

# Spin-1 Kitaev model in one dimension

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We study a one-dimensional version of the Kitaev model on a ring of size  $N$ , in which there is a spin  $S > 1/2$  on each site and the Hamiltonian is  $J \sum_n S_n^x S_{n+1}^y$ . The cases where  $S$  is integer and half-odd-integer are qualitatively different. We show that there is a  $\mathbb{Z}_2$  valued conserved quantity  $W_n$  for each bond  $(n, n+1)$  of the system. For integer  $S$ , the Hilbert space can be decomposed into  $2^N$  sectors, of unequal sizes. The number of states in most of the sectors grows as  $d^N$ , where  $d$  depends on the sector. The largest sector contains the ground state, and for this sector, for  $S = 1$ ,  $d = (\sqrt{5} + 1)/2$ . We carry out exact diagonalization for small systems. The extrapolation of our results to large  $N$  indicates that the energy gap remains finite in this limit. In the ground state sector, the system can be mapped to a spin-1/2 model. We develop variational wave functions to study the lowest energy states in the ground state and other sectors. The first excited state of the system is the lowest energy state of a different sector and we estimate its excitation energy. We consider a more general Hamiltonian, adding a term  $\lambda \sum_n W_n$ , and show that this has gapless excitations in the range  $\lambda_1^c \leq \lambda \leq \lambda_2^c$ . We use the variational wave functions to study how the ground state energy and the defect density vary near the two critical points  $\lambda_1^c$  and  $\lambda_2^c$ .

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## I. INTRODUCTION

In recent years, there have been many studies of quantum spin systems which are characterized by a high degree of frustration and topological order. The word ‘frustration’ here refers to systems with competing interactions having a large number of states with energy near the minimum energy. Topological order implies the existence of invariants which, for topological reasons, are robust against a large class of perturbations. Such systems are often associated with a novel structure of the ground state and low-lying excitations, and are interesting from the point of view of possible applications in quantum computation [1–5]. A particularly interesting model in this context is the two-dimensional frustrated spin-1/2 model introduced by Kitaev [3]. This model has several fascinating properties which have been studied in great detail [6–12]. For instance, the model and its variants constitute the only known class of spin models in two dimensions or more dimensions that is fully integrable, being reducible to a system of non-interacting Majorana fermions. A similar model, called the compass model, although not exactly solvable, was introduced by Kugel and Khomskii many years ago [13] to understand the magnetic properties of transition metal oxides which have orbital degeneracies. Recently physical realizations of the spin-1/2 Kitaev model have been proposed in optical lattice systems [14] and in quantum circuits [15]. Variants of the model have also been studied in two dimensions [16–24], three dimensions [25, 26] and also on quasi-one-dimensional lattices [27–29]. Finally, the spin- $S$  Kitaev model has been studied in the large  $S$  limit using spin wave theory [30], and the classical version of the Kitaev model has been studied at finite temperatures using analytical and Monte Carlo techniques [31]. Their

results indicate that while the phenomenon of order-by-disorder [32–35] may occur in the quantum mechanical Kitaev model, it does not in the corresponding classical model.

For the Kitaev model with spin  $S > 1/2$ , there is a  $\mathbb{Z}_2$  invariant associated with each plaquette for arbitrary spin- $S$ , which reduces to the conserved  $\mathbb{Z}_2$  gauge flux for the spin-1/2 case [30]. However, the model does not seem to be fully integrable. While some differences in the structure of the invariants between the models with half-odd-integer and integer spins have been pointed out [30], the issue of whether there are systematic differences in the nature of the low-energy spectrum is also of interest. In the present paper, we approach this problem by examining the spin-1 Kitaev model. The two-dimensional model appears difficult to analyze, but even the one-dimensional version of it has a lot of interesting structure, as we proceed to show.

The plan of this paper is as follows. In Sec. II, we consider the spin- $S$  Kitaev chain. In Sec. II A we show that this model has local, mutually commuting conserved quantities  $W_n$ , for integer  $S$ . The eigenvalues of  $W_n$  are  $\pm 1$ . For open boundary conditions, there are some additional conserved quantities at the ends of the system. The existence of these conserved quantities implies that the Hilbert space of a  $N$ -site system can be decomposed into a sum of  $2^N$  disjoint subspaces. The dimensions of these subspaces are not equal. In Sec. II B we develop a formalism to compute the dimension of these sectors. For large  $N$ , the dimension varies as  $d^N$  in most sectors, with the constant  $d$  depending on the sector. The sectors show complicated spatial structures, arising from the spatial structure of  $\{W_n\}$ . We show this in Sec. II C, by computing the non-trivial spatial dependence of expectation values of spin operators in some sectors, averaged

over all states in the sector. We then consider the spin-1 model in Sec. III. In Sec. III A, we consider the ground state and lowest excited state of the system. Exact diagonalizations of small systems show that the ground state lies in a sector in which  $W_n = +1$  for all  $n$ . In this sector, there is a gap between the ground state and the first excited state. The lowest excited state of the system is the ground state of a different sector; and the energy-gap seems to approach a non-zero value in the limit of the system size going to infinity. In Sec. IV, we consider the sector containing the ground state, and show that the Hamiltonian is equivalent to the Hamiltonian of a deposition-evaporation process of a nearest-neighbor-exclusion lattice gas model, which can be written as of a spin-1/2 system with local interactions with a range extending to at most next-nearest neighbors. The Hamiltonian seems to be difficult to diagonalize exactly, we present a variational study of the ground state in Sec. V. The variational estimate of the ground state energy is found to agree well with the results obtained numerically for small systems. We also analyze the first excited state of the Hamiltonian. In Sec. VI, we consider a more general Hamiltonian, obtained by adding a term  $\lambda \sum_n W_n$ , and discuss its ground states as a function of  $\lambda$ . We show that the ground state of this new Hamiltonian is gapless for a range of couplings  $\lambda_1^c \leq \lambda \leq \lambda_2^c$ , and gapped otherwise. We argue that for  $\lambda$  just above  $\lambda_1^c$ , in the sector containing the ground state, the density of negative  $W$ 's is of order  $|\frac{1}{\log(\lambda - \lambda_1^c)}|$ . For  $\lambda$  just below  $\lambda_2^c$ , the density of positive  $W$ 's goes to zero as  $(\lambda_2^c - \lambda)^{1/2}$ . In the final section, we summarize our conclusions, and discuss the relationship of this model with the Fibonacci chain.

## 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.

Let us begin with the Kitaev model on the honeycomb lattice. This is governed by the Hamiltonian

$$H_{Kit}^{hex} = J_x \sum_{\langle ij \rangle_x} S_i^x S_j^x + J_y \sum_{\langle ij \rangle_y} S_i^y S_j^y + J_z \sum_{\langle ij \rangle_z} S_i^z S_j^z, \quad (1)$$

where  $\langle ij \rangle_a$  denote the nearest-neighbor bonds in the  $a^{\text{th}}$  direction. If we set  $J_z = 0$ , we get a set of decoupled chains. We call this the Kitaev chain, and this is the topic of this paper. The Hamiltonian is by

$$H = \sum_n (J_{2n-1} S_{2n-1}^x S_{2n}^x + J_{2n} S_{2n}^y S_{2n+1}^y). \quad (2)$$

In general, the couplings  $J_m$  could be all different from each other. If some of the couplings are negative, we can change the signs of those couplings by performing the unitary transformation

$$S_m^x \rightarrow -S_m^x, \quad S_m^y \rightarrow -S_m^y, \quad \text{and} \quad S_m^z \rightarrow S_m^z \quad (3)$$

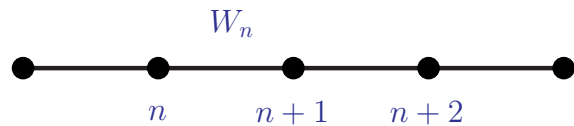


FIG. 1: Picture of the Kitaev chain showing one of the conserved quantities  $W_n$ .

on appropriate sites. We consider the simpler case, where all couplings have the same value,  $J_m = J$ . Without any loss of generality, we set  $J = 1$ . Finally, the Hamiltonian can be unitarily transformed to a more convenient form by the following transformation on the even sites,

$$S_{2n}^x \rightarrow S_{2n}^y, \quad S_{2n}^y \rightarrow S_{2n}^x, \quad \text{and} \quad S_{2n}^z \rightarrow -S_{2n}^z. \quad (4)$$

The Hamiltonian in Eq. (2) then takes the translation invariant form

$$H_{Kit} = \sum_n S_n^x S_{n+1}^y. \quad (5)$$

### A. Invariants

The Hamiltonian in Eq. (5) has the following local symmetries for all  $S$ . Let us introduce the operators on sites

$$\Sigma_n^a = e^{i\pi S_n^a}, \quad (6)$$

and operators on bonds

$$W_n = \Sigma_n^y \Sigma_{n+1}^x. \quad (7)$$

as shown in Fig. 1. We then find that

$$[W_n, H] = 0. \quad (8)$$

The eigenvalues of  $\Sigma_n^a$  are  $\pm 1$  for integer  $S$  and  $\pm i$  for half-odd-integer  $S$ . Thus for any value of the spin  $S$ , the eigenvalues of  $W_n$  are  $\pm 1$ .

