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Exact results of the Kitaev model on a hexagonal lattice: spin states, string and brane correlators, and anyonic excitations

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Abstract

In this work, we illustrate how a Jordan–Wigner transformation combined with symmetry considerations enables a direct solution of Kitaev's model on the honeycomb lattice. We (i) express the p-wave type fermionic ground states of this system in terms of the original spins, (ii) adduce that symmetry alone dictates the existence of string and planar *brane* type correlators and their composites, (iii) compute the value of such non-local correlators by employing the Jordan–Wigner transformation, (iv) affirm that the spectrum is inconsequential to the existence of topological quantum order and that such information is encoded in the states themselves and (v) express the local symmetries of Kitaev's model and the anyonic character of the excitations in terms of fermions.

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1. Introduction

Topological quantum order (TQO) [1, 2] is a new paradigm that lies beyond the realm of Landau's theory [3, 4] of local order parameters. TQO is intuitively associated with insensitivity to *local* perturbations: the order is *topological*. As such, TQO cannot be described by *local* order parameters. A quintessential example of a system with TQO is Kitaev's model on the honeycomb lattice [5–7]. In this paper, we will study this model. Our *new central results* are (a) an explicit form for the ground states in real space which extends and complements the works of [6, 7] as well as (b) our finding of non-local correlations (two-dimensional *string* or *brane* type correlators) in this system. We further show how the (c) known anyonic excitations of Kitaev's model can be examined anew by using a direct Jordan–Wigner transformation. Beyond providing a direct solution which highlights certain previously overlooked aspects, our results will flesh out some of the more general ideas [8, 9] regarding the general character of TQO.

2. Outline

This paper is organized as follows. In section 3, we review the fermionization of the Kitaev model on a hexagonal lattice [9, 10]. The original model of spins on a hexagonal lattice is mapped to a model of p-wave BCS model with a site-dependent chemical potential for spinless fermions on a square lattice. In section 4, we discuss the fermionic representation of symmetries embodied in the model. It is shown that the local conserved quantities on the plaquettes studied by Kitaev [6] are equivalent to the conserved bond quantities in the fermionic representation, up to a gauge fixing. In section 5, the ground-state configuration, which is vortex free in spin representation and with a uniform chemical potential in fermionic representation, is exactly solved in fermionic representation. The spin basis form of the ground state is also studied. It is shown that the ground state can be written as a projection of a given reference state over a sector of the Hilbert space that has a chosen set of topological numbers which are similar to, yet slightly more complicated than, other systems which exhibit TQO such as the Rokhsar–Kivelson dimer model [11] and the Kitaev toric code model [2]. The phase diagram and Bogliubov excitations are also obtained. In section 6, we show how the known results about the anyonic vortex excitation in the gapped state can be easily studied in the fermionic representation. In section 7, a symmetry argument is put forward concerning the vanishing correlation functions, which is also recently derived anew by a Majorana fermionization construction [12]. We also show that string correlators naturally appear in Kitaev's model. A brief summary in section 8 concludes this work. In the appendices, we provide technical details concerning the determination of the ground state and review Elitzur's theorem.

3. Fermionization

We begin with a fermionization of the Kitaev model on the hexagonal lattice [6, 7] which is defined by the following $S = 1/2$ Hamiltonian:

$$H = -J_x \sum_{x\text{-bonds}} \sigma^x_R \sigma^x_{R'} - J_y \sum_{y\text{-bonds}} \sigma^y_R \sigma^y_{R'} - J_z \sum_{z\text{-bonds}} \sigma^z_R \sigma^z_{R'}, \tag{1}$$

with R and R' the lattice sites. This system can be fermionized by a Jordan–Wigner transformation [9, 10]. This one-dimensional fermionization is made vivid by deforming the hexagonal lattice into a 'brick-wall lattice' which is topologically equivalent to it on which we may perform a one-dimensional Jordan–Wigner transformation. The schematics are shown in figure 1. In the upcoming, we will mark all sites by 'white' or 'black' (w/b) in order to denote to which sublattice they belong to. The distance between the two nearest-neighboring sites on this lattice will be set to unity.

Throughout, we will consider the system with open boundary conditions unless stated otherwise. The diagonal directions $\hat{e}_x$ and $\hat{e}_y$ shown in figure 1 will be of paramount importance in our final solution. Let us denote by (i, j) the Cartesian coordinates of each site R on the lattice of figure 1. Let us next consider the Jordan–Wigner transformation defined by a simple one-dimensional contour which threads the entire lattice (see figure 2):

$$\sigma^+_{ij} = 2 \left[\prod_{j'<j} \prod_{i'} \sigma^z_{i'j'} \right] \left[\prod_{i'<i} \sigma^z_{i'j} \right] c^\dagger_{ij} \tag{2}$$

$$\sigma^z_{ij} = 2c^\dagger_{ij} c_{ij} - 1. \tag{3}$$

This path goes through each lattice site exactly once as shown in figure 2. In equation (2), $\sigma^+ = \sigma_x + \mathrm{i}\sigma^y$ is twice the spin raising operator at a given site, hence the factor of 2.

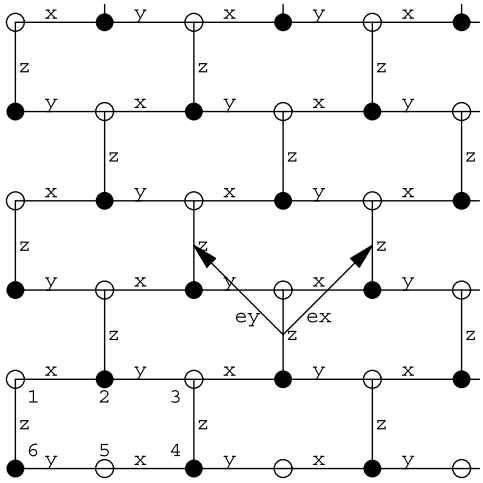

Figure 1. Deformed hexagonal lattice and three types of bonds.

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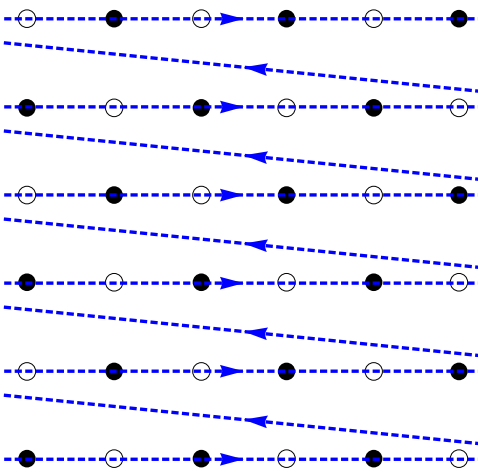

Figure 2. Schematics of the contour for the Jordan–Wigner transformation that we employ in the deformed hexagonal lattice—see text and equation (3) in particular.

The Kitaev model of equation (1) now becomes

$$H = J_x \sum_{x\text{-bonds}} (c^\dagger - c)_w (c^\dagger + c)_b - J_y \sum_{y\text{-bonds}} (c^\dagger + c)_b (c^\dagger - c)_w - J_z \sum_{z\text{-bonds}} (2c^\dagger c - 1)_b (2c^\dagger c - 1)_w. \tag{4}$$

Henceforth, the subscripts w and b, respectively, denote the white and black sites of a bond as illustrated in figure 1.

Let us next introduce the Majorana fermions

$$A_w = (c - c^\dagger)_w / \mathrm{i}, \qquad B_w = (c + c^\dagger)_w \tag{5}$$

for the white sites, and

$$B_b = (c - c^\dagger)_b / \mathrm{i}, \qquad A_b = (c + c^\dagger)_b \tag{6}$$

for the black sites. With all of these transformations in tow, the Hamiltonian now reads

$$H = -\mathrm{i} \left[\sum_{x\text{-bonds}} J_x A_w A_b - \sum_{y\text{-bonds}} J_y A_b A_w \right] - J_z \sum_{z\text{-bonds}} J_z (BA)_b (BA)_w. \tag{7}$$

It is easy to see that BB along the z-bond is a conserved quantity [10]. Thus, the Z_2 operator

$$\alpha_r = \mathrm{i} B_b B_w, \tag{8}$$

with r the coordinate of the midpoint of the bond connecting the black and red sites, is fixed for each vertical bond. The Hamiltonian of equation (1) now reads

$$H(\{\alpha\}) = -\mathrm{i} \left[\sum_{x\text{-bonds}} J_x A_w A_b - \sum_{y\text{-bonds}} J_y A_b A_w \right] - \mathrm{i} J_z \sum_{z\text{-bonds}} \alpha_r A_b A_w. \tag{9}$$

Here, r denote the centers of the vertical bonds. In section 4, We will show that $\{\alpha_r\}$ are intimately related to the local symmetries present in Kitaev's model of equation (1). This

identification, combined with reflection positivity arguments [6], will allow us to infer that, up to ($d = 1$ [13]) symmetry operations, $\alpha_r = 1$ for all r. The ground state does not contain any 'vortices' which are marked by one-dimensional in the Ising variables $\{\alpha_r\}$ along a row. Similar reflection positivity arguments regarding the absence of vortices in other systems and a bound on the energy penalties that they entail are, e.g., given in [14]. This, in turn, will allow us to explicitly diagonalize the Hamiltonian.

