Exact Results for Spin Dynamics and Fractionalization in the Kitaev Model

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We present certain exact analytical results for dynamical spin correlation functions in the Kitaev Model. It is the first result of its kind in nontrivial quantum spin models. The result is also novel: in spite of the presence of gapless propagating Majorana fermion excitations, dynamical two spin correlation functions are identically zero beyond nearest neighbor separation. This shows existence of a gapless but short range spin liquid. An unusual, *all energy scale fractionalization* of a spin-flip quanta, into two infinitely massive π fluxes and a dynamical Majorana fermion, is shown to occur. As the Kitaev Model exemplifies topological quantum computation, our result presents new insights into qubit dynamics and generation of topological excitations.

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In the field of quantum computers and quantum communications, practical realizations of qubits that are robust and escape decoherence is a foremost challenge [1]. In this context, Kitaev proposed [2] certain emergent topological excitations in strongly correlated quantum many body systems as robust qubits. In a fault tolerant quantum computation scheme [2–4], Kitaev constructed a nontrivial and exactly solvable two-dimensional spin model [2] and illustrated the basic ideas. In some limit it also becomes the celebrated "toric code" Hamiltonian. The Kitaev Model has come closer to reality, after recent proposals for experimental realizations [5,6] and schemes for manipulation and detection [7]. In initialization, error correction, and readout operations, it is "spins" rather than emergent topological degrees of freedom that are directly accessed from outside. Thus an understanding of dynamic spin correlations is of paramount importance.

We present certain exact analytical results for time dependent spin correlation functions in arbitrary eigenstates of the Kitaev Model. Our results are nontrivial and novel, with possible implications for new quantum computational schemes. Further, our result is unique in the sense that it is the first exact result for equilibrium dynamical spin correlation functions in a nontrivial 2D quantum spin model. Our result is valid for any lattice size with periodic boundary conditions.

We show that the dynamical two spin correlation functions are short ranged and vanish identically beyond nearest neighbor sites for all time t, for all values of the coupling constants J_x, J_y, and J_z, even in the domain of J's where the model is gapless. Our result shows rigorously that it is a short range quantum spin liquid and long range spin order is absent. We obtain a compact form for the time dependence, which makes the physics transparent.

The Kitaev Model supports dynamical Majorana fermion and static π-flux eigen excitations, having their own sharp quantum numbers. In particular, any component of local spin operator σ_i^α creates (Fig. 3) one Z_2 charge at site i and one pair of bound Z_2 fluxes in appropriate plaquettes sharing site i. We show that this composite undergoes quantum number fractionalization [8,9], in the sense that the Z_2 charge and flux get spatially separated.

In the present Letter we have restricted our calculation to dynamical correlation functions for time independent Hamiltonians, in arbitrary eigenstates and thermal states. In actual quantum computations, key manipulations such as braiding involve parametric change of the Hamiltonian and adiabatic transport of topological degrees of freedom [7]. In principle, some of the needed "nonequilibrium" dynamical correlation functions may be obtained by convolution of our results with suitable Berry phase factors.

In our work, we follow Kitaev [2] and use the Majorana fermion representation of spin-half operators and an enlarged Hilbert space. What is remarkable is that, because of the presence of certain local conserved quantities in the Kitaev Model, Hilbert space enlargement only produces "gauge copies", without altering the energy spectrum. This luxury is absent for standard 2D Heisenberg models when studied using an enlarged fermionic Hilbert space [9,10].

The Kitaev Hamiltonian is

$$H = -J_x \sum_{\langle ij\rangle_x} \sigma_i^x \sigma_j^x - J_y \sum_{\langle ij\rangle_y} \sigma_i^y \sigma_j^y - J_z \sum_{\langle ij\rangle_z} \sigma_i^z \sigma_j^z, \quad (1)$$

where i, j label the sites of a hexagonal lattice, $\langle ij\rangle_a$, $a = x$, y, z denotes the nearest neighbor bonds in the ath direction. The model has no continuous global spin symmetry. All bond interactions are Ising like, albeit in different quantization directions x, y, and z, in three different bond types, making the model quantum mechanical. Further, it renders a high degree of frustration; that is, even at a classical level a given spin cannot satisfy conflicting demands, from 3 neighbors, of orientations in mutually orthogonal directions. The model has a rich local symmetry. A specific product of 6 spin components in every elementary hexagon, $\sigma_1^y\sigma_2^z\sigma_3^x\sigma_4^y\sigma_5^z\sigma_6^x$ (Fig. 1), commutes with the full Hamiltonian. Thus there is one conserved Z_2 charge ± 1