However, there is a qualitative difference between integer and half-odd-integer values of  $S$ . For integer values of  $S$ , all the matrices  $\Sigma_n^a$  commute with each other, whereas for half-odd-integer values,  $\Sigma_n^a$  commutes with  $\Sigma_m^b$  for  $n \neq m$  but anticommutes with  $\Sigma_n^b$  for  $a \neq b$ . Consequently, for integer  $S$ , all the invariants  $W_n$  commute, but for half-odd-integer  $S$ ,  $W_n$  anti-commutes with its neighboring invariants,  $W_{n\pm 1}$ , and commutes with  $W_m$ ,  $m \neq n, n\pm 1$ . We will now show that this implies that all the eigenstates of the chain with half-odd-integer  $S$  are  $2^{N/2}$  fold degenerate.

The invariants for half-odd-integer  $S$  can be combined in the following way to form a set of mutually commuting angular momentum operators, one per every two bonds,

$$\mu_n^z = W_{2n}, \quad \mu_n^x = W_{2n-1} \prod_{m < n} W_{2m-1}, \quad \mu_n^y = i\mu_n^x \mu_n^z. \quad (9)$$

It can be verified that

$$[\mu_n^a, \mu_m^b] = 2i\delta_{nm}\epsilon^{abc}\mu^c, \quad (10)$$

$$\{\mu_n^a, \mu_n^b\} = 2\delta^{ab}. \quad (11)$$

The  $\mu_n^a$  commute with the Hamiltonian as they are made by multiplying conserved operators. Hence Eq. (10) shows that the Hamiltonian has a  $(SU(2))^{N/2}$  symmetry, where  $N$  is the number of sites. Eq. (11) shows that each of these  $SU(2)$  factors are realized in the spin-1/2 representation. Thus each eigenstate is  $2^{N/2}$ -fold degenerate. There is no reason for such a degeneracy for integer  $S$  and indeed, as we will see later, the ground state for  $S = 1$  is non-degenerate.

We note that the spin- $S$  Kitaev model in two dimensions also has a  $\mathbb{Z}_2$  valued invariant associated with every hexagon of the honeycomb lattice [30]. When they are restricted to a single chain, the invariants take the form

$$V_n = \Sigma_n^y \Sigma_{n+1}^z \Sigma_{n+2}^x \quad (12)$$

which involves three neighboring sites. The invariants given in Eq. (7) are simpler because they only involve two sites. For any spin  $S$ , we find that  $\Sigma_n^x \Sigma_n^y \Sigma_n^z = I$  and  $(\Sigma_n^a)^2 = (-1)^{2S}$ ; hence the invariants in Eqs. (7) and (12) are related to each other as

$$V_n = (-1)^{2S} W_n W_{n+1}. \quad (13)$$

Open chains have some extra symmetries at the edges. If the site labels of the open chain are  $1, \dots, N$ , then  $S_1^x$  and  $S_N^y$  also commute with the Hamiltonian. Thus at the first and last sites, we have a  $U(1)$  symmetry group generated by these operators. Note that a  $\mathbb{Z}_2$  subgroup of this group, consisting of the operators  $\Sigma_1^x$  and  $\Sigma_N^y$ , also commutes with all the invariants. If we combine the operators  $S_1^x$  and  $S_N^y$  with the  $W_n$  invariants on the first and last bonds, we have a larger symmetry group made of  $W_1$ ,  $S_1^x$  and their products at the first bond, and the group made of  $W_N$ ,  $S_N^y$  at the last bond. As we will show in Sec. III, for the  $S = 1$  case the group formed is  $SU(2) \times U(1)$  at each end.

### B. Counting of states for integer $S$

We will now develop a formalism to count the number of states in a given sector for integer  $S$ . In this case, the  $\Sigma$  matrices commute and hence can be simultaneously diagonalized. If  $|S, m\rangle$  denote the eigenstates of  $S^z$ , then

$$\Sigma^x |S, m\rangle = (-1)^S |S, -m\rangle, \quad (14)$$

$$\Sigma^y |S, m\rangle = (-1)^{S+m} |S, -m\rangle, \quad (15)$$

$$\Sigma^z |S, m\rangle = (-1)^m |S, m\rangle. \quad (16)$$

We can construct the eigenstates of the  $\Sigma$  matrices in the  $m \neq 0$  subspace,

$$|S, m\pm\rangle \equiv \frac{1}{\sqrt{2}} (|S, m\rangle \pm |S, -m\rangle), \quad (17)$$

where  $m = 1, \dots, S$ . The eigenvalues of the matrices are,

$$\Sigma^x |S, m\pm\rangle = \pm(-1)^S |S, m\pm\rangle, \quad (18)$$

$$\Sigma^y |S, m\pm\rangle = \pm(-1)^{S+m} |S, m\pm\rangle, \quad (19)$$

$$\Sigma^z |S, m\pm\rangle = (-1)^m |S, m\pm\rangle. \quad (20)$$

The states of a chain can be classified by the eigenvalues of  $\Sigma_n^x$  and  $\Sigma_n^y$  as

$$(y_N x_N) \cdots (y_2 x_2) (y_1 x_1), \quad (21)$$

where  $x_n, y_n = \pm 1$  are the eigenvalues of  $\Sigma_n^x$  and  $\Sigma_n^y$  respectively. The invariants are then  $W_n = x_{n+1} y_n$ .

We now calculate the number of states in a given sector  $\mathcal{W}$  using a standard transfer matrix technique. Consider the allowed states of  $r$  sites, when the values of  $r-1$  constants  $W_j$ , with  $j = 1$  to  $r-1$  have been specified. We denote this set of values by  $\mathcal{W}$ . Let  $Z_r(y|\mathcal{W})$  denote the number of allowed states of this set of sites with  $\Sigma_r^y = y$  where  $y$  takes values  $\pm 1$ . We now add a site  $r+1$  to the chain, and also specify  $W_r$ . Let the new set of  $\{W\}$  be denoted by  $\mathcal{W}'$ .

Consider first the case  $W_r = +1$ . Clearly, we can have two possibilities:  $\Sigma_{r+1}^x = \Sigma_r^y = +1$ , or  $\Sigma_{r+1}^x = \Sigma_r^y = -1$ . Let  $\nu(p, p')$  denote the number of states of a single site with  $\Sigma^y = p$ , and  $\Sigma^x = p'$ . Then, we clearly have the recursion equation

$$Z_{r+1}(y|\mathcal{W}') = \nu(y, +1)Z_r(+1, \mathcal{W}) + \nu(y, -1)Z_r(-1, \mathcal{W}). \quad (22)$$

This equation can be written as a matrix equation

$$\begin{bmatrix} Z_{r+1}(+1|\mathcal{W}') \\ Z_{r+1}(-1|\mathcal{W}') \end{bmatrix} = \mathbb{T}_+ \begin{bmatrix} Z_r(+1|\mathcal{W}) \\ Z_r(-1|\mathcal{W}) \end{bmatrix}, \quad (23)$$

where  $\mathbb{T}_+$  is a  $2 \times 2$  matrix given by

$$\mathbb{T}_+ = \begin{bmatrix} \nu(+1, +1) & \nu(+1, -1) \\ \nu(-1, +1) & \nu(-1, -1) \end{bmatrix}, \quad (24)$$

It then follows from Eqs. (18-20) that

$$\mathbb{T}_+ = \frac{1}{2} \begin{bmatrix} S-1 & S+1 \\ S+1 & S+1 \end{bmatrix} \quad \text{for } S \text{ odd}, \quad (25)$$

$$= \frac{1}{2} \begin{bmatrix} S+2 & S \\ S & S \end{bmatrix} \quad \text{for } S \text{ even}. \quad (26)$$

Similarly, when  $W_r = -1$ , the corresponding recursion equation is

$$\begin{bmatrix} Z_{r+1}(+1|\mathcal{W}') \\ Z_{r+1}(-1|\mathcal{W}') \end{bmatrix} = \mathbb{T}_- \begin{bmatrix} Z_r(+1|\mathcal{W}) \\ Z_r(-1|\mathcal{W}) \end{bmatrix}, \quad (27)$$

where the matrix  $\mathbb{T}_-$  is given by

$$\mathbb{T}_- = \mathbb{T}_+ \tau^x, \quad \text{with} \quad \tau^x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \quad (28)$$

It is then clear that for a given set of invariants  $\mathcal{W}$ , the number of states can be written in terms of a product of the matrices  $\mathbb{T}_+$  and  $\mathbb{T}_-$ .