4. Fermionic representation of local symmetries

As shown by Kitaev [6], the Hamiltonian of equation (1) has one conserved quantity for each plaquette (or hexagon) h,

$$I_h = \sigma^y_{1w}\sigma^z_{2b}\sigma^x_{3w}\sigma^y_{4b}\sigma^z_{5w}\sigma^x_{6b}. \tag{10}$$

Here, 1–6 denote the sites of a given plaquette, as illustrated in the plaquette of the lower corner in figure 1. In the subscripts, we also label the (w/b) sublattices of the sites. The conserved quantity I_h on the plaquette is equivalent to the bond conserved quantity α defined in the previous section, up to a gauge fixing as we shall show below. This can be shown by fermionizing I_h using the transformation we introduced in the previous section. Let us first fermionize the product of first three spins:

$$\begin{aligned}\sigma^y_{1w}\sigma^z_{2b}\sigma^x_{3w} &= \frac{1}{\mathrm{i}}(c^\dagger - c)_{1w}\sigma^z_{2b}\sigma^z_{1w}\sigma^z_{2b}(c^\dagger + c)_{3w}\\ &= \mathrm{i}(c^\dagger + c)_{1w}(c^\dagger + c)_{3w}\\ &= \mathrm{i}B_{1w}B_{3w}.\end{aligned} \tag{11}$$

Similarly,

$$\sigma^x_{6b}\sigma^z_{5w}\sigma^y_{4b} = \mathrm{i}B_{4b}B_{6b}. \tag{12}$$

Therefore,

$$I_h = \alpha_{34}\alpha_{16}. \tag{13}$$

This model has an extra degeneracy that links difference sectors parameterized by different sets of α's. The vortex (or anyon) variables are the product of two consecutive Ising bond variables. In other words, anyons (I_h) are none other than domain walls in the Ising variables ($\{\alpha_r\}$) that our system contains. Inverting all of the values of α_r for all sites r which lie along a horizontal row leaves the system unchanged. Physically, effecting the transformation $\alpha_r \to -\alpha_r$ for all bonds r along a row does not change the vorticity content of the system: all domain walls along the chain remain invariant (and as we show so does the spectrum). In the notation of [8, 13], this corresponds to a $d = 1$ dimensional operator (as it involves spin operators on a ($d = 1$ dimensional) line). For simplicity, let us divide α into different subsets: $\{\alpha\} = \cup_i[\alpha]_i$. Here, $[\alpha]_i$ denotes the set of bonds that are connected to white sites of the ith horizontal line of the brick-wall lattice. We next explicitly write down these $d = 1$ symmetry operators in both their fermionic and original spin language form. Towards this end, we construct the unitary operator U^w_i

$$U^w_i = \prod_{j\geqslant i}\prod_{n\in j} A_n. \tag{14}$$

In equation (14), n is a site index. We note that U^w_i effectively reverses the sign of $[\alpha]_i$ while leaving others untouched

$$\begin{aligned}&\left(U^w_i\right)^\dagger H(\ldots, [\alpha]_{i-1}, [\alpha]_i, [\alpha]_{i+1}, \ldots)\left(U^w_i\right)\\ &\qquad = H(\ldots, [\alpha]_{i-1}, -[\alpha]_i, [\alpha]_{i+1}, \ldots).\end{aligned} \tag{15}$$

Therefore, we have extra freedom to fix one α in each subset $[\alpha]_i$. This degree of freedom is closely related to the string-like conserved quantity in the original spin model, namely,

$$P_j = \prod_i \sigma_{ij}^z, \tag{16}$$

which rotates all spins on the jth line by 180° around z. Under the gauge fixing in which one α is fixed to +1 in each $[\alpha]_i$, the set of Kitaev conserved quantities $\{I_h\}$ is equivalent to $\{\alpha\}$.

5. Ground state

5.1. Diagonalization

Armed with a physical meaning of the bond variables α from section 4, we now proceed to solve the problem posed by equation (7) and diagonalize the problem.

It is interesting to introduce a fermion on the z-bond

$$d = (A_w + \mathrm{i}A_b)/2, \qquad d^\dagger = (A_w - \mathrm{i}A_b)/2, \tag{17}$$

where A_w and A_b are, respectively, the Majorana fermions on the white and black sites of a given z-bond. We thus have a model for fermions on a square lattice with a site-dependent chemical potential

$$H = J_x \sum_r \left(d_r^\dagger + d_r\right)\left(d_{r+\hat{e}_x}^\dagger - d_{r+\hat{e}_x}\right) + J_y \sum_r \left(d_r^\dagger + d_r\right)\left(d_{r+\hat{e}_y}^\dagger - d_{r+\hat{e}_y}\right) + J_z \sum_r \alpha_r \left(2d_r^\dagger d_r - 1\right). \tag{18}$$

The unit vector $\hat{e}_y$ connects two z-bonds and crosses a y-bond, see figure 1. A similar definition holds for $\hat{e}_x$. Note that

$$[\alpha_r, d_r] = \left[\alpha_r, d_r^\dagger\right] = 0. \tag{19}$$

For sufficiently large systems, the ground-state configurations are bulk vortex-free configurations [6] in which $I_h = 1$ for all plaquettes (hexagons) h. The ground state of the fermionic problem of equation (18) has $\alpha_r = 1$ everywhere (and all sectors of $\{\alpha_r\}$ related to it by the $d = 1$ operation of equations (14) and (16)) which corresponds to $I_h = 1$ for all plaquettes h. As shown in figure 3, reversing I_h to $I_h = -1$ leads to an inversion of the chemical potentials $\{\alpha_r\}$ along a horizontal string.

The exact solution for ground state is now easy to obtain for the bulk system by a Fourier transformation. Up to innocuous additive constants, the Hamiltonian of the vortex-free configuration now reads

$$H_g = \sum_q \left[\epsilon_q d_q^\dagger d_q + \mathrm{i}\frac{\Delta_q}{2}\left(d_q^\dagger d_{-q}^\dagger + \mathrm{H.c.}\right)\right], \tag{20}$$

where

$$\epsilon_q = 2J_z - 2J_x \cos q_x - 2J_y \cos q_y, \qquad \Delta_q = 2J_x \sin q_x + 2J_y \sin q_y. \tag{21}$$

The fermionized Hamiltonian (18) describes a p-wave type BCS pairing model with a site-dependent chemical potential. After a Bogliubov transformation, this Hamiltonian can be diagonalized and the quasiparticle excitation is

$$E_q = \sqrt{\epsilon_q^2 + \Delta_q^2}. \tag{22}$$

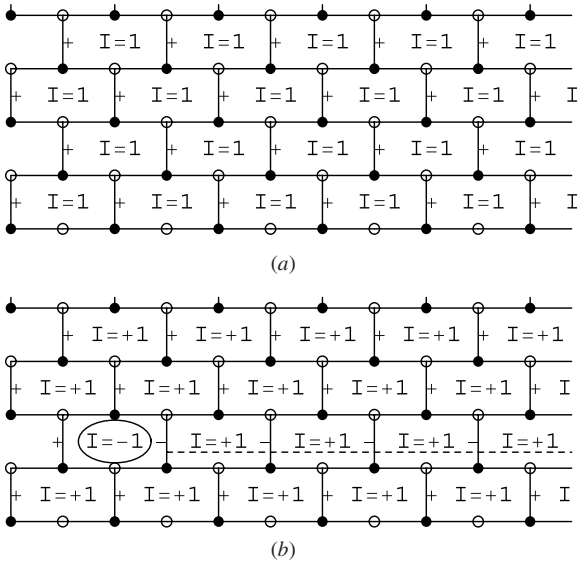

Figure 3. (*a*) Vortex-free configuration. (*b*) Reversing I in a plaquette corresponds to flip the chemical potential along a string.

5.2. *Spectrum*

The energy spectrum, in the low-energy vortex-less sector $\alpha_r = 1$ (and all sectors of $\{\alpha_r\}$ related to it by the $d = 1$ operation of equations (14) and (16)), which we found to be given by equations (21) and (22) obviously does not encode information about the topological nature of Kitaev's model. The equivalence of the lowest eigenvalues of the Hamiltonians in both (i) the simple BCS-type problem given by equations (21) and (22) and (ii) the Kitaev model of equation (1) vividly illustrates the maxim that the states themselves in a particular (operator language) representation and not their energies which determine whether or not the TQO exists [8, 9]. In other words, the same Hamiltonian in different representations which are related to one another by unitary transformations and thus preserve the same set of eigenvalues (the energy spectrum) [8] can describe both topologically quantum-ordered systems (such as Kitaev's model) or systems with no topological order [8, 9]. In the current context, these mappings are the Jordan–Wigner transformations that we apply [9].

