\sqrt{S}(q,-p)$, and $\sqrt{S}(-q,p)$.

The term coupling the two spins at the opposite ends of the vertical dimer is given by $S_i^zS_j^z=[S-(p_i^2+q_i^2)/2][-S+(p_j^2+q_j^2)/2]\simeq -S^2+(S/2)(p_i^2+q_i^2+p_j^2+q_j^2)$ up to order S. Thus there is no coupling between the two spins to this order in S.

For any dimer covering of the honeycomb lattice, there is a set of SAWs covering the lattice such that none of the bonds appearing on a SAW is a dimer. Hence the two spins appearing at the two ends of any dimer belong to different SAWs as shown in Fig. 3. (Notice that these SAWs are different from the ones we discussed earlier while finding our flat valley through the slide operation; in those SAWs, alternate bonds were dimers.) As we saw above, sites belonging to different SAWs are decoupled from each other up to order S. We can therefore carry out a spin-wave analysis for each SAW separately. Now consider a SAW which forms a closed loop with n sites where we saw earlier that n must be an even integer. (The minimum value of n is 6 corresponding to a hexagon.) Let $n=2m$. As we go around the loop, we choose the spin variables along the loops to be q and p, alternately, so that the couplings between nearest neighbors involve either q_m,q_n or p_m,p_n but not q_m,p_n. Because of the two cases (i) and (ii) discussed above, the loop may have either periodic boundary condition (PBC) or antiperiodic boundary condition (ABC). Ignoring a constant, we find the spin-wave Hamiltonian for the SAW to be

$$H_{sw}=\frac{J}{2}\sum_{i=1}^{n}(p_i^2+q_i^2)+J\sum_{i=1}^{m-1}(p_{2i-1}p_{2i}+q_{2i}q_{2i+1})+J(p_{n-1}p_n\pm q_nq_1), \tag{13}$$

with either PBC or ABC for the last bond connecting sites n and 1; the sign of the q_nq_1 term is + and − in the two cases, respectively. The SAW has m unit cells each consisting of two sites. The normal modes can be characterized by a momentum k, where $k=0,2\pi/m,\ldots,(2\pi m-2\pi)/m$ in the case of PBC and $k=\pi/m,3\pi/m,\ldots,(2\pi m-\pi)/m$ in the case of ABC. We now find the normal-mode frequencies by solving the classical Hamiltonian equations of motion. For each momentum k, we find that there are two frequencies given by 0 and $\omega_k=2J|\cos(k/2)|$. The existence of a zero-energy mode for each k is a signature of the enormous ground-state degeneracy at the classical level; the zero mode also implies that the spin-wave correction to the expectation value of the spin at each site diverges.

The spin-wave normal modes are interesting. Even though they are formally characterized by a wave vector, they are defined on self-avoiding strings of varying shapes and sizes on the lattice. Second, by construction, the classical interaction energy of the spins on a SAW is identically zero bond by bond; it is neither a minimum nor a maximum. We have a collection of *one-dimensional* spin waves living on SAWs. Further these spin waves have a linear dispersion $\omega_{\pi+q}\approx 2J|q|$ at low frequencies around $k=\pi$.

A linear dispersion is known in the spin-1/2 Heisenberg antiferromagnetic system in one dimension. However, the spin waves there are spin-1 excitations. In the Kitaev model under consideration, this linear dispersion occurs for both antiferromagnetic and ferromagnetic couplings and is nondegenerate indicating some kind of *spin-zero* or *real scalar* character of the spin-wave quanta. The frustration in the Kitaev model seems to induce an effective antiferromagnetic behavior along the SAW lines whatever the sign of J is. This linear spin-wave spectrum should be considered as a precursor to the linear Majorana spectrum that one gets for the spin-1/2 Kitaev model. It is likely that these scalar spin-wave quanta undergo quantum number fractionization leading to Majorana fermions.

We now calculate the zero-point energy per site $e_0=\Sigma_k\omega_k/(2n)$ as a function of $n\geq 6$. We find that (i) for m odd, $e_0/J=\mathrm{cosec}(\pi/n)/n$ for PBC and $\cot(\pi/n)/n$ for ABC, and (ii) for m even, $e_0/J=\cot(\pi/n)/n$ for PBC and $\mathrm{cosec}(\pi/n)/n$ for ABC.