For example, for an open chain of  $N$  sites, and  $\mathcal{W} = \{W_{N-1}, \dots, W_3, W_2, W_1\} = \{+1, \dots, +1, -1, -1\}$ , we have

$$\begin{bmatrix} Z_N(+1|\dots + --) \\ Z_N(-1|\dots + --) \end{bmatrix} = \mathbb{T}_+ \dots \mathbb{T}_+ \mathbb{T}_- \mathbb{T}_- \begin{bmatrix} Z_1(+1|\phi) \\ Z_1(-1|\phi) \end{bmatrix} \quad (29)$$

where  $\phi$  denotes the null string, and  $Z_1(y|\phi)$  denotes the number of states of the spin at site 1 with  $\Sigma_1^y = y$ . Thus  $Z_1(+1|\phi) = S + 1$ ,  $Z_1(-1|\phi) = S$ , when  $S$  is an even integer, and  $Z_1(+1|\phi) = S$ ,  $Z_1(-1|\phi) = S + 1$  when  $S$  is an odd integer. The total number of states in this sector is then given by

$$\Gamma(\mathcal{W}) = Z_N(+1|\mathcal{W}) + Z_N(-1|\mathcal{W}). \quad (30)$$

For a closed chain, there is an additional invariant  $W_N = y_N x_1$  and the number of states in the sector becomes

$$\Gamma(\mathcal{W}) = \text{Tr} \left( \prod_{n=1}^N \mathbb{T}_{W_n} \right), \quad (31)$$

where  $\mathbb{T}_{W_n} \equiv \mathbb{T}_\pm$  for  $W_n = \pm 1$  and  $\prod_{n=1}^N$  is an ordered product of  $\mathbb{T}_\pm$  matrices, from site 1 to  $N$  with the index increasing from right to left.

We now calculate the dimensions of some sectors for a closed chain of length  $N$ . It is easy to get an explicit answer for the two extreme limits when  $W_n = \pm 1$  for all  $n$ . In these cases, the number of states,  $\Gamma^\pm$ , is

$$\Gamma^\pm = (d_1^\pm)^N + (d_2^\pm)^N, \quad (32)$$

where  $d_1^\pm(S)$  and  $d_2^\pm(S)$  are the larger and smaller eigenvalues of  $\mathbb{T}_\pm$  respectively. The eigenvalues can be computed to give,

$$d_{1(2)}^+ = \frac{1}{2} \left( S \pm \sqrt{S^2 + 2S + 2} \right) \quad \text{for } S \text{ odd}, \quad (33)$$

$$= \frac{1}{2} \left( S + 1 \pm \sqrt{S^2 + 1} \right) \quad \text{for } S \text{ even}, \quad (34)$$

$$d_{1(2)}^- = \frac{1}{2} \left( S + 1 \pm \sqrt{S^2 - 1} \right) \quad \text{for } S \text{ odd}, \quad (35)$$

$$= \frac{1}{2} \left( S \pm \sqrt{S^2 + 2S} \right) \quad \text{for } S \text{ even}. \quad (36)$$

For  $S = 1$ ,  $d_1^+$  is equal to the golden ratio,  $\gamma = (1 + \sqrt{5})/2$ , and  $d_2^+ = -1/\gamma$ . As  $N \rightarrow \infty$ , the dimension of the Hilbert space in the sector with all  $W_n = 1$  grows as  $\gamma^N$ . On the other hand,  $d_1^- = d_2^- = 1$ . The dimension of the sector with all  $W_n = -1$  is therefore equal to 2.

With the exception of  $S = 1$ , the larger of the two eigenvalues  $d_1^\pm$  is always greater than 1, and in the  $N \rightarrow \infty$  limit, we have

$$\Gamma^\pm(S) = (d_1^\pm(S))^N. \quad (37)$$

$d_1^\pm(S)$  is referred to as the quantum dimension of the sector. As can be seen it is, in general, fractional for any  $S$ . In the limit  $S \rightarrow \infty$ , the quantum dimension tends to  $S + 1/2$  for both the sectors. It is interesting to note that it is a half-odd-integer in this limit.

### C. Expectation values of the $\Sigma$ operators in different sectors

In this section we find the expectation values of the  $\Sigma_n^a$  operators in various sectors. We will assume periodic boundary conditions. Our calculation will average over all the states of a given sector considered with equal weight; this can be considered as a calculation in the limit that the temperature  $T \rightarrow \infty$ , so that it does not depend on the Hamiltonian.

We evaluate the expectation values of  $\Sigma_n^a$  by inserting projection operators at site  $n$  in the product of transfer matrices in Eq. (31). This yields the following expression for the expectation value of the  $\Sigma_n^a$  operator in a general sector with a  $W$ -configuration  $\mathcal{W}$

$$\langle \Sigma_{n+1}^a \rangle_{\mathcal{W}} = \text{Tr} \left[ \left( \prod_{j=n+1}^N \mathbb{T}_{W_j} \right) \mathbb{T}_{W_n}^a \left( \prod_{i=1}^{n-1} \mathbb{T}_{W_i} \right) \right] / \Gamma(\{\mathcal{W}\})$$

where

$$\mathbb{T}_{W_n}^x = W_n \mathbb{T}_{W_n} \tau^z$$

$$\mathbb{T}_{W_n}^y = \tau^z \mathbb{T}_{W_n}$$

$$\mathbb{T}_{W_n}^z = W_n \tau^z \mathbb{T}_{W_n} \tau^z \quad (38)$$

and  $\tau^z$  and  $\tau^x$  are the well-known Pauli matrices.

We now compute the expectation values of  $\Sigma_n^a$  in two sectors: the sector  $\mathcal{W}_0$  with all  $W_n = +1$ , and the sector  $\mathcal{W}_1$  in which one of the  $W_n = -1$  and all the other  $W_n = +1$  (without loss of generality we pick  $W_N = -1$ ). The expressions for  $\langle \Sigma_n^a \rangle_{\mathcal{W}_{0,1}} \equiv \langle \Sigma_n^a \rangle_{0,1}$  can be evaluated in terms of the eigenvectors and eigenvalues of  $\mathbb{T}_+$ . The  $\mathbb{T}_+$  matrix is a linear combination of the Pauli matrices,  $\tau^z$  and  $\tau^x$ . Its eigenvectors are spinors polarized parallel and anti-parallel to a direction in the  $z_x$  plane, forming an angle  $\theta_S$  with the  $z$ -axis, where  $\theta_S$  is defined by,

$$\begin{aligned} \cos \theta_S &\equiv -\frac{1}{\sqrt{1 + (S+1)^2}} \quad \text{for } S \text{ odd}, \\ &\equiv \frac{1}{\sqrt{1 + S^2}} \quad \text{for } S \text{ even}, \end{aligned} \quad (39)$$

$$\begin{aligned} \sin \theta_S &\equiv \frac{S+1}{\sqrt{1 + (S+1)^2}} \quad \text{for } S \text{ odd}, \\ &\equiv \frac{S}{\sqrt{1 + S^2}} \quad \text{for } S \text{ even}. \end{aligned} \quad (40)$$