Let us now proceed to study when the spectrum of equations (21) and (22) describes a system with a spectral gap between the ground and the next excited states and delineate these boundaries between the gapped and gapless phases. Towards this end (see figure 4), we study the nominal solution to $E_q = 0$ which is

$$q_x = \pm \arccos\left[\frac{J_x^2 + J_z^2 - J_y^2}{2J_xJ_z}\right], \qquad q_y = \pm \arccos\left[\frac{J_y^2 + J_z^2 - J_x^2}{2J_yJ_z}\right]. \tag{23}$$

This solution makes sense only when the conditions

$$-2|J_y||J_z| \leqslant J_y^2 + J_z^2 - J_x^2 \leqslant 2|J_y||J_z|, \tag{24}$$

$$-2|J_x||J_z| \leqslant J_x^2 + J_z^2 - J_y^2 \leqslant 2|J_x||J_z| \tag{25}$$

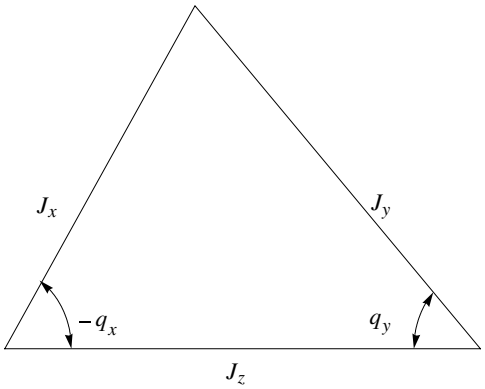

Figure 4. A geometric interpretation of equations (21) for the existence of gapless excitations. The two conditions $\epsilon_q = \Delta_q = 0$ imply that $q_{x,y}$ can be regarded as angles in the triangle formed by $\{J_x, J_y, J_z\}$ as shown. The law of cosines gives equations (23). This plot immediately leads to the triangle inequality condition of equation (28). When the triangle inequality is violated (the gapped phase), $q_{x,y}$ are imaginary and lead to a finite correlation length as we will discuss later (equation (68)).

are satisfied simultaneously. These inequalities can be easily solved to obtain the condition for gapless excitations

$$|J_x| \leqslant |J_y| + |J_z|, \tag{26}$$

$$|J_y| \leqslant |J_x| + |J_z|, \tag{27}$$

$$|J_z| \leqslant |J_x| + |J_z|. \tag{28}$$

This result is in agreement with Kitaev's original solution and Pachos' analysis [6, 7]. We can now view $q_{x,y}$ as (up to an inversion $q_a \to -q_a$ for one of the components of $\vec{q}$) as the angles in the triangle formed by the couplings J_x, J_y and J_z—see figure 4. Equation (23) is the law of cosines in this triangle which automatically satisfies $\Delta_q = \epsilon_q = 0$ of equation (21) and consequently has $E_q = 0$. It is also interesting to note that the cyclic symmetry between J_x, J_y, J_z is explicitly restored in the ground-state solution although its explicitness is lost in the fermionized model.

Next, we briefly remark on not only the low-energy spectrum of pertinence to the zero-temperature problem, but rather examine the entire spectrum of the theory. After tracing over the fermionic degrees of freedom present in equation (18), we obtain an effective two-dimensional Ising-type Hamiltonian (in $\{\alpha_r\}$) with long-range interactions. The full spectrum of this long-range Ising-type Hamiltonian is identical to that of Kitaev's model.

5.3. Real space form of the ground states

The BCS-type ground state corresponding to equation (22) is

$$|g\rangle = \prod_k \left(u_k + v_k d_k^\dagger d_{-k}^\dagger\right)|0\rangle, \tag{29}$$

where

$$|v_k|^2 = \frac{1}{2}\left[1 - \frac{\epsilon_k}{E_k}\right], \qquad |u_k|^2 = \frac{1}{2}\left[1 + \frac{\epsilon_k}{E_k}\right]. \tag{30}$$

Let us now invert the transformations that we have performed until now (Jordan–Wigner and others) in order to express the fermionic operators and the fermionic vacuum state in terms of the original spin degrees of freedom. In what follows, we will, when needed, keep explicit track of the (w/b) sublattices of each of the sites of each vertical bond whose center is at $\vec{r}$. Undoing all of the transformations that we employed thus far, we have

$$d_k^\dagger = -\frac{1}{2}\sum_{r_w}\left[\sigma_{r_w}^y\left(\prod_{r'<r_w}\sigma_{r'}^z\right) - \mathrm{i}\sigma_{r_b}^x\left(\prod_{r'<r_b}\sigma_{r'}^z\right)\right]\mathrm{e}^{-\mathrm{i}\vec{k}\cdot(\vec{r}_w-\frac{1}{2}\hat{e}_z)}. \tag{31}$$

(For a definition of $\hat{e}_z$, see figure 1.) The product $\prod_{r'<r_w}$ corresponds to the product of all lattice sites $\vec{r}'$ which appear before r_w on the Jordan–Wigner contour of equation (3) which traverses all sites of the two-dimensional lattice. A similar definition applies to $\prod_{r'<r_b}$: it is the product over all lattice sites which appear before r_b in the Jordan–Wigner product.

In the spin basis, a fermionic vacuum corresponds to

$$|0\rangle = \mathcal{N}\left(\prod_{r_w}\left[\frac{1}{2}(1+\mathcal{B}_{r_w})\right]\right)\left(\prod_h\left[\frac{1}{2}(1+I_h)\right]\right)\left(\prod_j\left[\frac{1}{2}(1+\overline{\alpha}_{r_{2w}^*})\right]\right)|\phi\rangle. \tag{32}$$

Here, the product over h is that over all elementary hexagons, $|\phi\rangle$ is an arbitrary reference state, e.g., in the σ^z basis, we may choose it to be the fully polarized state $|\phi\rangle = |\uparrow\uparrow\cdots\uparrow\rangle$, the operator

$$\mathcal{B}_{r_w} \equiv -\sigma_{r_w}^x\sigma_{r_w+1}^z\cdots\sigma_{r_b-1}^z\sigma_{r_b}^x \tag{33}$$

extends over all sites lying between (and including) r_w and r_b as labeled by the one-dimensional Jordan–Wigner contour that connects r_w with r_b, $\mathcal{N}$ is a normalization factor and the hexagonal operator I_h is as given by equation (10). Similarly, inverting the fermionization carried earlier, we find that

$$\overline{\alpha}_{r_w} = \left(\prod_{1<r_w}\sigma_1^z\right)\left[-\sigma_{r_w}^x + \left(\prod_{r_w\leqslant 1'<r_b}\sigma_{1'}^z\right)\left(-\mathrm{i}\sigma_{r_b}^y\right)\right] \tag{34}$$

is the spin representation of the operator α_r of equation (8). Equation (34) defines an operator $\overline{\alpha}_{r_w}$ for any white lattice site r_w. In the last product in equation (32), we have a product of $\frac{1}{2}(1+\alpha_{r_w})$ over one lattice site r_w in every row j. The symbol r_{jw}^* denotes the first leftmost white lattice site r_w in the jth row. In combination with equation (13) (valid for any plaquette), the conditions $\alpha_{r_{jw}^*} = 1$ and $I_h = 1$ ensure that $\alpha_r = 1$ for all r. A derivation of equations (32) and (33) is given in the appendix. It is noteworthy that

$$\left[I_h, \mathcal{B}_{r_w}\right] = [I_h, I_{h'}] = \left[\mathcal{B}_{r_w}, \mathcal{B}_{r_w'}\right] = \left[I_h, d_k^\dagger\right] = \left[I_h, \overline{\alpha}_{r_{jw}^*}\right] = \left[\mathcal{B}_{r_w}, \overline{\alpha}_{r_{jw}^*}\right]0. \tag{35}$$

Thus, $\{I_h\}$ and $\{\mathcal{B}_{r_w}\}$ lead to disjoint Z_2 algebras. Thus, when combined, equations (21), (22), (29)–(33) give us the explicit form of the ground state wavefunctions for the $S = 1/2$ system defined by equation (1).

5.4. Comparison to ground states of other topological-ordered systems

The spin basis form of the ground state of this topologically ordered system can be compared to that of the other systems exhibiting topological quantum order, e.g. both the Rokhsar–Kivelson (RK) [11] and the Kitaev toric code models [2] (as well as Wen's plaquette model [19] which is equivalent to Kitaev's toric code model) [8] have ground states of the form

$$|\psi\rangle = \mathcal{N}\sum_i |\chi_i\rangle, \tag{36}$$

with $\mathcal{N}$ a normalization constant and the sum over i performed over all states $|\chi_i\rangle$ which belong to a given topological sector which is evident by the real space representation (e.g., an even or odd number of dimers/positive bonds in the Rokhsar–Kivelson/Kitaev toric code models, respectively). In both the RK and Kitaev toric code models, these ground states may be expressed as a product of projection operators (related to a Z_2 algebra) acting on a given reference state. For instance, in the Kitaev's toric code model on the square lattice [2]

$$H = -\sum_s A_s - \sum_p B_p, \tag{37}$$

with $A_s = \prod_i \sigma_{is}^x$ and $B_p = \prod_{\langle ij\rangle \in p} \sigma_{ij}^z$, as stated earlier, all ground states may be expressed as

$$|g_{\text{toric code}}\rangle = \mathcal{N}\left(\prod_s \frac{1}{2}(1 + A_s)\right)\left(\prod_p \frac{1}{2}(1 + B_p)\right)|\phi\rangle, \tag{38}$$

with $|\phi\rangle$ a reference state. Similarly, the general equation (36) can be written as a projection of a given reference state over a sector of the Hilbert space that has a chosen set of topological numbers (those corresponding to a given topological sector). As seen from our solution of equation (29), the ground state of Kitaev's model on the hexagonal lattice (equation (1)) [6] is more complicated. This is so as it involves the fermionic operators of equation (31). The Fermi vacuum of equation (32) indeed already has a form similar to equation (38) but, as seen from equation (29), it needs to be acted on by fermionic string operators. This leads to a far more nontrivial state. Written longhand in the original spin basis, we have that the fermion pair creation operator

$$d_k^\dagger d_{-k}^\dagger = \frac{1}{4}\sum_{r_{w1}}\sum_{r_{w2}} \mathrm{e}^{\mathrm{i}k(r_{w2}-r_{w1})}\left(\sigma_{r_{w1}}^y\left(\prod_{r'<r_{w1}}\sigma_{r'}^z\right) - \mathrm{i}\sigma_{r_{b1}}^z\left(\prod_{r'<r_{b1}}\sigma_{r'}^z\right)\right)$$
$$\times\left(\sigma_{r_{w2}}^y\left(\prod_{r''<r_{w2}}\sigma_{r''}^z\right) - \mathrm{i}\sigma_{r_{b2}}^z\left(\prod_{r''<r_{b2}}\sigma_{r''}^z\right)\right) \tag{39}$$

needs to be augmented. Here, in the product signs we made explicit that along the Jordan–Wigner contour that we employ here $r_b = r_w + L$. When equation (39) is combined with equations (29), (32) and (33), we have a form for the real space spin states of the Kitaev model.