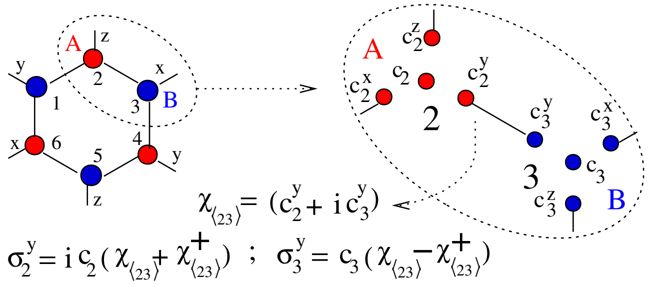

FIG. 1 (color online). Elementary hexagon and "bond fermion" construction. A spin is replaced with 4 Majorana fermions (c, c^x, c^y, c^z). Bond fermion $\chi_{\langle 23\rangle}$ and spin operator are defined. A and B denote the sublattice index.

at every dual lattice site of the hexagonal lattice. The model is exactly solvable and becomes noninteracting Majorana fermions, propagating in the background of static Z_2 gauge fields. Different possible Z_2 charges separate the Hilbert space into super selected sectors. The ground state corresponds to all Z_2 charges $= +1$. In this sector, for a range of J's, Majorana fermions are gapless, including the special point $J_x = J_y = J_z$.

Following Kitaev, we represent the spins in terms of Majorana fermions. At each site, we define 4 Majorana fermions, c^α, $\alpha = 0, x, y, z$, with $\{c^\alpha, c^\beta\} = 2\delta_{\alpha\beta}$. Four Majorana (real) fermions make two complex fermions, making the Hilbert space four dimensional. Notionally, Hilbert space dimension of a Majorana fermion is $\sqrt{2}$, an irrational number, reminding us that Majorana fermions have to occur in pairs (leading to a $\sqrt{2}\times\sqrt{2} =$ 2-dimensional Fock space) in physical problems.

The dimension of Hilbert space of N spins is 2^N. The enlarged Hilbert space has a dimension $4^N = (\sqrt{2}\times\sqrt{2}\times\sqrt{2}\times\sqrt{2})^N$. State vectors of the physical Hilbert space satisfy the condition

$$D_i|\Psi\rangle_{\rm phys} = |\Psi\rangle_{\rm phys}; \qquad D_i \equiv c_i c_i^x c_i^y c_i^z. \tag{2}$$

Henceforth we will denote c_i^0 by c_i. The spin operators can then be represented by

$$\sigma_i^a = i c_i c_i^a, \qquad a = x, y, z. \tag{3}$$

When projected into the physical Hilbert space, the operators defined above satisfy the algebra of spin 1/2 operators, $[\sigma_i^a, \sigma_j^b] = i\epsilon_{abc}\sigma^c\delta_{ij}$. The Hamiltonian written in terms of the Majorana fermions is

$$H = -\sum_{a=x,y,z} J_a \sum_{\langle ij\rangle_a} i c_i \hat{u}_{\langle ij\rangle_a} c_j, \tag{4}$$

with $\hat{u}_{\langle ij\rangle_a} \equiv i c_i^a c_j^a$. Kitaev showed that $[H, \hat{u}_{\langle ij\rangle_a}] = 0$ and $u_{\langle ij\rangle a}$ become constants of motion with eigenvalues $u_{\langle ij\rangle_a} = \pm 1$. The variables $u_{\langle ij\rangle_a}$ are identified with static (Ising) Z_2 gauge fields on the bonds. Kitaev Hamiltonian [Eq. (6)] has a local Z_2 gauge invariance in the extended Hilbert space. For practical purposes, the local Z_2 gauge transformation amounts to $u_{\langle ij\rangle a} \to \tau_i u_{\langle ij\rangle a}\tau_j$, with $\tau_i \pm 1$. Equation (2) is the Gauss law and the physical subspace is the gauge invariant sector.