In all cases, $e_0/J\to 1/\pi\simeq 0.318$ as $n\to\infty$. We find that the minimum value of e_0 occurs if $n=6$ and we have ABC. In that case, $e_0/J=\sqrt{3}/6\simeq 0.289$.

Now we show that the above minimum for the zero-point energy per site can actually be achieved for the entire honeycomb lattice. Consider a dimer covering such that the corresponding SAWs cover the lattice with hexagons as shown in Fig. 4. (There are three such dimer coverings; this will contribute a factor of three when we compute the ground-state degeneracy below.) For each such dimer covering, we take the two spins on all dimers on bonds of type n to point in the same way, say, the top spin pointing along $\hat{\mathbf{n}}$ and the bottom spin pointing along $-\hat{\mathbf{n}}$ (here $n=x,y$, or z). Then we find that each hexagon has ABC and therefore $e_0=0.289J$.

Next, we note that for each of the three dimer coverings, the SAWs cover the lattice with $N/6$ hexagons. These hexagons form a triangular lattice containing $N/3$ triangles. We then see that the ABC of the Hamiltonian in Eq. (13) continues to hold if we flip both the spins on all the three dimers, which pairwise join three hexagons which form a triangle. So even after the dimer covering is fixed, we still have an exponentially large number of ground states given by $2^{N/3}$ corresponding to the different ways in which pairs of spins on different dimers can point. Since there are three possible dimer coverings, the total degeneracy of the quantum ground states is $3\times 2^{N/3}$, which goes as $(1.260)^N$ for large N. This is a smaller exponential than the number of discrete classical ground states, which goes as $(1.662)^N$ as stated earlier.

To conclude, we have shown that the dimer coverings which have the minimum zero-point energy per site given by $0.289J$ are the ones which correspond to SAWs covering the lattice with hexagons. The number of quantum ground states picked out by the zero-point energy of the spin waves still grows exponentially with the number of sites, but it grows more slowly than the number of classical ground states.

Finally, we can again consider what happens if the couplings on the three kinds of bonds are different, say, J_x, J_y, and J_z. We again find that if one of these, say J_z, is larger than the other two, then the classical ground states are given by the state with purely vertical dimers; in each such dimer, the two spins can point along the $+\hat{\mathbf{z}}$, $-\hat{\mathbf{z}}$ or $-\hat{\mathbf{z}}$, $+\hat{\mathbf{z}}$ directions. Hence the number of classical ground states is $2^{N/2}$. We find that this degeneracy is not broken by the zero-point energy of the spin waves.

IV. CONSERVED Z_2 FLUXES

In this section we construct commuting operators for the spin-S Kitaev model and also generalize the Jordan-Wigner transformation for the spin-S case. In the process we get exact results and some new insights.

For the spin-1/2 Kitaev model in two dimensions, it is known that there is a conserved quantum number associated with each hexagon. When the model is rewritten as a Z_2 gauge theory, these conserved quantities correspond to the Z_2 fluxes passing through the hexagon. Since the number of such quantum numbers (or hexagons) is $N/2$, the Hilbert space decomposes into $2^{N/2}$ independent sectors corresponding to each flux independently taking the values ± 1. We will now show that all this continues to hold for arbitrary values of the spin S, integer, or half-odd integer.

We first note that the three spin operators S^x, S^y, S^z satisfy the identities,

$$e^{i\pi S^a}S^b e^{-i\pi S^a} = S^b \text{ if } a=b,$$

$$= -S^b \text{ if } a\neq b, \tag{14}$$

for $a,b=x,y,z$. Now consider a hexagon h with sites labeled as $1,\ldots,6$ with the Hamiltonian

$$H_h = S_1^x S_2^x + S_2^y S_3^y + S_3^z S_4^z + S_4^x S_5^x + S_5^y S_6^y + S_6^z S_1^z. \tag{15}$$

If we define an operator

$$W_p \equiv e^{i\pi(S_1^y+S_2^z+S_3^x+S_4^y+S_5^z+S_6^x)} \tag{16}$$

(see Fig. 1), then it follows from Eq. (14) that

$$W_p H_h (W_p)^{-1} = H_h. \tag{17}$$

Thus W_p commutes with the Hamiltonian H_h. It is easy to check that W_p also commutes with the other terms of the full Hamiltonian coming from other plaquettes. For $S=1/2$, we observe that

$$W_p = -\sigma_1^y\sigma_2^z\sigma_3^x\sigma_4^y\sigma_5^z\sigma_6^x, \tag{18}$$

where σ^a denote the Pauli matrices.

