

Dynamic Response in the 2D Kitaev Model

Preliminary Oral Examination Paper

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Abstract

This report reviews the dynamic properties of the Kitaev model on the honeycomb lattice. The place of this exactly solvable model in the search for spin liquids is discussed along with the recent prospects for realization of the spin liquid state in the $A_2\text{IrO}_3$, $A=\text{Na, Li}$ materials. The exact solution of the model is given and the recent calculation of the two-spin dynamic correlation function is reviewed. We outline some technical advances in the calculation of spin correlation functions for the model. This leads to the possibility of a perturbative framework to calculate the dynamic structure factor, which could help distinguish a spin liquid state in an inelastic scattering experiment.

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I. MAGNETIC MATERIALS: ORDER AND CORRELATIONS

Most magnetic materials order at low temperatures. When competing interactions favor different simple orderings that cannot be simultaneously satisfied the system is said to be frustrated. These systems typically order at much lower temperatures. In the most

interesting cases the frustration leads to a large degeneracy in classical ground states so that only quantum fluctuations can distinguish a single ground state. If the system orders at zero temperature by some spontaneous symmetry breaking (SSB) to a state chosen by quantum fluctuations we call it order by disorder. Instead, we are interested in systems in which this degeneracy leads to fractionalized excitations without SSB and in this case we call the system a quantum spin liquid [1]. Below we will consider the concept of fractionalization in a review of the fractional excitations in the resonant valence bond state.

Experimental detection of a spin liquid state has proven difficult. Unlike the situation for conventional order, there is no local order parameter from which to detect this rare state. However, as we discuss more below, fractional excitations give rise to a distinct spectrum when compared to their ordered counterparts that can be seen in the dynamic structure factor. Structure factors can be measured so it is theoretically interesting to compute these to allow comparison with experiment. This is the main motivation for this project.

Here we consider an exactly solvable model system on the 2D honeycomb lattice due to Kitaev [2] for which an exact spin liquid state has been proven [2]. Only recently has the dynamic structure factor been computed for this model [3, 4] and work remains to compute the contributions to the structure factor from possible perturbing Hamiltonians [5]. Here we consider using the simple properties of this model to compute n -spin correlation functions, which can be used to study the dynamic structure factor perturbatively around the exact Kitaev point.

A. RVB and Fractionalization

To illustrate the physics of a spin liquid state and the types of properties we look for we begin with a review of the resonant valence bond (RVB) state. The RVB state first became important when Anderson used it to try and describe high temperature superconductivity [6] finding that the RVB states can give rise to superconductivity upon doping [7]. These exotic states were found interesting on their own soon after that and the RVB state still provides an intuitive picture of a spin liquid ground state [1].

In the presence of antiferromagnetic (AFM) exchange a pair of spin-1/2 particles prefers to be in the total spin-0 singlet state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ with the triplet (spin-1) state as an excited state. A valence bond state is one where spin-1/2 moments pair into these dimer