5.5. *Time reversal symmetry breaking*

Our expressions show that the state $|g\rangle$ of the open boundary condition system is generally not time reversal invariant for any size system—whether it contains an odd or even number of spins. In the expressions above for the ground state, this is seen by taking $\sigma^a \to -\sigma^a$ for all components $a = x, y, z$ under time reversal. If any of the indices in equation (39) are such that $(r_{w1} - r_{w2})$ or L are odd, then equation (39) is not time reversal invariant. Similarly, the operator $\mathcal{B}_{r_w}$ of equation (33) contains $(L + 1)$ spin operators and is not time reversal invariant for even L. A reference state $|\phi\rangle$ of equation (32) on an even-size lattice can be chosen to be time reversal invariant. For the odd-size lattice, the considerations are more immediate.

As a concrete example, let us consider three hexagons that span a total of 13 vertices as shown in figure 5. This example serves to illustrate the presence of time reversal symmetry breaking even without doing any calculations. It is impossible to write down a ground state of Kitaev's model of 13 $S = 1/2$ spins of this 13 site 'disc-like geometry' that is non-degenerate. The same considerations apply also to instances in which we have various topologies. For

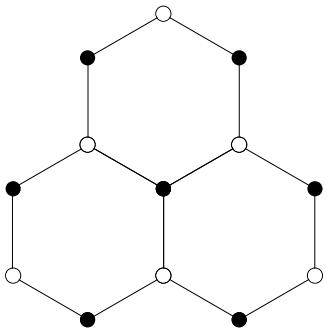

Figure 5. The geometry of 3 hexagons that span a total of 13 vertices. By Kramers' theorem, ground states of this system that contains an odd number of $S = 1/2$ spins must break time reversal invariance.

instance, we can put the figure above of three hexagons with a total of 13 sites on a three-fold torus—that of three handles (the genus number $g = 3$). Here, there will be a hole at the center of each of the hexagons. One of the sites is common to three ordinary tori and three other sites are common to two tori. There is periodicity around each of the hexagons (hence the designation of $g = 3$) in this case. This 13 site system on the plane corresponds to a system with open boundary conditions, while if it is a $g = 3$ torus it corresponds to a system that has nontrivial periodicity around three hexagonal rings (along with the same number of trivial periodicity of period one along three other directions). In both cases, as the Hamiltonian H is time reversal invariant (because $T^{-1}S_{a;i}T = -S_{a;i}$ with T the time reversal operator and $S_{a;i}$ the $a = x, y, z$ component of the spin operator at spin i and the Hamiltonian is quadratic in the spins) and there is an odd number of spins in these particular examples ($n = 13$), by Kramers' theorem, the ground state—and in fact any energy eigenstate—must be, at least, two-fold degenerate. General considerations for constructing a torus of genus g from individual ordinary ($g = 1$) tori are outlined[3]. We emphasize that this degeneracy is mandated for an odd size system by Kramers' theorem for any time reversal invariant Hamiltonian. Time reversal symmetry breaking similarly occurs in extensions of Kitaev's model that allow for odd cycles [6, 15] (e.g., a triangular decoration of the lattice).

In any half-integer spin system whether or not it has topological order (i.e., one which cannot display any global symmetry breaking with local order parameters) [1] in which the number of particles is odd, the ground states must, by Kramers' theorem, exhibit time reversal symmetry breaking. This conclusion may be fortified for general gapped systems with short-range Hamiltonians. In such systems, there is an exponential clustering of correlations [16]. This clustering, in turn, implies that the ground state can, up to exponentially small corrections [17], be written as a matrix product state constructed of low-lying states on finite size blocks. The block size may, in principle, be taken arbitrarily large, so long as is smaller than the

[3] Generally, in a fusion of a general individual tori of genus $g = 1$ each having N_a sites into a general genus of genus g, the total number of spins is

$$N_s = \sum_{a=1}^{g} N_a - \sum_i (n_i - 1).$$

Here, n_i is the number of tori to which a given site i is common to. The second term above removes the multiple counting of a given site if it appeared in several tori prior to the fusion. The total number N_s of $S = 1/2$ spins can be either even or odd. The 13 site geometry discussed earlier is a particular instance of this with $N_{1,2,3} = 6$ (three hexagons) which has three sites common to two tori and one point common to all three tori. There, we obviously have $N_s = 3 \times 6 - 3 - 2 = 13$ (odd).

system. Consider a general Hamiltonian $H = \sum_R h_R$, with R labeling different blocks and h_R a Hamiltonian that has its support on R. Spins can be shared by different blocks R. By Hastings' theorem [17], the ground state of H is up to exponential corrections a matrix product state. Let us now examine what this implies when combined with time reversal. If all blocks R are chosen to have an odd number of sites in the decomposition of any short-range $S = 1/2$ Hamiltonian H, then all states of the different blocks R will be, at least, doubly degenerate. This is because of the (at least) two-fold degeneracy of each level in the odd-sized blocks R implied by Kramers' theorem. We see here that the matrix product construction then implies that the ground state of large systems (also if they are of even size) must also be, at least, two-fold degenerate up to corrections which are exponentially small in the size of the system. This degeneracy is dictated by the time reversal non-invariance of the local energy eigenstates in each of the odd-sized blocks R. The considerations above are general and apply to both systems with or without toplogical order. Topological order pertains to systems such as Kitaev's which do not display global symmetry breaking associated with local order parameters, [1]. The existence of degeneracy in Kitaev's model can also be seen by the non-commutativity of existent symmetries: this non-commutativity lies at the heart at Kitaev's inception of this model. We will detail symmetry considerations for this model in a later section.

5.6. Boundary terms

For infinite open systems, the previous discussion will be sufficient for the analysis of bulk properties. However, in a closed system, boundary terms will lead to a topological dependency of the ground state degeneracy. In this subsection, we shall consider the toroidal geometry, which can be viewed as periodic boundary conditions along both directions. For the Jordan–Wigner transformation defined in equation (3), the periodic boundary condition along the vertical direction will have no effect since the phase terms of two nearest-neighboring terms along x or y bonds cancel out and there is no phase term for the z-bond coupling. For the periodic boundary condition, the boundary terms read

$$H_{\text{boundary}} = \sum_j \left[J_x \sigma^x_{1,2j} \sigma^x_{L_h,2j} + J_y \sigma^y_{1,2j+1} \sigma^y_{L_h,2j+1} \right]. \tag{40}$$

Here, L_h is the size of the system along the horizontal direction. After the Jordan–Wigner transformation (3), the coupling strength of the boundary terms acquires a phase

$$H_{\text{boundary}} = \sum_j [J_x \phi(2j) A_{1,2j} A_{L_x,2j} + J_y \phi(2j+1) A_{1,2j+1} A_{L_x,2j+1}], \tag{41}$$

with the phase term given by

$$\phi(j) = \prod_{1 \leqslant i \leqslant L_h} \sigma^z_{i,j}. \tag{42}$$

This phase does not commute with the Z_2 bond operator α on the z-bonds attached to the jth horizontal line. The phase factor $\phi(j)$ reverses all α of the z-bonds attached to the sites on the jth horizontal line. The boundary terms thus lift the degeneracy characterized by different choices of α bonds. The gauge freedom discussed in section 4 is now fixed by the boundary terms and the ground state degeneracy acquires a topological dependence. On the other hand, the boundary term commutes with the plaquette quantity defined by Kitaev. Therefore, the discussion about the correlator in a later section is still valid when the boundary term is included. The momentum components (k_x, k_y) employed in the solution of the previous

subsections above are related by a 45° rotation to the discrete values (k_h, k_z) for the system with periodic boundary conditions along the vertical and horizontal directions discussed here.