For the sector with all  $W_n = +1$  it is easy to see that  $\langle \Sigma_n^x \rangle_0 = \langle \Sigma_n^y \rangle_0$ . For large  $N$ , we obtain

$$\langle \Sigma_n^{x(y)} \rangle_0 = \cos \theta_S, \quad (41)$$

$$\langle \Sigma_n^z \rangle_0 = \cos^2 \theta_S + \frac{d_1^+}{d_1^-} \sin^2 \theta_S. \quad (42)$$

In the sector where  $W_N = -1$  and the rest are equal

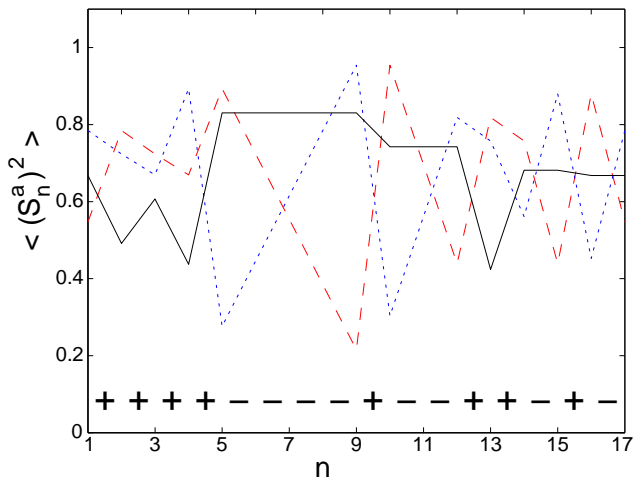


FIG. 2: Plot of  $\langle S_n^{x2} \rangle$  (dotted line),  $\langle S_n^{y2} \rangle$  (dashed line) and  $\langle S_n^{z2} \rangle$  (full line) as a function of  $n$  for  $S = 1$ , on a ring with 16 sites in the sector  $++++- - - -+ - - + + - + -$ , with periodic boundary conditions (site 17 = site 1).

to  $+1$ , we get, for large  $N$ ,

$$\langle \Sigma_n^x \rangle_1 = \langle \Sigma_n^x \rangle_0 \left( 1 - \left( \frac{d_2^+}{d_1^+} \right)^{n-1} \right), \quad (43)$$

$$\langle \Sigma_n^y \rangle_1 = \langle \Sigma_n^y \rangle_0 \left( 1 - \left( \frac{d_2^+}{d_1^+} \right)^n \right), \quad (44)$$

$$\langle \Sigma_n^z \rangle_1 = \langle \Sigma_n^z \rangle_0 \left( 1 + \frac{2 \cos \theta_S}{d_1^+ \cos \theta_S + d_2^+ \sin^2 \theta_S} \left( \frac{d_2^+}{d_1^+} \right)^{n-1} \right). \quad (45)$$

Note that in the limit  $n \rightarrow \pm\infty$ ,  $\langle \Sigma_n^a \rangle$  in Eqs. (43-45) approach the values given in Eqs. (41-42) exponentially quickly.

While in general  $\Sigma_n^a$  are complicated multi-spin operators, for  $S = 1$  we have  $\Sigma_n^a = 1 - 2(S_n^a)^2$ . Thus, for  $S = 1$  we are essentially computing the expectation values of  $(S_n^a)^2$ . To see what the spin textures are like in a typical sector, we have plotted in Fig. 2 the expectation values of  $S_n^{x2}$ ,  $S_n^{y2}$  and  $S_n^{z2}$  for  $S = 1$ , as a function of the spatial coordinate  $n$  for a ring of size 16, in the sector where the sequence of  $W$ 's is  $++++- - - -+ - - + + - + -$ . This sequence was chosen as it is a de Bruijn sequence [36] of length 16, in which each of the 16 possible binary sequences of length 4 occur exactly once, taking the periodic boundary conditions into account.

### III. $S = 1$ MODEL

We will now focus on the Kitaev chain with spin-1's at each site. We will work with the natural spin-1 representation in which

$$(S^a)_{bc} = i\epsilon_{abc}. \quad (46)$$

In this representation, the matrices  $\Sigma^a$  are diagonal and are given by

$$\begin{aligned} \Sigma^x &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \\ \Sigma^y &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \\ \Sigma^z &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \end{aligned} \quad (47)$$

We note that these matrices satisfy  $\Sigma^x \Sigma^y \Sigma^z = I$ . We denote the basis vectors by  $|x\rangle$ ,  $|y\rangle$  and  $|z\rangle$  defined as

$$|x\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |y\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |z\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \quad (48)$$

We then see that the 9 possible states at sites  $(n, n+1)$  are given by:

$$|xy\rangle, |xz\rangle, |yx\rangle, |zy\rangle \text{ and } |zz\rangle \text{ with } W_n = 1, \quad (49)$$

and

$$|xx\rangle, |yy\rangle, |yz\rangle \text{ and } |zx\rangle \text{ with } W_n = -1. \quad (50)$$

From Eq. (46) we have,

$$\begin{aligned} S^x|x\rangle &= 0, & S^y|x\rangle &= i|z\rangle, & S^z|x\rangle &= -i|y\rangle, \\ S^x|y\rangle &= -i|z\rangle, & S^y|y\rangle &= 0, & S^z|y\rangle &= i|x\rangle, \\ S^x|z\rangle &= i|y\rangle, & S^y|z\rangle &= -i|x\rangle, & S^z|z\rangle &= 0. \end{aligned} \quad (51)$$

Eqs. (47) and (51) imply that  $(S^a)^2 = (1 - \Sigma^a)/2$ .

For the 5 states in Eq. (49) satisfying  $W_n = 1$ , we have the following actions of the relevant term in the Hamiltonian,

$$\begin{aligned} S_1^x S_2^y |xy\rangle &= 0, \\ S_1^x S_2^y |xz\rangle &= 0, \\ S_1^x S_2^y |zy\rangle &= 0, \\ S_1^x S_2^y |zz\rangle &= |yx\rangle, \\ S_1^x S_2^y |yx\rangle &= |zz\rangle. \end{aligned} \quad (52)$$

For the 4 states in Eq. (50) satisfying  $W_n = -1$ , the actions of the relevant term in the Hamiltonian are given by

$$\begin{aligned} S_1^x S_2^y |xx\rangle &= 0, \\ S_1^x S_2^y |yy\rangle &= 0, \\ S_1^x S_2^y |yz\rangle &= -|zx\rangle, \\ S_1^x S_2^y |zx\rangle &= -|yz\rangle. \end{aligned} \quad (53)$$

As mentioned earlier, for an open chain with site numbers going from 1 to  $N$ , we find that  $S_1^x$  and  $S_N^y$  commute with  $H$ . We define the operators,

$$\tau^1 \equiv iW_1 S_1^x, \quad \tau^2 \equiv S_1^x, \quad (54)$$

$$\tau^3 \equiv -S_1^x W_1 S_1^x, \quad \tau^0 \equiv \frac{1}{2} (1 - (S_1^x)^2). \quad (55)$$

It can be verified that these operators obey a  $SU(2) \times U(1)$  algebra. Exactly the same construction on the last bond, with  $S_1^x \rightarrow S_N^y$  and  $W_1 \rightarrow W_N$ , yields the same algebra on that bond.

### A. Numerical studies

We have carried out exact diagonalization studies of small systems with periodic boundary conditions in order to find the energies of the ground state and the lowest excited state of the spin-1 Kitaev chain. We find that the ground state lies in the sector with all  $W_n = 1$  and has zero momentum (momentum is a good quantum number in this sector since the values of the  $W_n$ 's are translation invariant). The ground state energy per site as a function of the system size  $N$  is presented in Table I. We see that  $E_0/N$  shows odd-even oscillations as a function of  $N$  but seems to converge quite fast. The fast convergence indicates that the ground state must have a fairly short correlation length. The  $N$ -dependence of  $\bar{E}_N = E_0/N$  can be fitted to the form

$$\bar{E}_N = E_\infty + B(-\alpha)^N. \quad (56)$$

A simple plot of  $\log |\bar{E}_N - E_\infty|$  versus  $N$  (Fig. 3), gives a good straight line for  $E_\infty = -0.60356058$ , which we take to be the best estimate of  $E_\infty$ . The corresponding values of  $B$  and  $\alpha$  are 0.07 and 0.51. The estimated errors of extrapolation are about 1 in the last significant digit.

| $N$ | $E_0/N$      | $N$ | $E_0/N$      |
|-----|--------------|-----|--------------|
| 2   | -0.707106770 | 11  | -0.603525102 |
| 3   | -0.577350259 | 12  | -0.603578389 |
| 4   | -0.612372458 | 13  | -0.603551567 |
| 5   | -0.600000024 | 14  | -0.603565216 |
| 6   | -0.605046094 | 15  | -0.603558183 |
| 7   | -0.602888465 | 16  | -0.603561819 |
| 8   | -0.603869855 | 17  | -0.603559971 |
| 9   | -0.603412688 | 18  | -0.603560924 |
| 10  | -0.603632331 | 19  | -0.603560388 |

TABLE I: Ground state energy per site versus  $N$ .