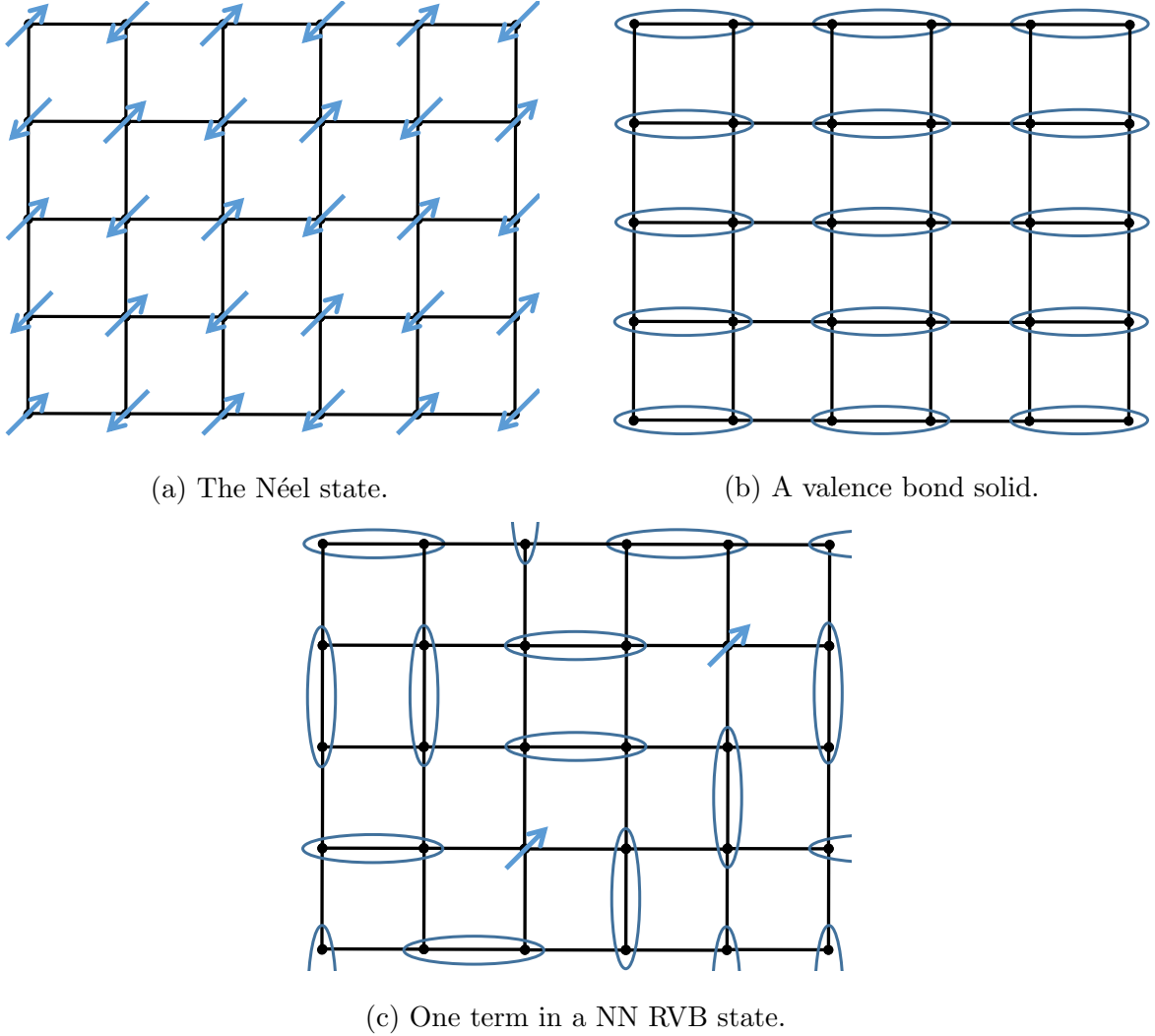


FIG. 1: Examples of different spin states on the square lattice [8].

states to minimize AFM exchange [7]. Two such states are illustrated on the square lattice in Figure 1 in contrast with the Néel ordered state in Figure 1a [8]. A system with the valence bond ground state in Figure 1b spontaneously breaks the translational symmetry and $\pi/2$ rotation symmetry forming a valence bond solid (VBS). One may wonder if it is possible for a valence bond ground state not to break translational symmetry. The nearest neighbor (NN) RVB state is given by the superposition of all dimer coverings of the lattice, one of which is illustrated in Figure 1c along with an excitation. An RVB ground state does not spontaneously break any lattice symmetries.

Of the three states just described the RVB has the most interesting excitation spectrum. Near the Néel state we may flip a single spin which is a spin-1 excitation. In the VBS state

we also have spin-1 excitations, such as the breaking a singlet dimer into two up spins. In the VBS if you try to separate two spin-1/2s you pay an energy cost that grows with distance to rearrange the crystal structure of dimers. However, in the resonating valence bond state the situation is very different. The spin-1 excitation of a dimer into two ‘up’ spins can break into two independently propagating parts, as illustrated in Figure 1c. Once separated these spin-1/2 excitations propagate freely at no energy cost. This is an example of fractionalization of excitations. In the spin liquid state the spin-1/2 excitations are known as spinons. Other excitations in the VBS are spin-1 excitations and have a well-defined dispersion relation such as small disturbances of the ordered state which are known as magnons or spin waves. However, the fractionalization of spin-1 particles into separate spin-1/2 particles is unique to valence bond systems in the spin liquid RVB state.