We conclude with brief remarks about the symmetries of equation (16) in the case of periodic boundary conditions and on a candidate trial state. The spin system of equation (1) on the torus has the $\phi(j)$ operators of equations (16) and (42) as exact symmetries. On the torus, the symmetry of equation (16) corresponds to the product of spin operators along an entire toric cycle. These operators satisfy the following identity:

$$\phi(j)\phi(j+1) = \prod_{h\in S} I_h. \tag{43}$$

Here, S is a ribbon of width 1 on the torus which contains all hexagons (plaquettes) lying between the two consecutive rows j and $j+1$. As the ground states of the Kitaev model are vortex free ($I_h = 1$ for all h), the right-hand side of equation (43) is 1. Thus, for all rows j, we have that $\phi(j) = \phi(j+1)$. A variational state for the periodic system is given by

$$|\psi_{\text{var}}\rangle = \mathcal{N}\sum_{\alpha'} |g_{\alpha'}\rangle = \mathcal{N}\Big(\prod_j [1+\phi(j)]\Big)|g\rangle, \tag{44}$$

with $\mathcal{N}$ a normalization constant and $\{\alpha'\}$ all configurations, which up to the symmetry operations of equations (14) and (16), correspond to the uniform sector $\alpha_r = 1$ for all bonds r. Here, $|g_{\alpha'}\rangle$ is the ground state in a given α' sector of the open boundary system. Such a state is related to the general uniform $\alpha_r = 1$ ground state which we derived earlier (the state $|g\rangle$ of equations (29)–(33)) by the application of the symmetry operators $\phi(j)$ of equations (16) and (42). The variational state of equation (44) is an eigenstate of all of the symmetries $\{\phi(j)\}$ of equations (16) and (42) (with a uniform eigenvalue which is equal to 1).

6. Anyons in the gapped phase

We will now derive and study anyons in the gapped phase of Kitaev's model by relying directly on the Jordan–Wigner transformation. The existence of anyons in this phase has long been recognized [6] and, due to the prospect of fault tolerant quantum computing, is one of the main motivations for studying this system. The current appendix illustrates how these anyons may be directly studied and derived within our framework.

Besides the Bogliubov quasiparticles, other excitations—the vortex excitation illustrated in figure 3(*b*)—are also manifest. It is more interesting to study these excitations within the gapped state. In this section, we shall follow Kitaev's original argument [6] and now demonstrate, in our fermionic representation, the anyonic nature of these vortex excitations. Let us start in the limit where $J_x = J_y = 0$. In this limit, the fermionized Hamiltonian reads

$$H = J_z \sum_r \alpha_r \big(2d_r^\dagger d_r - 1\big). \tag{45}$$

The ground state is thus $2^{N/2}$ degenerate, where N is the number of sites. This degeneracy can also be understood in the original spin language. In this limit, all vertical bonds are disconnected. Let us consider a single bond $\big(J_z\sigma_1^z\sigma_2^z\big)$. Without loss of generality, let us consider $J_z > 0$. There are two degenerate ground states $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$. This degeneracy is related to the local Z_2 symmetry which is present for $J_x J_y = 0$. Without losing generality, let us set $J_x = 0$. In this case, we can define a local unitary transformation which is just $\sigma_1^x\sigma_2^x$ on one of the x-bonds. The effect of this operator is to transform J_z to $-J_z$ on the two vertical bonds connected to the x-bond. If $J_x J_y \neq 0$, such transformation is impossible and we expect the degeneracy to be lifted. The lowest order contribution from J_x and J_y terms is thus

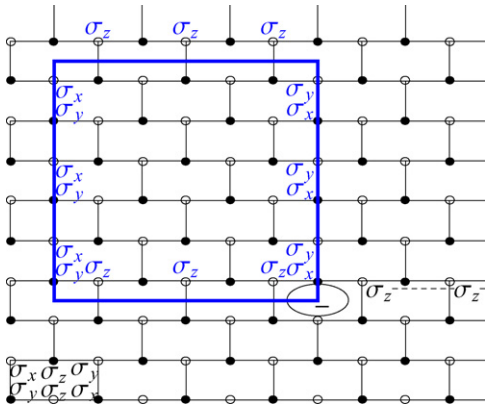

Figure 6. Loop operator to move a vortex along a loop.

expected to be in the second order of $J_x J_y$, i.e., $J_x^2 J_y^2 / J_z^3$. This corresponds to a fourth-order perturbation. Indeed, Kitaev has shown this is true in the language of spin operators [6]. The non-constant effective Hamiltonian up to fourth order is thus proportional to the product of the four horizontal bonds of a given plaquette, $\left(\sigma_1^x \sigma_2^x\right)\left(\sigma_2^y \sigma_3^y\right)\left(\sigma_6^y \sigma_5^y\right)\left(\sigma_5^x \sigma_4^x\right)$. In the language of our Majorana fermions A, this is

$$\begin{aligned} H_{\text{eff}}^{(4)} &\propto (A_1 A_2)(A_2 A_3)(A_6 A_5)(A_5 A_4) \\ &= (\mathrm{i} A_1 A_6)(\mathrm{i} A_3 A_4). \end{aligned} \tag{46}$$

Here, we have dropped the sublattice subscripts b and w for the A fields. If we introduce a dual spin on vertical bonds,

$$\mu_r^z = 2 d_r^\dagger d_r - 1, \tag{47}$$

then the effective Hamiltonian H_{eff} will be nothing but an Ising coupling between two neighboring spins along the horizontal direction $H_{\text{eff}}^{(4)} \propto \mu_{i,j+1/2}^z \mu_{i+2,j+1/2}^z$. The total perturbative Hamiltonian thus reads

$$H = \sum_{ij} \left[2 J_z \alpha_i \mu_i^z - \frac{J_x^2 J_y^2}{16 J_z^3} \mu_{ij}^z \mu_{i+2,j}^z \right] + \text{const} \tag{48}$$

on the lattice of vertical bonds. The coefficient $-1/16$ is worked out by Kitaev [6]. As one would expect, the J_x and J_y terms lift the degeneracy and the ground state is the one with $\alpha_i = 1$ in our aforementioned gauge fixing of the extra freedom in section 4. The interesting excitation state that corresponds to the anyon studied by Kitaev [6] is thus the ground state of the Hamiltonian of the configuration sketched in figure 3(*b*). This is exactly the same vortex state in the plaquette p defined by Kitaev [6], where one conserved quantity I is reversed in the plaquette p. In this state, to save (positive) J_z contributions to the energy, the effective spins $\{\mu_i\}$ on the cut where $\alpha_i = -1$ are also flipped and the resultant configuration is a domain wall structure at p. The energy penalty associated with this domain wall is $J_x^2 J_y^2 / 8 J_z^3$. For convenience, let us define

$$\tilde{I}(i, j + 1/2) = \mu_{i-1,j+1/2}^z \mu_{i+1,j+1/2}^z. \tag{49}$$

In terms of the original spin operators, $\tilde{I}$ is, similar to equation (10),

$$\tilde{I} = \sigma_1^x \sigma_2^z \sigma_3^y \sigma_4^x \sigma_5^z \sigma_6^y. \tag{50}$$

An illustration is provided in the lower-corner plaquette of figure 6.

We shall now demonstrate that the anyonic nature of the vortex excitation. A vortex on the plaquette centered at $(i, j + 1/2)$ is characterized by two kinks on the same bond, one in the channel of α and another in the channel of μ^z. There are four equivalent ways to create a vortex on the plaquette centered at $(i, j + 1/2)$:

$$P_w^R(i, j + 1/2) = \prod_{i'>i} iA_wB_w(i', j + 1), \tag{51}$$

$$P_w^L(i, j + 1/2) = \prod_{i'<i} iA_wB_w(i', j + 1), \tag{52}$$

$$P_b^R(i, j + 1/2) = \prod_{i'>i} iA_bB_b(i', j), \tag{53}$$

$$P_b^L(i, j + 1/2) = \prod_{i'<i} iA_bB_b(i', j). \tag{54}$$

The operators $P_w^R\left(P_b^R\right)$ are related to $P_w^L\left(P_b^L\right)$ by the gauge transformations encapsulated by $U_i^w\left(U_i^b\right)$ of equation (14). We also note that $\left(P_{b,w}^{R,L}\right)^2 = 1$. Therefore, $P_{b,w}^{R,L}$ can either create a vortex or annihilate an existing vortex at $(i, j+1/2)$. A naive way to move an anyon vertically from $(i, j + 1/2)$ to $(i, j + 5/2)$ is to apply $P_b^L(i, j + 5/2)P_w^L(i, j + 1/2)$. It turns out that it is more convenient to multiply two extra phase terms, the first one contains the multiplication of z-bonds centered at $(i', j + 3/2)$ with $i' < i$

$$\left(\prod_{i'<i}[(iA_bB_b)(iA_wB_w)]_{z\text{-bonds}}\right),$$

and the second one contains the multiplication of $\tilde{I}$ centered at $(i', j + 3/2)$ with $i' \leqslant i, \prod_{i'\leqslant i}\tilde{I}(i', j + 3/2)$. After including these two phases, the shifting operator $\mathcal{T}_y$ from $(i, j + 1/2)$ to $(i, j + 5/2)$ takes a simple form in terms of spin operators

$$\mathcal{T}_y = \sigma^x(i, j + 1)\sigma^y(i, j + 2). \tag{55}$$

We are now ready to construct the loop operator that moves vortex around and study the statistic properties of vortex excitations. Let us first create a vortex on the plaquette centered at $(i, j + 1/2)$ with $P_w^R(i, j + 1/2)$, which applies S^z on all site-3 (white site at the top-right corner) of the plaquettes $(i', j + 1/2)$ with $i' \geqslant i$ as shown in figure 6. To move this vortex along a closed loop C, we can construct a loop operator L_C by multiplying $\mathcal{T}_y$ along vertical lines and σ^z along horizontal parts of the loop, as illustrated in figure 6. The loop operator can be expressed by

$$L_C = \left(\prod_{\substack{(i',j')\in C,\\ j'+j=\text{odd}}} \tilde{I}(i', j' + 1/2)\right)\left(\prod_{l_b\in C}\left[\sigma_w^z\sigma_b^z\right]_l\right). \tag{56}$$