In the sector with all  $W_n = 1$ , the first excited state has momentum equal to  $\pi$  if  $N$  is even. We find that the gap separating it from the ground state is given by 1.0353 for  $N = 4$  and 0.9845 for  $N = 6$ . These values also seem to be converging rapidly, and the large value is consistent with a short correlation length. However, this is *not* the lowest excited state of the system. Rather, we find that the state nearest in energy to the ground state is the ground state of the sector with exactly one  $W_n = -1$  and all the other  $W_n = 1$ . (We cannot use momentum to classify the states in this sector since it is not translation invariant). The energy gap  $\Delta E$  between the lowest energy state in this sector and the ground state of the sector with all  $W_n = 1$  is shown in Table II. We

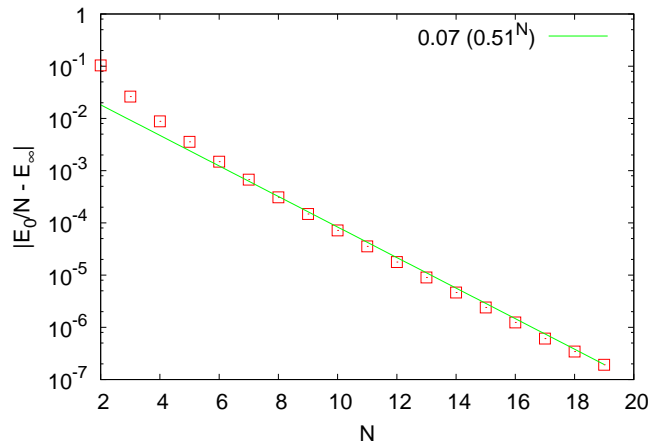


FIG. 3: Graph of  $|E_0/N - E_\infty|$  with  $N$ , where  $E_\infty = -0.60356058$ , showing an exponential convergence to the value of the ground state energy with  $N$ .

see that these also oscillate between even and odd values of  $N$  but seem to converge quite fast to a small but non-zero value. This is evidence that the spin-1 Kitaev chain has a finite gap in the thermodynamic limit  $N \rightarrow \infty$ .

| $N$ | $\Delta E$ |
|-----|------------|
| 3   | 0.1141     |
| 4   | 0.2025     |
| 5   | 0.1671     |
| 6   | 0.1802     |

TABLE II: Energy gap between ground state and first excited state versus  $N$ .

## IV. MAPPING THE SPIN-1 CHAIN TO A SPIN-1/2 CHAIN

For a given value of the state of the spin at site  $n$ , and a given value of  $W_n$ , there are at most two choices for the spin state at site  $n + 1$ . Hence it is clear that the Hilbert space of a given sector can be mapped into the Hilbert space of a spin-1/2 chain, with some states excluded which correspond to infinite energy. However, in general, the corresponding Hamiltonian would have a rather complicated form, with long-ranged interactions. The mapping is easy to construct explicitly in the sector with all  $W_n = +1$ , and the corresponding Hamiltonian has only local interactions. This is what we now proceed to show.

Consider the state  $zzzz \dots$  that belongs to the sector with all  $W_n = +1$ . The only allowed process in this sector is  $zz \rightleftharpoons yx$  [Eqs. (52)]. We may think of this process as a quantum dimer deposition-evaporation model. The  $z$ -spins are treated as empty sites; two empty sites can be changed to being occupied by a dimer  $yx$  by a ‘deposition’ process, and conversely,  $yx$  can ‘evaporate’ and become

$zz$  again. The dimers have a hard-core constraint, and a site cannot be shared by two dimers. The dimers are oriented: the ‘head’  $x$  being to the right of the ‘tail’  $y$ .

This dimer deposition-evaporation model can also be described as a deposition-evaporation of a nearest-neighbor exclusion lattice gas. We just think of the heads as particles, and do not distinguish between the tails and empty sites, except for ensuring that we deposit a particle at a site only if it is empty and both its nearest neighbors are also empty. Then this model is described by the Hamiltonian

$$H_d = -\frac{1}{4} \sum_n (1 - \sigma_{n-1}^z) \sigma_n^x (1 - \sigma_{n+1}^z). \quad (57)$$

We note that this model is different from the dimer deposition-evaporation models studied earlier [37], in that the two ends of the dimer are distinct, and there is no reconstitution. Also, this Hamiltonian does not have an interpretation as the evolution operator of a classical Markov process, as there are no diagonal terms corresponding to probability conservation.

We have introduced a minus sign in the Hamiltonian for later convenience. This does not change the eigenvalue spectrum as the eigenvalues of  $H_d$  occur in pairs  $\pm e_i$ .

## V. VARIATIONAL STUDY OF SECTOR WITH ALL $W_n = 1$

We will now use a variational approach to study the ground state of the Hamiltonian  $H_d$  with periodic boundary conditions. We use the  $z$ -basis, and denote the  $\uparrow$  state at the site  $i$  by an occupied site ( $n_i = 1$ ), and the  $\downarrow$  state by an empty state ( $n_i = 0$ ). Since two adjacent sites cannot be simultaneously occupied, the state space is that of hard-core particles with nearest-neighbor exclusion on a line. A configuration  $\mathbf{C}$  is specified by an  $N$ -bit binary string  $0010010101 \dots$ , which gives the values of all the  $N$  occupation numbers  $n_i$ . We note that in the basis where all the  $n_i$  are diagonal, the Hamiltonian  $H_d$  has all matrix elements non-positive. This implies that the (real) eigenvector corresponding to the lowest energy will have all components of the same sign in this basis.

For the ground state of  $H_d$ , we consider a variational wave function of the form

$$|\psi\rangle = \sum_{\mathbf{C}} \sqrt{\text{Prob}(\mathbf{C})} |\mathbf{C}\rangle, \quad (58)$$

where  $\text{Prob}(\mathbf{C})$  is chosen as the probability of the lattice gas configuration  $\mathbf{C}$  in some classical equilibrium ensemble corresponding to a suitably chosen lattice gas Hamiltonian. Clearly, this trial vector is normalized, with

$$\langle\psi|\psi\rangle = 1. \quad (59)$$

With this choice,  $\text{Prob}(\mathbf{C})$  is also the probability of the configuration  $\mathbf{C}$  in the quantum mechanical variational state  $|\psi\rangle$ .

The simplest choice of the lattice-gas Hamiltonian is that of a classical lattice gas with nearest-neighbor exclusion, and a chemical potential  $\mu$ , with a Hamiltonian given by

$$H_{cl} = +\infty \sum_i n_i n_{i+1} - \mu \sum_i n_i, \quad (60)$$

where we use the convention that  $0 \cdot \infty = 0$ ; hence the first term in Eq. (60) allows states with  $n_i n_{i+1} = 0$  but disallows states with  $n_i n_{i+1} = 1$ . Let us denote  $z = \exp(\beta\mu)$ . It is straightforward to determine various correlation functions in the thermal equilibrium state corresponding to  $H_{cl}$ . The probability of a configuration  $\mathbf{C}$  is given by

$$\text{Prob}(\mathbf{C}) = \exp[-\beta H_{cl}(\mathbf{C})] / \Omega_N(z), \quad (61)$$

where  $\Omega_N(z)$  is the grand partition function for a ring of  $N$  sites.