Since $e^{\pm i2\pi S^a}=(-1)^{2S}$, we have $e^{i\pi S^a}=(-1)^{2S}e^{-i\pi S^a}$. It then follows from Eq. (14) that

$$e^{i\pi S^a}e^{i\pi S^b} = (-1)^{2S}e^{i\pi S^b}e^{i\pi S^a} \text{ if } a\neq b. \tag{19}$$

It then follows that W_p will commute with $W_{p'}$ since the two will share an even number of sites. It also follows that $W_p^2=1$. Thus the W_p's are a set of mutually commuting conserved operators with eigenvalues equal to ± 1.

We note that for $S=1/2$, these operators are the same as the conserved flux operators. We will henceforth refer to these operators as the flux operators for all S. While we do not have a gauge theoretic formalism of the model for $S>1/2$, we note that we can associate a conserved Z_2 quantum number with every closed loop on the lattice as follows. For every site on the closed loop, we define the normal direction as the direction associated with the bond that does not belong to the loop. If $(i_1,i_2,\ldots,i_N)$ are the sites for that loop and $(a_1,a_2,\ldots,a_N)$ are the corresponding normal directions, then the conserved quantity is

$$W_L = \prod_{n=1}^{N} e^{i\pi S_{i_n}^{a_n}}. \tag{20}$$

It is interesting to note that these closed-string operators are very similar to those defined by Den Nijs and Rommelse[16] in the context of $S=1$ chains and generalized to arbitrary values of S by Oshikawa.[17]

A. Ground-state fluxes

In the $S=1/2$ model, it has been proven that the values of the flux operators are the same for all the elementary hexagonal plaquettes and are equal to +1. Our semiclassical results indicate that this may be true for all values of S.

Consider the quantum state constructed by taking the direct product of the spin coherent states corresponding to any of the classical ground-state configurations defined by a dimer covering of the lattice. We will refer to these states as the semiclassical ground states. Consider a dimer covering which defines a set of closed self-avoiding loops such that the dimers form the normal directions to these loops. The semiclassical ground state corresponding to such a dimer covering is a simultaneous eigenstate of the flux operators corresponding to the closed loops defined by the dimer covering. The eigenvalues are given by

$$\prod_{n=1}^{N} e^{i\pi S_{i_n}^{a_n}}|\psi\rangle = e^{i\pi S\Sigma_{n=1}^{N} p_n}|\psi\rangle, \tag{21}$$

where $p_n = \pm 1$ depending on the polarization of the spin at the nth site. Since the honeycomb lattice is bipartite, all closed loops have an even number of sites. The eigenvalues are thus $e^{i2\pi lS}$, where l is an integer. If S is an integer, then we see that the eigenvalues are always 1. If S is a half-odd integer, then it is $(-1)^l$. It can be checked that the classical configurations, which lead to ABC in the spin-wave Hamiltonian, correspond to even l.

Thus we see that the spin-wave fluctuations pick out the states, which are simultaneous eigenstates of the flux operators corresponding to one third of the elementary plaquettes. It further picks out the states which have an eigenvalue +1 for these operators. We note that the semiclassical ground states can never be the simultaneous eigenstate of all the flux operators. The spin-wave fluctuations seem to pick out the states, which are the simultaneous eigenstates of the maximal number of elementary plaquette flux operators with eigenvalue +1. In the $S=1/2$ case, the exact ground state is a simultaneous eigenstate of all the flux operators with eigenvalue +1. Our results indicate that this may be the case for all S also.