An explanation of the notation is due. Without losing generality, let us assume the anyon is located on an even row, $j = 2n$. L_C can be separated into two parts. The first part is the product of $\tilde{I}$ that covers the plaquettes on the odd rows enclosed by the loop C. The second part is the product of $\sigma_b^z\sigma_w^z$ on the vertical bonds whose black site is enclosed inside the loop C. In the projected subspace on which the effective Hamiltonian lives, the vertical bond part is the identity 1. Therefore, the loop operator is just the product of $\tilde{I}$ over the plaquettes on the odd rows enclosed by C, $L_C = (-1)^{n_C}$, where n_C is the number of vortices that are located

on the odd rows and inside the loop C. In another words, if we bring a vortex on an odd row around another vortex on an even row, an extra minus sign is generated, while no such minus sign is generated if we bring a vortex on an even (odd) row around another vortex also on an even (odd) row. Putting all of the pieces together, we fleshed out, by building on the fermionic representation, the anyonic nature of the vortex excitations.

7. String and brane type correlators dictated by local symmetry

In this section, we shall apply symmetry considerations [8, 13] and review condensed remarks from [13] concerning the symmetries of this model and general considerations regarding non-vanishing correlators in similar matter coupled theories which are reviewed in appendix B. We will show directly from symmetry considerations that the Kitaev model on the hexagonal lattice [6] does not exhibit any two point correlations of length larger than 1 and that any non-vanishing correlation function generally amounts to a string operator (either closed or open). The fermionization that we employ here [9, 10] gives rise to precisely such string-like correlators whose form is dictated by symmetry. In the matter coupled gauge analogy of appendix B, all possible correlators correspond to open meson or closed photon lines. We will show that Kitaev's model supports finite-valued *brane* type correlators. By *brane* correlators, we allude to correlators which span portions of the two-dimensional plane. This result—as it applies for only the two point correlations—was also recently derived by a Majorana fermion construction [12]. In what follows, we show how gauge symmetry considerations effortlessly mandate this result.

7.1. Two point correlators

We claim that both at finite and at zero temperature the spin–spin correlation between any two spins which are separated by more than one lattice constant must vanish. To see this, we note that this system displays the local symmetries of equation (10). We now fuse these symmetries together and see that we have a symmetry associated with any closed contour C, by

$$\hat{O}_C = \prod_{p \in C} \sigma_p^{\gamma_{p^C}}. \tag{57}$$

In equation (57), the polarization index γ_{p^C} is chosen to correspond to the direction ($\gamma = x, y, z$) of the single bond emanating from site p which does not lie in the contour C. Any given site p forms the endpoint of three bonds; two of these bonds lie in the contour C and only a single bond ending in p does not lie in C.

We now briefly relate these symmetries to degeneracies. If two curves C and C' share an odd number of sites in common then O_C and $O_{C'}$ anticommute. Thus if, e.g., we choose to simultaneously diagonalize H and O_C and determine a ground state $|g_1\rangle$ in that common eigenbasis, then $O_{C'}|g_1\rangle$ is a new degenerate ground state. This degeneracy applies not only to the ground state sector but to all energy levels.

7.1.1. $T > 0$. By employing these symmetries along with Elitzur's theorem [18] at temperatures $T > 0$, we find that the finite temperature correlator $\langle \sigma_p^a \sigma_q^b \rangle$ vanishes unless (i) p and q are the nearest-neighbor sites and that (ii) $a = b$ corresponds to the direction ($a = x, y, z$) between the two lattice sites i and j in question. This is so as unless conditions (i) and (ii) are satisfied, there is at least one loop C for which $[\sigma_p^a \sigma_q^b]$ is not invariant under $\hat{O}_C$ of equation (57) and for which

$$\hat{O}_C [\sigma_p^a \sigma_q^b] \hat{O}_C = -[\sigma_p^a \sigma_q^b]. \tag{58}$$

7.1.2. $T = 0$. The $T = 0$ relation (even for different times [12]) is similarly derived. All of the operators $\hat{O}_c$ commute with one another. (This is seen as for the minimal loop C which contains a single hexagon, two neighboring hexagons leading to the operators $\hat{O}_1$ and $\hat{O}_2$ which contain two common sites which lead to two anti-commutation relations between the different Pauli matrices [6]. The product of operators each acting on a single hexagon leads to the most general symmetry operator of equation (57) with an arbitrary path C.) Consequently, we may simultaneously diagonalize H of equation (1) with all of the operators $\hat{O}_c$. The dynamical $T = 0$ two-spin correlation function

$$\begin{aligned}\langle\psi|\sigma_p^a(0)\sigma_q^b(t)|\psi\rangle &= \langle\psi|\sigma_p^a(0)\exp(\mathrm{i}Ht)\sigma_q^b(0)\exp(-\mathrm{i}Ht)|\psi\rangle \\ &= \Big(\langle\psi|\sigma_p^a\sigma_q^b|\psi\rangle + \mathrm{i}t\langle\psi|\sigma_p^a\big[H,\sigma_q^b\big]|\psi\rangle \\ &\quad + \frac{(\mathrm{i}t)^2}{2!}\langle\psi|\sigma_p^a\big[H,\big[H,\sigma_j^b\big]\big]|\psi\rangle + \cdots\Big) \end{aligned} \tag{59}$$

with $|\psi\rangle$ any ground state which is a simultaneous eigenstate of H and $\hat{O}_C$. The eigenvalues of $\hat{O}_C$ can only be ± 1. We can now show that unless p and q are linked by a single step along a direction a each of the expectation values in equation (59) vanishes. For example, for the first term in the final expression, we have

$$\begin{aligned}\langle\psi|\sigma_p^a\sigma_q^b|\psi\rangle &= (\langle\psi|\hat{O}_C)\sigma_p^a\sigma_q^b(\hat{O}_C|\psi\rangle) \\ &= \langle\psi|(\hat{O}_C\sigma_p^a\sigma_q^b\hat{O}_C)|\psi\rangle = -\langle\psi|\sigma_p^a\sigma_q^b|\psi\rangle, \end{aligned} \tag{60}$$

unless p and q which are linked by a single step along a direction a. Similarly, the second term in equation (59) is seen to vanish. Here, the commutator $\big[H,\sigma_q^b\big]$ leads to the sums of bilinears which involve the lattice site j and a nearest-neighbor site k. When multiplied by σ_p^a, this leads to an expression which is cubic in the spin operators. If all of the three lattice sites are different, we can choose a path C such that this expression changes sign under a unitary transformation corresponding to $\hat{O}_C$. Similar higher order terms in equation (59) are obtained, unless p and q which are linked by a single step along a direction a. This result reaffirms (from a purely symmetric point of view) the more detailed derivation of [12].

7.2. Higher order string and brane type correlators

We now turn to higher order spin correlations. A moment's reflection reveals that invariance under the general local symmetries of equation (10) allows only for the string or *brane* operators (either closed or open) to be finite: in other words, all spins must form continuous clusters along lines (strings) or lie in a fragment of the two-dimensional plane.

String and *brane* type correlators may involve, in the thermodynamic limit, an infinite number of fields and allow different topologies than that of closed loops alone. The fields may be ordered along an open string (or collection of such strings) or in higher dimensions may involve sophisticated combinations of fields at all lattice sites which we term as *brane* type correlators.

The best-known example of such a string correlator is that in the spin $S = 1$ AKLT chain [20, 21] in which

$$\left\langle S_i^z\left(\prod_{j=i+1}^{k-1}\mathrm{e}^{\mathrm{i}\pi S_j}\right)S_k^z\right\rangle = \frac{4}{9}. \tag{61}$$

This equation (61) holds for arbitrarily far separated sites i and k. As this correlator is, asymptotically, far larger than the usual spin–spin correlator, it is often said to capture a

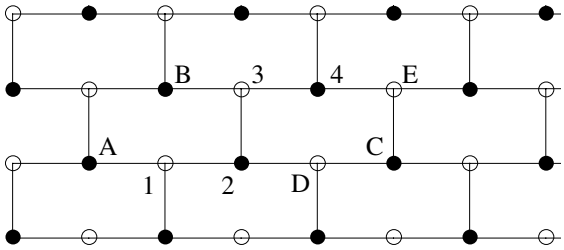

Figure 7. A non-vanishing open loop correlator of the form given by equation (62). Here, the correlator is equal $\langle(\sigma_1^x\sigma_2^x)(\sigma_2^z\sigma_3^z)(\sigma_3^x\sigma_4^x)\rangle = \langle\sigma_1^x\sigma_2^y\sigma_3^y\sigma_4^x\rangle$. All correlators are of the form of continuous string correlators such as this or of their union. See equation (61). As we review in the appendix, precisely such string correlators are the only non-vanishing correlation functions in matter coupled gauge theories.

hidden order. We may construct string operators which are more sophisticated variants of the operator appearing in equation (61). Apart from spin chains [20–22], such correlators also appear, amongst others, in doped Hubbard chains and related systems [23–25], cold atom chains [26], in spin leg ladders [27], and may be related to non-local constructs in Quantum Hall systems [28]. In doped Hubbard chains, the string correlator decays asymptotically with distance but with a power which is smaller than that of the usual spin–spin correlators. To date, nearly all appearances of string correlators are confined to one-dimensional or quasi-one-dimensional systems. The only known exceptions which we are aware of are [23] and possible links to the density matrix construct of [28] for Quantum Hall systems. In what follows, we show that the Kitaev model is a rigorous two-dimensional example of a system in which various string correlators can either attain a finite value or decay asymptotically in a slow manner (explicitly so for gapless systems).