The grand partition function  $\Omega_N(z)$  can be determined using the standard transfer matrix technique. We find the largest eigenvalue of the  $2 \times 2$  matrix  $\mathbf{T}_2$  given by

$$\mathbf{T}_2 = \begin{bmatrix} 1 & 1 \\ z & 0 \end{bmatrix}. \quad (62)$$

We now calculate  $\langle\psi|H_d|\psi\rangle$ . The matrix element of the  $i$ -th term is clearly zero, unless  $n_{i-1} = n_{i+1} = 0$ . Then the only non-zero matrix element is

$$\langle H_d \rangle / N = -2\sqrt{z} \text{Prob}(000) = \frac{-2}{\sqrt{z}} \text{Prob}(010). \quad (63)$$

Here  $\text{Prob}(000)$  denotes the probability that randomly selected three consecutive sites in the ring will be empty in the classical ensemble, and similar definition for  $\text{Prob}(010)$ . This is easily calculated for the Hamiltonian  $H_{cl}$  in the limit of large  $N$ . We get

$$\text{Prob}(010) = \text{Prob}(1) = \rho. \quad (64)$$

The largest eigenvalue  $\Lambda$  of  $\mathbf{T}_2$  is given by

$$\Lambda = (1 + \sqrt{1 + 4z})/2, \quad (65)$$

and  $\rho$  is the density per site given by  $\rho = z d \log(\Lambda) / dz$ . Extremizing  $\langle H_d \rangle$  with respect to  $z$ , we find that the minimizing value occurs for  $z = 0.405$ , yielding  $\langle H_d \rangle = -0.60057$ . This gives us the variational bound on the ground state energy per site  $E_0$

$$E_0 \leq -0.60057. \quad (66)$$

This energy is somewhat higher than the energy obtained in the previous section (see Fig. 3), indicating that the correlations in the classical Hamiltonian  $H_{cl}$  do not exactly reproduce the correlations in the quantum ground state of  $H_d$ .

We can make a better variational calculation by considering a classical lattice gas with an additional next-nearest-neighbor interaction. The Hamiltonian of this lattice gas is

$$H'_{cl} = +\infty \sum_i n_i n_{i+1} - K \sum_i n_i n_{i+2} - \mu \sum_i n_i. \quad (67)$$

Let us denote  $z = \exp(\beta\mu)$ , and  $u = \exp(\beta K)$ . In this case, the transfer matrix is a  $3 \times 3$  matrix given by

$$\mathbf{T}_3 = \begin{bmatrix} 1 & 0 & 1 \\ z & 0 & zu \\ 0 & 1 & 0 \end{bmatrix}. \quad (68)$$

The probability of the configuration  $\mathbf{C}$  in the equilibrium ensemble is given by

$$\text{Prob}(\mathbf{C}) = \exp[-\beta H'_{cl}(\mathbf{C})] / \Omega_N(z, u), \quad (69)$$

where  $\Omega_N(z, u)$  is the grand partition function for a ring of  $N$  sites. We then get

$$-\langle H_d \rangle / N = 2\text{Prob}(00000)\sqrt{z} + 4\text{Prob}(10000)\sqrt{zu} + 2\text{Prob}(10001)\sqrt{zu^2}, \quad (70)$$

Here  $\text{Prob}(00000)$  is the probability of finding a randomly selected set of five consecutive sites all unoccupied in the equilibrium ensemble corresponding to the Hamiltonian  $H'_{cl}$ . These probabilities are also easily calculated. Treating  $z$  and  $u$  as variational parameters, we find that  $\langle H_d \rangle$  is minimized for  $z = 0.35198$  and  $u = 1.3752$ . For these values one finds that the density is  $\rho = 0.1952$ ,  $\text{Prob}(00000) = 0.28066$ ,  $\text{Prob}(10000) = 0.082804$ , and  $\text{Prob}(10001) = 0.02443$ . These give

$$E_0 \leq -0.60333 \quad (71)$$

which is an improvement over Eq. (66), and quite close to the extrapolated value of  $-0.60356$  obtained from Table I. This may be further improved by taking third-neighbor interactions in the classical Hamiltonian, but this will not be attempted here.

## VI. STUDY OF GROUND STATES IN OTHER SECTORS

We define a more general Hamiltonian

$$H(\lambda) = H_{Kit} + \lambda \sum_n W_n. \quad (72)$$

Since the  $W_n$ 's commute with  $H_{Kit}$ , all the eigenvectors of  $H_{Kit}$  can be chosen to be simultaneous eigenvectors of  $H(\lambda)$ , for all  $\lambda$ . However, if we vary  $\lambda$ , we can get different eigenvectors to have the lowest energy.

Clearly, if  $\lambda$  is large and positive, the ground state will lie in the sector with all  $W_n = -1$ . Conversely, if  $\lambda$  is large and negative, the ground state is the lowest energy

eigenvector in the sector with all  $W_n = +1$ . In both these regions, the gap in the excitation spectrum is of order  $|\lambda|$ . As we vary  $\lambda$  from  $-\infty$  to  $+\infty$ , initially the gap decreases and becomes zero at some value  $\lambda_1^c$ . We then expect a gap to open up again when  $\lambda$  is greater than a second critical point  $\lambda_2^c > \lambda_1^c$ .

### A. Sectors with most $W_n$ 's positive

Since the ground state for  $\lambda = 0$  lies in the sector with all  $W_n = +1$ , we have  $\lambda_1^c > 0$ . In fact, if the lowest excitation energy in the Hamiltonian  $H_{Kit}$  is  $\Delta E$ , we have  $\lambda_1^c = \Delta E/2$ . At this point, the energy required to change a single  $W_n$  from  $+1$  to  $-1$  becomes zero. We now study this sector using the variational techniques of Sec. V and try to estimate the difference between the ground state energy of this sector and the sector with all  $W_n = 1$ .

Without loss of generality, we may assume that in this sector,  $W_N = -1$ , and the rest of the  $W$ 's are  $+1$ . The basis vectors in this sector are of type  $|xU\rangle$ , or  $|Vy\rangle$ , where  $U$  and  $V$  are all possible strings of length  $N-1$  obtainable from the string  $zzz\dots z$  of length  $N-1$ , using the substitution rule  $zz \rightarrow yx$ . Let  $|\psi\rangle$  be the eigenvector corresponding to the lowest eigenvalue of  $H$  in this sector. It is easy to verify that  $\langle xU|H|xU'\rangle$  and  $\langle Vy|H|V'y\rangle$  are negative, for all  $U$  and  $U'$ , and  $V$  and  $V'$ . But,  $\langle Vy|H|xU\rangle$  are positive. This implies that  $\langle xU|\psi\rangle$  and  $\langle xU'|\psi\rangle$  have the same sign for all  $U$  and  $U'$ . Similarly  $\langle Vy|\psi\rangle$  and  $\langle V'y|\psi\rangle$  have the same sign for all  $V$  and  $V'$ . This suggests a variational wave function of the form

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left[ \sum_U \sqrt{\text{Prob}(U)} |xU\rangle - \sum_V \sqrt{\text{Prob}(V)} |Vy\rangle \right]. \quad (73)$$

Here  $\text{Prob}(U)$  and  $\text{Prob}(V)$  are arbitrary functions, satisfying the constraint

$$\sum_U \text{Prob}(U) = \sum_V \text{Prob}(V) = 1. \quad (74)$$

Each configuration  $U$  is in one-to-one correspondence with the configurations of a nearest-neighbor-exclusion lattice gas on a linear chain of length  $(N-2)$ . Define a chain configuration as  $C = \{n_i\}$ . We put  $n_i = 1$  if and only if there is a  $y$  in  $U$  in the position  $i+1$ , otherwise  $n_i = 0$ . Note that the last element of  $U$  cannot be a  $y$ . We specify  $C$  by a binary string of length  $(N-2)$ . To go from  $C$  to  $U$ , we first add a single 0 to the binary string of  $C$  at the right end, and then use the substitution rule  $10 \rightarrow yx$ . The remaining zeros in  $C$  are replaced by  $z$ 's. Similarly, we specify  $V$  also by a binary string of length  $(N-2)$ , with  $x \rightarrow 1$ ,  $y, z \rightarrow 0$ , and as the leftmost element of the resulting string is always a zero, it may be deleted.

As in the previous calculation, we construct a classical Hamiltonian to variationally estimate the parameters



Prob( $C$ ). In this case, there is no translational symmetry, and in general, the lattice gas will have a non-trivial density profile. This is taken into account by making the activities of the lattice gas in the classical Hamiltonian site-dependent. We write

$$H_{cl}^C = +\infty \sum_{i=1}^{N-3} n_i n_{i+1} - \sum_{i=1}^{N-2} \mu_i n_i. \quad (75)$$

The probability of each configuration  $C$  of the lattice gas is then given by

$$\text{Prob}(C) = \exp[-\beta H_{cl}^C(C)] / \Omega_{N-2}(\{z_i\}), \quad (76)$$

with  $z_i = \exp(\beta \mu_i)$ , and  $\Omega_{N-2}(\{z_i\})$  is the grand partition function of the open chain of  $N - 2$  sites.