In the gauge field sector we have gauge invariant Z_2 vortex charges ± 1 (0 and π fluxes), defined as product of $u_{\langle ij\rangle a}$ around each elementary hexagonal plaquette.

Equation (6), with conserved $\hat{u}_{\langle ij\rangle_a}$, is the Hamiltonian of free Majorana fermions in the background of frozen Z_2 vortices or π fluxes. Since Z_2 gauge fields have no dynamics, all eigenstates can be written as products of a state in the $2^{(1/2)N}$-dimensional Fock space of the c_i Majorana fermions and the $(2)^{(3/2)N}$-dimensional space of Z_2 link variables. We will refer to the former as *matter sector* and the latter as *gauge field sector.* Gauge copies (eigenstates with same energy eigenvalues) spanning corresponding extended Hilbert space are obtained by local gauge transformations $u_{\langle ij\rangle a} \to \tau_i u_{\langle ij\rangle a}\tau_j$.

Now to facilitate the exact computation of all spin correlation functions we introduce a simple but key transformation. We call this as "bond fermion" formation. In the process we also discover a "quantum fractionalization" phenomenon in the Kitaev Model that has an unusual validity at all energy scales. Hereinafter, we follow the convention that i in the bond $\langle ij\rangle_a$ belongs to A and j to B sublattice. We define complex fermions on each link as

$$\chi_{\langle ij\rangle_a} = \tfrac{1}{2}(c_i^a + i c_j^a). \tag{5}$$

The link variables are related to the number operator of these fermions, $\hat{u}_{\langle ij\rangle_a} \equiv i c_i^a c_j^a = 2\chi^\dagger_{\langle ij\rangle_a}\chi_{\langle ij\rangle_a} - 1$. All eigenstates can therefore be chosen to have a definite χ fermion occupation number. The Hamiltonian is then block diagonal, each block corresponding to a distinct set of χ fermion occupation numbers. Thus all eigenstates in the extended Hilbert space take the factorized form,

$$|\tilde{\Psi}\rangle = |\mathcal{M}_{\mathcal{G}}; \mathcal{G}\rangle \equiv |\mathcal{M}_{\mathcal{G}}\rangle|\mathcal{G}\rangle \tag{6}$$

and

$$\chi^\dagger_{\langle ij\rangle_a}\chi_{\langle ij\rangle_a}|\mathcal{G}\rangle = n_{\langle ij\rangle_a}|\mathcal{G}\rangle, \tag{7}$$

where $n_{\langle ij\rangle_a} = \frac{u_{\langle ij\rangle_a}+1}{2}$ and $|\mathcal{M}_{\mathcal{G}}\rangle$ is a many body eigenstate in the matter sector, corresponding to a given Z_2 field of $|\mathcal{G}\rangle$. In terms of bond fermions, spin operators become

$$\sigma_i^a = i c_i(\chi_{\langle ij\rangle_a} + \chi^\dagger_{\langle ij\rangle_a}); \qquad \sigma_j^a = c_j(\chi_{\langle ij\rangle_a} - \chi^\dagger_{\langle ij\rangle_a}). \tag{8}$$

Three components of a spin operator at a site get connected to three different Majorana fermions defined on the three different bonds. Written in the above form, the effect of σ_i^a on any eigenstate, which we refer to as a "spin flip", becomes clear. In addition to adding a Majorana fermion at site i, it changes the bond fermion number from 0 to 1 and vice versa (equivalently, $u_{\langle ij\rangle a} \to -u_{\langle ij\rangle a}$), at the bond $\langle ij\rangle a$. The end result is that one π flux each is added to two plaquettes that are shared by the bond $\langle ij \rangle a$ (Fig. 2). We denote this symbolically as

$$\sigma_i^a = ic_i(\chi_{\langle ij \rangle_a} + \chi^\dagger_{\langle ij \rangle_a}) \to ic_i \hat{\pi}_{1\langle ij \rangle a} \hat{\pi}_{2\langle ij \rangle a} \quad (9)$$

with $\hat{\pi}_{1\langle ij \rangle a}$ and $\hat{\pi}_{2\langle ij \rangle a}$ defined as operators that add π fluxes to plaquettes 1 and 2 shared by a bond $\langle ij \rangle a$ (Fig. 2). Further $\hat{\pi}^2_{1\langle ij \rangle a} = 1$, since adding two π fluxes is equivalent to adding (modulo 2π) zero flux.