B. Flux basis and spin-spin correlations

One of the intriguing features of the Kitaev model is the peculiar form of the spin-spin correlation functions.[6] Only the nearest-neighbor correlations are nonzero. Further, only $S_i^x S_j^x$ on the x bonds, $S_i^y S_j^y$ on the y bonds, and $S_i^z S_j^z$ on the z bonds have nonzero values. These results are true for not only the ground state but also for any eigenstate of the model. In fact, as we will show, this form of the correlation function characterizes the set of simultaneous eigenstates of the flux operators.

Consider any simultaneous eigenstate of all the elementary flux operators denoted by $|\{p_n\}\rangle$, where $p_n = \pm 1$ is the eigenvalue of the flux operator of the nth plaquette. The spin operator S_i^a acting on this state produces another simultaneous eigenstate of the flux operators with the eigenvalues of the two plaquettes, which share the bond $(i, i+\hat{a})$ flipped. This follows from Eqs. (19) and (16). As two states with different sets of values of p_n are orthogonal, the only nonzero spin-spin correlations are

$$\langle S_i^x S_{i+\hat{x}}^x\rangle, \quad \langle S_i^y S_{i+\hat{y}}^y\rangle, \quad \text{and} \quad \langle S_i^z S_{i+\hat{z}}^z\rangle. \tag{22}$$

Thus, as stated earlier, the flux operators define a basis of a peculiar kind of spin liquid. This basis is formally constructed in the fermionic formalism of the spin-1/2 model. We will now show that it is possible to have an analogous Jordan-Wigner construction to construct this basis in the spin-S model also. However, unlike the spin-1/2 case our construction will not exhaust all the states in the Hilbert space and thus does not lead to an exact solution of the model.

Consider a Hamilton path running through the lattice. For simplicity, we consider an infinite lattice and take the path to go through the x and y bonds only. The construction can be generalized to any SAWs.[18] Define the "disorder operators" on the nth site to be

$$\mu_{i_n} = \prod_{m<n} e^{i\pi(S_{i_m}^z + S)}, \tag{23}$$

where the μ_{i_n}'s commute with each other and $\mu_{i_n}^2 = 1$. At each site i_n, the Hamilton path is used to classify the three bonds as *incoming, outgoing,* and *normal*. The normal bond for our path is the z bond. We denote the spin operator in the incoming and outgoing bond directions by $S_{i_n}^{t_1}$ and $S_{i_n}^{t_2}$, respectively. We now define two operators at each site,

$$\xi_{i_n} \equiv e^{i\pi(S_{i_n}^{t_1} + S)}\mu_{i_n},$$

$$\chi_{i_n} \equiv e^{i\pi(S_{i_n}^{t_2} + S)}\mu_{i_n}. \tag{24}$$

It then follows that

$$\xi_{i_n}\xi_{i_m} - (-1)^{2S}\xi_{i_m}\xi_{i_n} = \delta_{nm},$$

$$\chi_{i_n}\chi_{i_m} - (-1)^{2S}\chi_{i_m}\chi_{i_n} = \delta_{nm},$$

$$\xi_{i_n}\chi_{i_m} - (-1)^{2S}\chi_{i_m}\xi_{i_n} = 0. \tag{25}$$

Thus the ξ and χ operators are Majorana fermions for half-odd-integer spins and hard-core bosons for integer spins.

We now consider the commutators of the ξ_{i_n} and χ_{i_n} with the Hamiltonian. Consider the terms $\xi_{i_n} H \xi_{i_n}$ and $\chi_{i_n} H \chi_{i_n}$. All the terms in the Hamiltonian involving spins at sites i_m for $m<n$ are left invariant. This is because either both or none of the spins have their signs flipped. So we have

$$\xi_{i_n} H \xi_{i_n} = H - 2J_{t_2} S_{i_n}^{t_2} S_{i_{n-1}}^{t_2} - 2J_{a_n} S_{i_n}^{a_n} S_{i_n+\hat{a}_n}^{a_n},$$

$$\chi_{i_n} H \chi_{i_n} = H - 2J_{a_n} S_{i_n}^{a_n} S_{i_n+\hat{a}_n}^{a_n}. \tag{26}$$

It then follows that the operators defined on the normal bonds,

$$u_{ij} = e^{i\pi S}\chi_i \chi_j, \tag{27}$$

form a set of mutually commuting operators, which also commute with the Hamiltonian. The flux operator on any elementary plaquette is equal to the product of the u_{ij} operators on the two z bonds of the hexagon just as in the $S=1/2$ case.