Let us now turn back to Kitaev's model of equation (1). The only gauge-invariant (symmetry of equation (10)) quantities which, by Elitzur's theorem [18], can attain a finite expectation value are given by

$$\left\langle \prod_{pq\in C} [\sigma_p^{\alpha_{pq}}\sigma_q^{\alpha_{pq}}] \right\rangle, \tag{62}$$

with C a general contour which may be open or closed (or a union of such contours) and α_{pq} denotes the direction of the physical bond between the two nearest-neighbor sites p and q. When C is a closed loop, the argument of the average in equation (62) is, up to a multiplicative phase factor, equal to the symmetry operator of equation (57).

An example of such a correlator is furnished in figure 7. In figure 7, we show the only non-vanishing correlator which has four spins with sites 1 and 4 as its endpoints. To see that this string correlator is invariant under all local symmetries, consider first sites 1 and 4. Considering hexagons $h = E, D$ (see figure), we see that only the fields σ_1^x and σ_4^x are invariant under the local symmetry of equation (10). Next, we note that this particular choice of these fields at sites 1 and 4, the symmetry of equation (10) for both hexagons $h = A$ and $h = B$, enables the introduction of a field at site 2, 3 of the form $\sigma_{2,3}^y$. Thus, $\langle\sigma_1^x\sigma_2^y\sigma_3^y\sigma_4^x\rangle$ is a correlator which is invariant under all local symmetries. As such, it is not prohibited from attaining a non-zero expectation value at finite temperatures by Elitzur's theorem. Similarly, the product of two disjoint bonds $\langle(\sigma_1^x\sigma_2^x)(\sigma_x^3\sigma_x^4)\rangle$ is invariant under all local symmetries. In a similar fashion, we can proceed to consider longer contours invariant under local symmetries-all of which must be of the form of equation (61). Replicating the $T = 0$ considerations of equation (59) to multi-spin correlators, we see that string correlators of the form of equation (61) are

similarly symmetry allowed within the ground state sector but others are not. By construction, the string correlator is invariant under all products of the local symmetries $\{I_h\}$-the symmetries of equation (61). The contour C may consist of disjoint open segments (e.g. disjoint bonds with each bond containing two sites). Of all of the correlators of equation (62) that we found to be allowed by Elitzur's theorem, only those with an even number of spins are time reversal invariant. String correlators of the form of equation (61) with an odd number of spins are not time reversal invariant and consequently must vanish when time reversal symmetry is unbroken. We are grateful to J Vidal, S Dusuel and K Schmidt for prompting us to note what occurs under time reversal for our string correlators of equation (61).

For closed contours C, the quantity to be averaged in equation (62) becomes none other than the symmetry of equation (57). In appendix B, we review similar selection rules for lattice gauge theories. Though all non-vanishing correlators must be of the form of equation (62), systems with open boundary conditions, further allow for additional string correlators of this form with only the boundary site(s) on the contour C not adhering to this form. The appearance of only such non-vanishing open or closed continuous string correlators (involving all sites between sites p and q) is reminiscent of the gauge-invariant correlators appearing in matter coupled gauge theories, e.g. [13]. As stated earlier, all non-vanishing correlators must be of the form of equation (62) on a system with periodic boundary conditions or, in a system with open boundary conditions, further allow for additional string correlators of this form with only the boundary site(s) on the contour C not adhering to this form. The ideas underlying the constructs which we introduce next were reviewed in [8].

7.2.1. Correlators of maximal value. We next construct several such string correlators by relying on the mapping to the Fermi problem. This mapping transforms correlators which involve only several Fermi fields into those which involve an extensive number of spin fields and vice versa.

In the Kitaev model, the Fermi vacuua states $|0\rangle$ can be chosen to simultaneously diagonalize all of the symmetry operators $\{I_h\}$ and $\{\mathcal{B}_{r_w}\}$. Here, we will have that

$$\left|\langle 0|\prod_{r'=r_{w1}}^{r_{w2}} B_{r'}|0\rangle\right| = \left|\langle 0|\sigma^x_{r_{w1}}\sigma^y_{r_{w1}+1}\sigma^x_{r_{w1}+2}\ldots\sigma^x_{r_{b2}-1}\sigma^y_{r_{b2}}|0\rangle\right| = 1 \tag{63}$$

(for an even number of sites). The string correlator of equation (63) is equal to a constant value irrespective of its length (the number of spin operators that it contains). Different Jordan–Wigner contours may also be chosen which lead to the paths other than those in equation (63) which connect the two endpoints. The Fermi vacuua become ground states only in the limit of $|J_z/J_{x,y}| \gg 1$ (and permutations thereof). Physically in this limit, the large value of $|J_z|$ forces consecutive chains to be fully correlated. The open string correlator of equation (63) augments the closed loop correlators of equation (57) for any closed contour C. Of course, combinations of various closed loops and open string operators are possible.

We now discuss the situation for arbitrary $J_{x,y,z}$. Given a general ground state $|g\rangle$ of the form of equation (29), we can transform it into a Fermi vacuum state by a unitary transformation

$$U = \prod_k \left(u_k + v_k(b_k^\dagger + b_k) - u_k n_k\right), \qquad U|g\rangle = |0\rangle. \tag{64}$$

Here, $n_k \equiv d_k^\dagger d_k$. For a general ground state $|g\rangle$, the non-local *brane* expectation value

$$|\langle g|U^\dagger\sigma^x_{r_{w1}}\sigma^y_{r_{w1}+1}\sigma^x_{r_{w1}+2}\ldots\sigma^x_{r_{b2}-1}\sigma^y_{r_{b2}}U|g\rangle| = 1. \tag{65}$$

The operator of equation (65) has maximal correlations (the modulus of the expectation value of these operators cannot exceed 1). The maximal correlations exceed the standard string correlators found in the AKLT chain. Written in terms of the original spin fields at each site, this operator generally (for finite $J_{x,y,z}$) spans all sites of the lattice.

7.2.2. Non-maximal correlators. We can similarly construct other operators which would reduce to other open string operators if the system were one-dimensional (if, e.g., $J_z = 0$). These form other generalizations of the familiar one-dimensional string operators. In what follows, we discuss string operators which are not maximally, and indeed decay with increasing separation between the two endpoints of the string. To this end, let us start by writing

$$d^\dagger_{r_1} d_{r_2} = \pm\frac{1}{4}\left(\prod_{r_{w_1}\leqslant r'''<r_{w_2}} \sigma^z_{r'''}\right)\left\{-\mathrm{i}\sigma^y_{r_{b_1}} + \sigma^x_{r_{b_1}}\left(\prod_{r_{w_1}\leqslant r'<r_{b_1}-1} \sigma^z_{r'}\right)\right\} \times \left\{\mathrm{i}\sigma^y_{r_{w_2}} + \sigma^x_{r_{b_2}}\left(\prod_{r_{w_2}\leqslant r''<r_{b_2}-1} \sigma^z_{r''}\right)\right\}. \tag{66}$$

Here, the + sign is chosen if $r_{w_2} < r_{b_1}$ along the contour on which the Jordan–Wigner transformation is performed and the − sign is chosen otherwise. Here, we have that

$$\left\langle d^\dagger_{r_1} d_{r_2}\right\rangle = \frac{1}{2}\int \frac{\mathrm{d}^2k}{(2\pi)^2}\,\mathrm{e}^{-\mathrm{i}\vec{k}\cdot(\vec{r}_1-\vec{r}_2)}\left[1-\frac{\epsilon_k}{E_k}\right], \tag{67}$$

with the definitions of equation (22) for ϵ_k and E_k. The form of this expression follows directly from the state of equation (29), $\langle n_k\rangle = v_k^2$. Looking at equation (67), we see that for gapless systems, a power-law behavior may be sparked. In the presence of a gap, the branch points in the complex q plane of E_q of equation (22) along a chosen direction may determine the asymptotic long-distance correlation length along that direction. Rather explicitly, in the gapped phase, we have from equation (23) that the logarithm of the correlator of equation (67) scales asymptotically, along the x, y directions as $[-(|r_{2;a} - r_{1;a}|/\xi_a)]$ (where $\{r_a\}$ are $\vec{r}\cdot\hat{e}_a$ with $a = x, y$ (see figure 1)) with

$$\frac{1}{\xi_x} = \cosh^{-1}\left[\frac{J_x^2 + J_z^2 - J_y^2}{2J_xJ_z}\right], \qquad \frac{1}{\xi_y} = \cosh^{-1}\left[\frac{J_z^2 + J_y^2 - J_x^2}{2J_yJ_z}\right]. \tag{68}$$

Along any given direction a, in the complex q_a plane, there are two branch points along the imaginary q_a axis. There is a simple signature of the $T = 0$ critical phase that occurs when we cross from the gapped to the non-gapped phases when $|J_x \pm J_y| = |J_z|$. Here, the branch points merge at $q_a = 0$ and there is a divergent correlation length ξ_a. Within the gapless phase, the two branch points lie along the real q_a axis.