Now we wish to calculate spin-spin correlation functions in physical subspace. Since the spin operators are gauge invariant, we can compute the correlation in any gauge fixed sector and the answer will be the same as in the physical gauge invariant subspace. (We have confirmed this by a calculation in the projected physical subspace.) So we consider the 2-spin dynamical correlation functions, in an arbitrary eigenstate of the Kitaev Hamiltonian in some fixed gauge field configuration $\mathcal{G}$,

$$S_{ij}^{ab}(t) = \langle \mathcal{M}_{\mathcal{G}} | \langle \mathcal{G} | \sigma_i^a(t) \sigma_j^b(0) | \mathcal{G} \rangle | \mathcal{M}_{\mathcal{G}} \rangle. \quad (10)$$

Here $A(t) \equiv e^{iHt} A e^{-iHt}$ is the Heisenberg representation of an operator A, keeping $\hbar = 1$. As discussed above,

$$\sigma_j^b(0) | \mathcal{G} \rangle | \mathcal{M}_{\mathcal{G}} \rangle = c_i(0) | \mathcal{G}^{ia} \rangle | \mathcal{M}_{\mathcal{G}} \rangle \quad (11)$$

$$\sigma_i^a(t) | \mathcal{G} \rangle | \mathcal{M}_{\mathcal{G}} \rangle = e^{i(H-E)t} c_j(0) | \mathcal{G}^{jb} \rangle | \mathcal{M}_{\mathcal{G}} \rangle, \quad (12)$$

where $|\mathcal{G}^{ia(jb)}\rangle$ denote the states with extra π fluxes added to $\mathcal{G}$ on the two plaquettes adjoining the bond $\langle ik \rangle_a$, $\langle lj \rangle_b$ and E is the energy eigenvalue of the eigenstate $|\mathcal{G}\rangle|\mathcal{M}_{\mathcal{G}}\rangle$. Since the Z_2 fluxes on each plaquette are conserved quantities, it is clear that the correlation function in Eq. (10) which is the overlap of the two states in Eqs. (11) and (12) is zero unless the spins are on neighboring sites. Namely, we have proved that the dynamical spin-spin correlation has the form

$$S_{ij}^{ab}(t) = g_{\langle ij \rangle_a}(t) \delta_{a,b}, \quad ij \text{ nearest neighbors}$$
$$= 0 \quad \text{otherwise.} \quad (13)$$

Computation of $g_{ij}(0)$ is straightforward in any eigenstate $|\mathcal{M}_{\mathcal{G}}\rangle$. For the ground state where conserved Z_2 charges

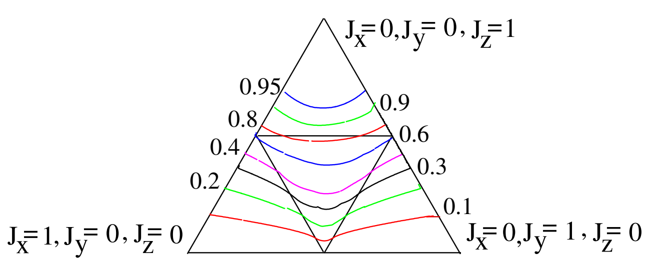

FIG. 2 (color online). Contour plot of nonzero $\langle \sigma_i^z \sigma_j^z \rangle$ in the parameter space. The distances from any point in the outer triangle to its three sides are in the ratio J_x:J_y:J_z. Numerical number attached with the contour is the value of $\langle \sigma_i^z \sigma_j^z \rangle$. The middle triangle is the gapless phase.