We note that the matrix  $H$  is unchanged under the space reflection  $i \leftrightarrow N + 1 - i$ , and at the same time exchanging  $x$  and  $y$ . This can be built into our eigenvector by assuming that if  $V$  are strings corresponding to lattice gas configurations  $C$ , we set

$$\text{Prob}(V) = \text{Prob}(U), \quad (77)$$

where  $U$  is the string corresponding the lattice gas configuration  $C^T$ , the transpose of  $C$ .

The rest of the calculation is done as before. By construction, we have

$$\langle \psi_{\text{var}} | \psi_{\text{var}} \rangle = 1. \quad (78)$$

It is straightforward to express  $\langle \psi | H | \psi \rangle$  in terms of the marginal probabilities of the different local configurations of the lattice gas, remembering that there is no translational invariance. For example, we get

$$\langle \psi | S_N^x S_1^y | \psi \rangle = -\text{Prob}_C(n_1 = 0). \quad (79)$$

In the simplest case, we work with only two parameters, and set  $z_1 = z'$ , and  $z_i = z$  for  $i \neq 1$ . We would like to estimate the difference of the ground state energy in this sector and the ground state over all sectors. These energies are of order  $N$ , and to cancel the leading linear  $N$ -dependence, we have to set  $z$  equal to the optimal value  $z^* = 0.4045$  to get the best energy value of Eq. (66). We assume that  $N$  is large, so that only the term in the partition function corresponding to the largest eigenvalue is kept. Extremizing over  $z'$  we obtain  $z' = 0.2537$ , and for this value

$$\langle \psi_{\text{var}} | H | \psi_{\text{var}} \rangle = -0.6005N + 0.1875. \quad (80)$$

This implies the following bound on the lowest eigenvalue in this sector

$$E'_0 \leq NE_0 + \Delta. \quad (81)$$

with  $\Delta = 0.1875$  providing an estimate of the energy gap between the ground state and the first excited state of the Hamiltonian. This estimate can be improved by

adding more parameters in the variational wave function, or equivalently in the classical lattice gas Hamiltonian. A two parameter wave function would have  $z'$  and  $z''$  at the two opposite ends. Extremizing with respect to these parameters we find the energy gap to be 0.1642 with  $z' = 0.2537$  and  $z'' = 0.6670$ . A four parameter wave function would have fugacities  $z_1, z_2, z_{N-3}$  and  $z_{N-2}$  adjustable, and the rest of the  $z_i$ 's set equal to  $z^*$ . Table III shows the improvement in the value of the energy gap with the number of parameters used.

We thus obtain a variational estimate of the energy gap of the first excited state from the ground state energy. This matches quite well with the numerical estimates obtained in the previous section.

| Number of parameters | $\Delta$ |
|----------------------|----------|
| 1                    | 0.18751  |
| 2                    | 0.16419  |
| 4                    | 0.15845  |
| 6                    | 0.15642  |
| 8                    | 0.15578  |
| 10                   | 0.15556  |

TABLE III: Estimate of the energy gap with the number of parameters used.

It is straightforward to extend this treatment to sectors with two or more  $W_n$ 's negative. There is an energy  $\Delta$  required to create a single negative  $W_n$ . Thus  $\lambda_1^c = \Delta/2$ . If two defects are spaced far apart, the energy required to create two defects will be nearly  $2\Delta$ , with the correction term decreasing exponentially with the distance between the defects. For  $n$  defects, the energy would be minimized if the defects are equally spaced. Thus the distance between the defects is  $N/n$ , and the energy cost of creating  $n$  defects  $\Delta E(n)$  in  $H(\lambda)$ , for small  $n$ , is well approximated by

$$\Delta E(n) \approx -2n\lambda + n\Delta + nA \exp(-BN/n), \quad (82)$$

where  $A$  and  $B$  are some constants. This then implies that for  $\lambda = \lambda_1^c + \epsilon$ , the density of defects in the true ground state of  $H(\lambda)$  will vary as  $1/|\log \epsilon|$ .

## B. Sectors with most $W_n$ 's negative

We now discuss the behavior of the ground state energy near the critical point  $\lambda_2^c$ . This depends on the behavior of the ground state energy in sectors in which only a few of the  $W_n$ 's are  $+1$ .

For a ring of  $N$  sites, the sector with all  $W_n = -1$  contains only two states,  $xxxxx \dots$  and  $yyyyyy \dots$ . The two are degenerate, with eigenvalue equal to  $-\lambda N$ .

Now consider the sector with only one  $W_n = +1$ , say  $W_0 = +1$ . Consider the state  $\psi_1 = |zxxxx \dots\rangle$  in this sector. From Eqs. (53), under  $H_{Kit}$ , we have  $zx \rightleftharpoons yz$ ,

and this state can make a transition only to the state  $\psi_2 = |yzxxx \dots\rangle$ . And  $\psi_2$  can return to  $\psi_1$  or go to  $\psi_3 = |yyzxx \dots\rangle$ . Thus, the dynamics may be considered as the dynamics of a particle  $z$ , which can hop to a nearest neighbor under the action of the Hamiltonian. There is a string of  $y$ 's connecting the current position of the particle to the leftmost allowed position which is  $n = 1$ . This string can become longer, or shorter, as the particle moves, with no energy cost. When the  $z$ -spin is at the site  $N$ , it cannot move further to the right. The ground state energy  $E_{1\text{-sector}}^g$  if this sector is seen to be the same as that of a particle with nearest-neighbor hopping, confined to move in the space  $1 \leq x \leq N$ . It is thus given by

$$E_{1\text{-sector}}^g = -(N-2)\lambda - 2J \cos\left(\frac{\pi}{N+1}\right). \quad (83)$$

Thus, we see that for large  $N$ , the state with all  $W_n$ 's equal to  $+1$  is no longer the ground state for  $\lambda < J$ .

We now consider a sector with exactly two of the  $W_n$ 's equal to  $+1$ , and the rest negative. Let us start with the state  $|zxxx \dots zxxx \dots\rangle$ , where the spins at two sites  $i = 1$  and  $i = m+1 \leq N$  are in the state  $z$  (these states will be referred to as  $z$ -spins in the following). This corresponds to  $W_N = W_m = +1$ . Then, under the action of  $H(\lambda)$ , this state mixes with other states where the positions of the  $z$ -spins can change; the general state in this sector may be labeled by the positions of the  $z$ -spins,  $r_1$  and  $r_2$ . We will write the vector as  $|r_1, r_2\rangle$ , where  $1 \leq r_1 \leq m < r_2 \leq N$ . Then, for  $1 < r_1 < m$  and  $m+1 < r_2 < N$ , we get

$$\begin{aligned} H_{Kit}|r_1, r_2\rangle = & -|r_1, r_2+1\rangle - |r_1+1, r_2\rangle \\ & -|r_1, r_2-1\rangle - |r_1-1, r_2\rangle. \end{aligned} \quad (84)$$

If the first  $z$ -spin is at  $m$  and the second is not at  $m+1$ , the first spin cannot move to  $m+1$ , as that site would be in spin state  $y$ , and the state  $zy$  cannot change [Eqs. (52)]. Similarly, if  $r_2 = N$ , and  $r_1 \neq 1$ , then the second spin cannot move to the right. However, if the two  $z$ -spins are adjacent, then they can change to a state  $zz \rightleftharpoons yx$  [Eqs. (52)]. But from the state  $yx$  the state can only return to  $zz$ .