Fusing equations (66) and (67) together, we have an expression for the expectation value of the string operator which lives on all sites linking r_{w_1} up to (and including) r_{b_2}. The left-hand side of equation (66) is given by the Fourier transform in equation (67). Similar transformations may be applied to other fermionic correlators which when translated into the spin variables lead to other string correlators.

The ground-state form of equation (29) enables a direct computation of the expectation value of any general product of the form $\langle\prod_i d_{k_i}\prod_j d^\dagger_{k_j}\rangle$. This is so as the state of equation (29) is a direct product in k space. For each value of k, we have a binomial distribution for each occupancy, v_k^2 for the occupancy of the pair $(k, -k)$ and a probability of u_k^2 for it to be empty. Thus, any general multi-spin correlator can be trivially computed—we first Fourier transform it, then express the product in terms of the Fermi variables

following the Jordan–Wigner transformation, and then compute the average for the states of equation (29) where each average for a given value of k becomes decoupled from all other values of k. In a related vein, Wick's theorem for equation (22) ensures the decomposition of general correlator into a product of pair correlators for $(k, -k)$ pairs.

8. Conclusion

In conclusion, we presented an exact solution of Kitaev's toric code model which allows for various new results:

(1) We fermionize Kitaev's model to render it into a p-wave type BCS pairing problem.
(2) We derive the exact *ground state wavefunction in terms of the spin degrees of freedom*. With it, we examine the zero-temperature correlation functions and derive the exact correlation lengths within the gapped phase. We further show that the wavefunction in this case is more complicated than in the other prototypical models of topological quantum order (e.g., the Rokhsar–Kivelson quantum dimer model and Kitaev's or Wen's square-lattice models).
(3) We prove that local symmetries only enable string (open or closed) and *brane* type correlators (and their unions) to be non-zero in this system. We show how string correlators may be directly evaluated in terms of the exact ground state wavefunction. Kitaev's model is one of the very few two-dimensional systems with string or *brane* type correlators. Nearly all known examples of string correlators to date centered on one-dimensional systems.
(4) We identify the local symmetries of this system in terms of bond variables in the fermionic problem.
(5) We illustrate, in terms of fermions, the anyonic character of the vortex excitations in the gapped phase by an explicit construction.

Many possible extensions of our results follow from our fermionic wavefunctions. For instance, we can consider impurity bound states in systems engineered to have Hamiltonians which deviate slightly from equation (1). For spatially non-uniform J_x, J_y, J_z, so long as no new interactions are added, the toric symmetries remain in tact (as does the fermionization). In the vortex-free sector, the problem reduces to that of an impurity in a BCS-type system which may lead to fermionic bound states. In subsequent work, we will further aim to detail the Ising-type Hamiltonian that results for the vortex variables by tracing out over the fermionic degrees of freedom in equation (18).

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Appendix A. The fermionic vacuum in the spin representation

In what follows, we briefly outline the derivation of equation (32). For the fermionic vacuum, we have $d_k|0\rangle = 0$ for all k or equivalently

$$d_r|0\rangle = 0 \tag{A.1}$$

for all vertical bond centers r. Equation (A.1) implies that in the original spin basis,

$$\left[\left(\prod_{r'<r_b} \sigma^z_{r'}\right)\sigma^x_{r_b} + \mathrm{i}\sigma^y_{r_w}\left(\prod_{r'<r_w} \sigma^z_{r'}\right)\right]|0\rangle = 0. \tag{A.2}$$

Now, let us write the state $|0\rangle$ as a general superposition of states in the σ^z basis:

$$|0\rangle = \sum_{\sigma_1\sigma_2\cdots\sigma_N} A_{\sigma_1\sigma_2\cdots\sigma_N}|\sigma_1\sigma_2\cdots\sigma_N\rangle. \tag{A.3}$$

Inserting equation (A.2) into (A.3), we find that for all four possible spin orientations at r_w and r_b (up/down at each of these two sites) we have that the amplitudes satisfy

$$\begin{aligned} &A_{\sigma_1\sigma_2\cdots\sigma_{r_w}\cdots\sigma_{r_b}\cdots\sigma_{r_N}} = -\left(\sigma_{r_w+1}\cdots\sigma_{r_b-1}\right) \\ &A_{\sigma_1\sigma_2\cdots\sigma_{r_w-1}(-\sigma_{r_w})\sigma_{r_w+1}\cdots\sigma_{r_b-1}(-\sigma_{r_b})\sigma_{r_b+1}\cdots\sigma_N}. \end{aligned} \tag{A.4}$$

If and only if equation (A.4) is satisfied does the state of equation (A.3) satisfy equation (A.2). Equation (A.4) is equivalent to the demand that

$$\sigma^x_{r_w}\sigma^x_{r_b}|0\rangle = -\left(\sigma^z_{r_w+1}\cdots\sigma^z_{r_b-1}\right)|0\rangle. \tag{A.5}$$

In turn, equation (A.5) is equivalent to the condition

$$|0\rangle = \mathcal{B}_{r_w}|0\rangle, \tag{A.6}$$

for all sites $\vec{r}_w$ with the operator definition of equation (33). Equation (A.6) along with the condition of no vortices as dictated by reflection positivity [6] ($I_h = 1$) or an easier immediate direct inspection of equation (18) leads to the general solution for the Fermi vacuum state in the spin basis (equation (32)).

It is noteworthy that in the particular limit $J_z \geqslant 0$ with $J_x = J_y = 0$, any of the $2^{N/2}$ states having $\sigma^z_{r_w}\sigma^z_{r_b} = 1$ is a ground state. Here, N is the number of sites and $N/2$ is the number of vertical $\sigma^z\sigma^z$ bonds. As seen from our fermionization (e.g. equation (18), this corresponds to the condition $\alpha_r(2n_r - 1 = 1$ for each vertical bond r with $n_r = d^\dagger_r d_r$ the fermionic occupancy. In the sector $\alpha_r = 1$ for all r, the remaining ground state is that of the fermionic vacuum derived above. As shown in section 4, the inversion of α_r on all sites r of a given row leaves the spectrum invariant. If there are L horizontal rows then there are 2^L fermionic sectors that share the same spectrum.

Appendix B. String correlators in matter coupled gauge theories

Here, we briefly review, the well-known local symmetries of lattice gauge theories in order to clarify their similarity and the similarity of the string correlators that they mandate to the string correlators in Kitaev's model. In section 7, we invoke precisely this analogy. The crux of the selection rule on the allowed correlations (which forces all correlators be string type operators in both gauge theories and Kitaev's model) is Elitzur's theorem. Elitzur's theorem states that any quantity which does not transform as a singlet under local (gauge) symmetries must have a vanishing expectation value.

We now review Elitzur's theorem [18] in its more prominent use—that of gauge theories. In the theories of matter at lattice sites (σ_p) which are coupled to gauge fields (U_{pq}) which reside on links of the lattice [29, 30], the action is a sum of (i) a plaquette product of the gauge fields and (ii) a minimal coupling between the matter fields and the gauge fields. To illustrate, consider the simplest gauge theory (the Ising gauge theory) in which Ising gauge fields are coupled to Ising matter fields. Here, the action

$$S = -K\sum_{\square} U_{pq}U_{ql}U_{ln}U_{np} - J\sum_{pq}\sigma_p U_{pq}\sigma_q, \tag{B.1}$$

with $U_{pq} = \pm 1$ and $\sigma_p = \pm 1$. Many early results were found by [30]. This action is invariant under the local (gauge) transformations $\sigma_p \to \eta_p\sigma_p$, $U_{pq} \to \eta_p U_{pq}\eta_q$ with, at any site p, $\eta_p = \pm 1$. Let us define gauge-invariant link variables by $z_{pq} \equiv \sigma_p U_{pq}\sigma_q$. The action

is a functional of $\{z_{pq}\}$. Any correlator which involves a product of any number of z's is invariant under the local gauge transformations and consequently does need not vanish by Elitzur's theorem [18]. In matter coupled gauge theories with $J \neq 0$ in equation (B.1), any correlator of the form

$$\left\langle \prod_{pq \in C} z_{pq} \right\rangle \tag{B.2}$$

for any contour C (either open or closed or a contour C which is the union of smaller open/closed contours) is gauge-invariant and need not vanish by Elitzur's theorem. For closed contours C, the average of equation (B.2) is the 'Wilson loop' [29] which makes an appearance also in 'pure' ($J = 0$) gauge theories. These *string* type correlators (as well as related topological percolation transitions and crossovers [31]) provide the only means for probing the behavior of this system. Precisely such *string* operators (both closed- and open-ended variants) are the sole nonzero correlators than are allowed by symmetry in Kitaev's model (see section 7.2).

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