are unity at all plaquettes, the equal time 2-spin correlation function for the bond $\langle ij \rangle z$ is given by the analytic expression:

$$\langle \sigma_i^z \sigma_j^z \rangle \equiv S^{zz}_{\langle ij \rangle z}(0) = \frac{\sqrt{3}}{16\pi^2} \int_{BZ} \cos\theta(k_1, k_2) dk_1 dk_2, \quad (14)$$

where $\cos\theta(k_1, k_2) = \frac{\epsilon_k}{E_k}$, $E_k = \sqrt{(\epsilon_k^2 + \Delta_k^2)}$, in the Brillouin zone. $\epsilon_k = 2(J_x \cos k_1 + J_y \cos k_2 + J_z)$, $\Delta_k = 2(J_x \sin k_1 + J_y \sin k_2)$, $k_1 = \mathbf{k} \cdot \mathbf{n}_1$, $k_2 = \mathbf{k} \cdot \mathbf{n}_2$, and $\mathbf{n}_{1,2} = \frac{\sqrt{3}}{2} \mathbf{e}_y \pm \frac{1}{2} \mathbf{e}_x$ are unit vectors along x and y type bonds. At the point, $J_x = J_y = J_z$, we get $S^{zz}_{\langle ij \rangle a}(0) = 0.52$. The contour plot of $\langle \sigma_i^z \sigma_j^z \rangle$ in the parameter space is shown in Fig. 2. $\langle \sigma_i^x \sigma_j^x \rangle$ and $\langle \sigma_i^y \sigma_j^y \rangle$ can be obtained from Eq. (14) by the substitutions $J_x \to J_z \to J_y \to J_x$ and $J_x \to J_y \to J_z \to J_x$, respectively.

To compute $g_{\langle ij \rangle_a}(t)$ we substitute for the σ's from Eqs. (5) and (6). We choose a gauge where $u_{\langle ij \rangle_a} = -1$ implying $\chi^\dagger_{\langle lj \rangle_b} | \mathcal{G} \rangle = \chi^\dagger_{\langle ik \rangle_b} | \mathcal{G} \rangle = 0$. We note that the above conditions imposed at $t = 0$ will continue to be true at all times since the bond fermion numbers are conserved. We then have

$$g_{\langle ij \rangle a}(t) = \langle \mathcal{M}_{\mathcal{G}} | \langle \mathcal{G} | ic_i(t) \chi^\dagger_{\langle ij \rangle_a}(t) \chi_{\langle ij \rangle_a}(0) c_j(0) | \mathcal{G} \rangle | \mathcal{M}_{\mathcal{G}} \rangle. \quad (15)$$

The time dependence evolution can be expressed in terms of the Hamiltonian, and noting it is diagonal in the number operators $\chi^\dagger \chi$, we get

$$g_{\langle ij \rangle a}(t) = \langle \mathcal{M}_{\mathcal{G}} | e^{iH[\mathcal{G}^{ia}]t} ic_i(0) e^{-iH[\mathcal{G}^{ia}]t} (-1) c_j(0) | \mathcal{M}_{\mathcal{G}} \rangle, \quad (16)$$

where $H[\mathcal{G}^{ia}]$ is the tight binding Hamiltonian in the background of the static gauge field configuration $\mathcal{G}^{ia}$. The (-1) factor is $u_{\langle ij \rangle_a}$. This expression can be written in terms of the time evolution under $H[\mathcal{G}]$ as follows:

$$g_{\langle ij \rangle_a}(t) = \langle \mathcal{M}_{\mathcal{G}} | ic_i(t) T(e^{-2J_a \int_0^t u_{\langle ij \rangle a} c_i(\tau) c_j(\tau) d\tau})$$
$$\times u_{\langle ij \rangle_a} c_j(0) | \mathcal{M}_{\mathcal{G}} \rangle. \quad (17)$$

The above equation is written in an arbitrary gauge.

We have thus derived a simple but exact expression for the spatial dependence of the two spin dynamical correlation function. We have also obtained an exact expression for the time dependence in terms of the correlation functions of noninteracting Majorana fermions in the background of static Z_2 gauge fields. Equation (17) represents the propagation of a Majorana fermion in the presence of two injected fluxes. It can be treated as an x-ray edge problem and computed in terms of the Toeplitz determinant. We will not do this now but proceed to discuss some general features of our results.