If we disallow the transitions to state  $yx$ , the  $z$ -spins act as independent particles moving in two disjoint regions of space,  $1 \leq r_1 \leq m$  and  $m+1 \leq r_2 \leq N$ . In this case, the minimum energy of this system is just the sum of the energies of two particles. This energy is an upper bound on the true ground state energy of this system. Thus, we find that the ground state energy in this sector,  $E_{2\text{-sector}}^g$ , has the upper bound

$$\begin{aligned} E_{2\text{-sector}}^g \leq & -2J \cos\left(\frac{\pi}{m+1}\right) - 2J \cos\left(\frac{\pi}{N-m+1}\right) \\ & -\lambda(N-4). \end{aligned} \quad (85)$$

Next, suppose that the state with the  $m$ -th site in the  $y$ -state and the  $(m+1)$ -th in the  $x$ -state is called the state  $r_1 = m+1, r_2 = 1$ , and a similar definition for the other end. Then the range of  $r_2$  is at most  $m+1$ , and

the range of  $r_2$  is at most  $l - m + 1$ . By excluding some states (here  $r_1 = m+1, r_2 \neq r_1$ ), the kinetic energy can only increase, and hence we have

$$\begin{aligned} E_{2\text{-sector}}^g \geq & -2J \cos\left(\frac{\pi}{m+2}\right) - 2J \cos\left(\frac{\pi}{N-m+2}\right) \\ & -\lambda(N-4). \end{aligned} \quad (86)$$

For  $N, m \gg 1$ , these bounds can be expanded in powers of  $1/m$ , and have the same leading order correction. Also, the minimum energy corresponds to equally spaced defects, with  $m = N/2$ .

We can easily extend the discussion to sectors with three, four or more  $W_n$ 's equal to  $+1$ . In case the lengths of the intervals between the positive  $W_n$ 's are  $m_1, m_2, m_3, \dots, m_r$ , the bounds on the lowest energy in this sector  $E_{r\text{-sector}}^g$  become

$$\begin{aligned} -2J \sum_{i=1}^r \cos\left(\frac{\pi}{m_i+2}\right) - \lambda(N-2r) & \leq E_{r\text{-sector}}^g \\ & \leq -2J \sum_{i=1}^r \cos\left(\frac{\pi}{m_i+1}\right) - \lambda(N-2r). \end{aligned} \quad (87)$$

Thus, we see that for  $\lambda > J$ , the ground state belongs to the sector with all  $W_n$ 's equal to  $-1$ . If  $\lambda = J(1 - \epsilon)$ , the ground state will be in the sector with  $n$  equispaced bonds with  $W_n = +1$ , where the spacing  $\ell$  between them  $\approx N/n$  is given by  $\epsilon^{-1/2}$ . The minimum energy per site of  $H(\lambda)$  for  $\lambda = J(1 - \epsilon)$  varies as  $\epsilon^{3/2}$  for small  $\epsilon$ . Equivalently, if we restrict ourselves to sectors with only a fraction  $\epsilon$  of  $W_n$ 's having the value  $+1$ , the minimum energy per site varies as  $-\epsilon^{3/2}$ . This is equivalent to the statement that for  $H_{Kit}$  corresponding to  $\lambda = 0$ , in the sector with the fractional number of positive  $W_n$ 's being equal to  $\Delta$ , the minimum energy per site varies as  $\Delta^{3/2}$ .

## VII. DISCUSSION

In this paper, we first analyzed the symmetries of a spin- $S$  Kitaev chain. We found a  $\mathbb{Z}_2$  invariant,  $W_n$ , associated with every link  $(n, n+1)$ , namely,  $N$  invariants for the model defined on a ring with  $N$  sites. For integer  $S$ , these invariants commute with each other and the Hamiltonian. The Hilbert space can therefore be split into  $2^N$  sectors, where the Hamiltonian is block diagonal. For half-odd integer  $S$ ,  $W_n$  anti-commutes with  $W_{n\pm 1}$  and commutes with the rest. We showed that this implies that all the eigenstates of the half-odd-integer spin models are  $2^{N/2}$ -fold degenerate, thus showing a qualitative difference between the integer and half-odd-integer models. We have developed a formalism to compute the dimensions of the invariant sectors. We showed that the dimension of most of the sectors can be calculated in terms of products of  $2 \times 2$  matrices  $\mathbb{T}_+$  and  $\mathbb{T}_-$ . For  $S = 1$  the quantum dimension of the sector with all  $W_n = 1$  is the golden ratio,  $(1 + \sqrt{5})/2$ . For  $S \rightarrow \infty$ , the quantum dimension tends to  $S + 1/2$  in both the  $W_n = 1$  and the  $W_n = -1$  sectors.

We have then studied the spin-1 case in detail. We have found that the ground state lies in a sector which can be mapped to a quantum lattice gas model with nearest-neighbor exclusion. We developed a variational wave function that relates the quantum mechanical averages to the correlation functions of a classical lattice gas with nearest-neighbor exclusion. We considered a more general Hamiltonian with a term proportional to the sum of the conserved quantities, and showed that as a function of the coupling constant  $\lambda$ , this would show gapless excitations in the range  $\lambda_1^c \leq \lambda \leq \lambda_2^c$ . We extended our variational calculation to study how the ground state energy and the defect density would vary near the two critical points  $\lambda_1^c$  and  $\lambda_2^c$ . At  $\lambda = \lambda_1^c$ , Eq. (82) implies that the energy of the lowest excited state in a system of length  $L$  goes as  $E \sim \exp(-BL)$ , corresponding to a state in which one  $W_n = -1$  while all the other  $W_n = 1$ . By the usual scaling arguments, the gap to the first excited state goes as  $1/L^z$ , where  $z$  is the dynamical critical exponent. We therefore conclude that  $z = \infty$ . At  $\lambda = \lambda_2^c$ , the low-energy excitations form a low-density gas of hard-core particles. In one dimension, this can be mapped to a system of non-interacting spinless fermions with a non-relativistic spectrum  $E \sim k^2$ . Hence in a system of size  $L$ , the gap to the lowest energy states goes as  $1/L^2$  corresponding to  $k \sim 1/L$ ; thus  $z = 2$ . It would be interesting to find the value of  $z$  in the critical region  $\lambda_1^c < \lambda < \lambda_2^c$ .

Finally, we note that there is another interesting one-dimensional spin model called the golden or Fibonacci chain [38, 39], for which the number of states on a ring of size  $N$  is the same as that of the spin-1 Kitaev chain in the sector with all  $W_n = 1$ . The Hamiltonian for this model is

$$H_{GC} = \sum_i ((n_{i+1} + n_{i-1} - 1) - n_{i-1}n_{i+1}(\gamma^{-3/2}\sigma_i^x + \gamma^{-3}n_i + 1 + \gamma^2)), \quad (88)$$

where  $n_i = (1 - \sigma_i^z)/2$ . It has been shown [38, 39] that this model is critical. Its long-range correlations are de-

scribed by a  $SU(2)$  level 3 Wess-Zumino-Witten model, which is a conformally invariant field theory with central charge equal to  $7/10$ . The Hamiltonian in Eq. (88) differs from the spin-1 Kitaev chain in the  $W_n = 1$  sector by terms which are products of the  $n_i$  operators. We have shown that the spin-1 Kitaev chain is gapped. Thus these terms correspond to some relevant operators which take the golden chain Hamiltonian away from criticality.

We can show that it is possible to add multi-spin terms to the minimal Kitaev chain which reduce to the extra terms in the  $W_n = 1$  sector. We need to add products of the  $n_i$  operators to the minimal Kitaev chain to obtain the golden chain in the sector with all  $W_n = 1$ . The basis states  $|\uparrow\rangle, |\downarrow\rangle$  that we use in Sec. IV are eigenstates of the  $n_i$  operators with eigenvalues 1 and 0 respectively. The  $|\uparrow\rangle$  state represents a state with the head, namely  $|x\rangle$ . The  $|\downarrow\rangle$  state represents either an empty site,  $|z\rangle$ , or a tail,  $|y\rangle$ . It is clear from Eqs. (47) and (48) that the operator  $P^x \equiv (1 + \Sigma^x)/2$  has eigenvalues 1 for  $|x\rangle$  and 0 for  $|y\rangle$  and  $|z\rangle$ . Since all the  $\Sigma$  matrices commute for integer  $S$ , they commute with the invariants and are block diagonal within the invariant sectors. Thus, the Hamiltonian,

$$H_{KGC} = \gamma^{-3/2}H_{KC} - \sum_i (1 - P_{i+1}^x - P_{i-1}^x + \gamma^2 P_{i-1}^x P_{i+1}^x + \gamma^{-3} P_{i-1}^x P_i^x P_{i+1}^x), \quad (89)$$

when restricted to the  $W_n = 1$  sector, is exactly the golden chain Hamiltonian discussed by Feiguin *et al.* and others [38, 39]. We have thus constructed a realization of the golden chain model as a spin-1 chain.

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