Thus, just as in the $S=1/2$ case, the flux basis is easy to construct in terms of the χ_i operators. However, writing it in a simple form in terms of the original spins remains a challenge.

V. EXACTLY SOLVABLE HIGHER SPIN MODEL WITH FREE MAJORANA FERMIONS

For the case of half-odd-integer spin S, we find that it is not possible to write the spin-S Kitaev model in Eq. (9) in terms of local interactions between the Majorana fermions introduced above. The difficulty arises from not being able to invert Eq. (24) to obtain the spin operators. However, for any

finite value of half-odd-integer spin, we can define a modified Kitaev Hamiltonian for which we can give the exact spectrum and degeneracies. Our modified Kitaev Hamiltonian has the form

$$H = \frac{J}{S} \sum_{j+l=\text{even}} (\tau^x_{j,l}\tau^x_{j+1,l} + \tau^y_{j-1,l}\tau^y_{j,l} + \tau^z_{j,l}\tau^z_{j,l+1}), \qquad (28)$$

where $\tau^a \equiv e^{i\pi S^a}$ is the π-rotation operator introduced in Eq. (14). Now, the operators τ^a only connect states, which have the same magnitude of S^z, in the S^z basis; this is because $e^{i\pi S^x}$ and $e^{i\pi S^y}$ acting on $|S_z=m\rangle$ give $|S_z=-m\rangle$. Hence the τ^a's reduce to 2×2 blocks in the basis of eigenstates of S^z; the number of such blocks is equal to $S+1/2$ corresponding to $m=1/2,3/2,\ldots,S$. For example, in the case of $S=3/2$, we find that in the basis of the two states with $S^z=\pm 3/2$, $\tau^x=-i\sigma^x$, $\tau^y=i\sigma^y$, and $\tau^z=-i\sigma^z$, while in the basis of the two states with $S^z=\pm 1/2$, $\tau^x=-i\sigma^x$, $\tau^y=-i\sigma^y$, and $\tau^z=i\sigma^z$.

In view of this, the $(2S+1)^N$ dimensional Hilbert space for N spins decomposes into $(S+1/2)^N$ copies of 2^N dimensional Hilbert spaces. Inside each copy, the Hamiltonian in Eq. (28) behaves exactly like the Kitaev Hamiltonian in Eq. (9) leading to the identical spectrum and physical properties. The degeneracy of $(S+1/2)^N$ of the Hamiltonian (which is not a gauge degeneracy) is an unusual decomposition of the eigenstates and may have some special use in quantum computation.

In the case of integer spins, Eq. (19) shows that the τ^a operators commute with each other for all the values of $a=x,y,z$. Hence, they can be diagonalized simultaneously; each of the diagonal entries is equal to ± 1. The integer spin version of Eq. (28) therefore reduces to a kind of Ising spin model, which is classical rather than quantum mechanical.

VI. DISCUSSION

In this paper we have presented a large spin analysis of the Kitaev model whose spin-1/2 end is exactly solvable. We find a classical ground-state structure, which has a nontrivial geometry in the N-spin space. There are discrete sets of points that are connected by flat valleys. Our spin-wave analysis gives either zero or positive-energy excitations indicating local stability of the degenerate set of vacuua. Further, depending on the vacuum chosen (which depends on the dimer covering pattern), the spin waves are localized on the SAW curves. It would be interesting to see how and when quantum number fractionization occurs and Majorana fermions emerge when one goes beyond harmonic spin-wave theory.

A class of excitations that we have not studied in this paper is the one involving dimer coverings containing one or more defects. By definition, a defect site does not lie on a dimer. We can consider ground states about these defective dimer coverings; these will define ground states containing a topological spin defect. As the energy of one topological defect is of the order of JS, there is a finite gap to these excitations. It would be interesting to study whether such a defect might be related to a Majorana fermion excitation.

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