The notion of fractionalization of spin-flip quanta is the natural interpretation of our results [8,9]. Consider time

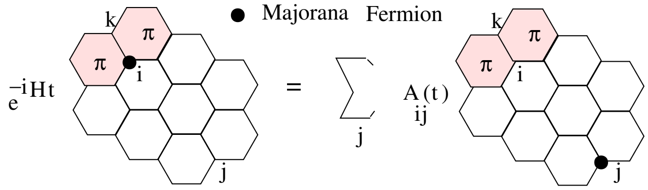

FIG. 3 (color online). Time evolution and fractionalization of a spin flip at $t = 0$ ($\sigma_i^z|\mathcal{M}_{\mathcal{G}}; \mathcal{G}\rangle$) at site i, into a π-flux pair and a propagating Majorana fermion.

evolution of a single "spin flip" at site i given in Eq. (12). Using the notation introduced in Eq. (9) we have

$$\sigma_i^a|\hat{\Psi}\rangle \equiv ic_i(t)T(e^{2u_{\langle ik\rangle a}J_a \int_0^t c_i(\tau)c_k(\tau)d\tau})\hat{\pi}_{\langle ik\rangle a1}\hat{\pi}_{\langle ik\rangle a2}|\hat{\Psi}\rangle. \tag{18}$$

A spin flip at site i at time $t = 0$ is a sudden perturbation to the matter (Majorana fermion) sector, as it adds two static π fluxes to adjoining plaquettes. The time ordered expression represents how a bond perturbation term, $i2u_{\langle ik\rangle a}J_a c_i c_k$, evolves the Majorana fermion state, in "interaction representation." At long time scale the resulting "shakeup" is simple and represents a rearrangement (power law type for gapless case) of the Majorana fermion vacuum to added static π-flux pairs. The Majorana fermion, produced by a spin flip, $c_i(t)$ propagates freely as a function of time.

As a spin flip at site i is a composite of a Majorana fermion and a π-flux pair [Eq. (13)], two spin correlation functions define the probability that we will detect the added composite at site j after a time t. As the added π-flux pairs do not move, the above probability is identically zero, unless sites i and j are nearest neighbors and spin components are $a = b$. This is why the spatial dependence of two spin correlation functions are sharply cut off at nearest neighbor separation. The asymptotic response to an added π-flux pair and free dynamics of the added Majorana fermion control the long time power law behavior of our only nonvanishing nearest neighbor two spin correlation function.

Further, for a given pair of nearest neighbor sites, only one Ising spin pair of a corresponding component is nonzero. Other pairs and cross correlation functions vanish. More specifically, for a given bond the only nonzero two spin correlation function is the bond energy.

What is unusual is that the above result is true in all eigenstates of the Kitaev Model, irrespective of energies. It follows that it is fundamental in topological quantum computation. In the presence of external magnetic field, the gauge fields $\hat{u}_{\langle ij\rangle}$ and the Z_2 flux operators do not commute with the Hamiltonian. The π fluxes acquire their own dynamics and have a bandlike motion. While the correlation functions are no longer exactly calculable we find that, at least for weak magnetic fields, the short range character of spin-spin correlation and quantum number fractionalization phenomenon survive.

Multispin correlation functions can be calculated in our formalism. Further, quantum entanglement, a key notion in quantum computation and quantum information, is ultimately connected with some complicated multispin correlation function. Preliminary calculations show that concurrence is zero for any two sites.

To summarize, this Letter presents certain exact analytical results for the spin dynamics and a spin-flip fractionalization scheme for the Kitaev Model. As this nontrivial spin model is also a model for topological quantum computation, our exact results should provide insights into qubit dynamics and possible ways of generating emergent topological qubits. Our formalism, which uses the factorized character of the eigenfunctions in the extended Hilbert space, is easily adapted to the calculation of multispin correlation functions, which is a key step in the calculation and understanding of quantum entanglement properties.

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