B. Detecting a spin liquid

The fractionalization of excitations in a spin liquid state can be probed with a number of spectroscopic techniques. One of the most common techniques for measuring dynamic spectra is inelastic neutron scattering (INS). Neutrons are convenient due to charge neutrality and the energy scale at which their wavelength is on the order of a few lattice constants (0.01 eV \leftrightarrow 100 K). For an inelastic scattering experiment like INS the essential physical property being measured is the Fourier transform of the dynamic correlation function, which we call the structure factor.

$$S_{ij}^{ab}(t) = \langle S_i^a(t) S_j^b(0) \rangle. \quad (1)$$

$$S^{ab}(\omega, q) = \int_{BZ} \frac{d^d q}{(\text{Area of BZ})} e^{iq} \int dt e^{i\omega t} S_{ij}^{ab}(t). \quad (2)$$

In the scattering experiment q is the momentum and ω the energy, which is deposited on some excitation in the system. The static structure factor $S(q) = \int d\omega S(\omega, q)$ reveals any order that the system has in the form of peaks at the points in the Brillouin zone at the ordering wave-vectors, around which the low-energy spin waves are excited.

The detection of a lack of Bragg peaks down to a small temperature is an important result for any magnetic material. However, measurement of the dynamics of the fractional excitations can provide positive evidence for a spin liquid state, especially when paired with a theoretical description or prediction. For one dimension the effects of fractionalization on

the dynamic spectrum are known and have been verified experimentally [9]. Both magnons and spinons themselves have a well-defined dispersion relation $\omega(q)$ appearing as a single curve in a 2D plot of $S(\omega, q)$. However, in the fractional excitations are created in pairs, say by a neutron interaction, whose total energy and total momentum are determined by the sum of two energies and two momenta that can add any vectorial way. Therefore, the dynamic structure factor due to the spinon continuum allows more than a single energy for a given momentum and ultimately corresponds to a continuum of cross section $S(\omega, k)$ for fixed k . A broad spectrum has already been measured in 2D by neutron scattering in herbertsmithite [10] (a Kagome-lattice antiferromagnet). Ultimately one would like to match the observed spectrum with a theoretical model. For herbertsmithite there has been some progress already, although work is still ongoing [11].

II. THE HEISENBERG-KITAEV MODEL AND THE IRIDATES

Now we discuss the Kitaev model, which is the model we start from to compute $S(q, \omega)$. We first review the model and then discuss the iridates where it is believed to be relevant.

The Kitaev model is tailored for its exact solvability. We consider nearest neighbor (NN) spins interacting on the honeycomb lattice, but instead of an anisotropic interaction we have only one of the three components of the spin coupled along each of the three types of bonds according to the labels in Figure 2. We write

$$H_K = - \sum_{\langle ij \rangle^a} S_i^a S_j^a, \quad (3)$$

Frustration in the Kitaev model comes from competition between different anisotropic interactions with neighbors, or competing non-commuting spin operators forcing dynamic frustration [12]. The benefit of the precise form of interaction is that each operator S_i^a appears in only one term in the Hamiltonian. As will be seen below, in a certain fermionic representation of the spins we can take advantage of this operator separation to find a number of conserved quantities. This is what makes the model exactly solvable and the reason it has become an extremely important example for a theoretical understanding of many concepts around spin liquids physics, as well as topological phases.

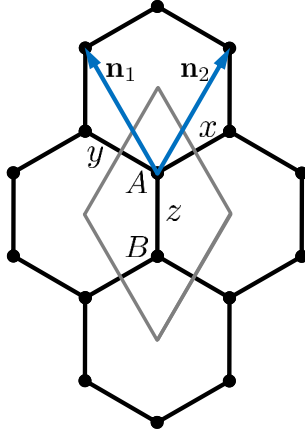


FIG. 2: The different bonds and sublattices and our choice of reciprocal lattice vectors and unit cell.

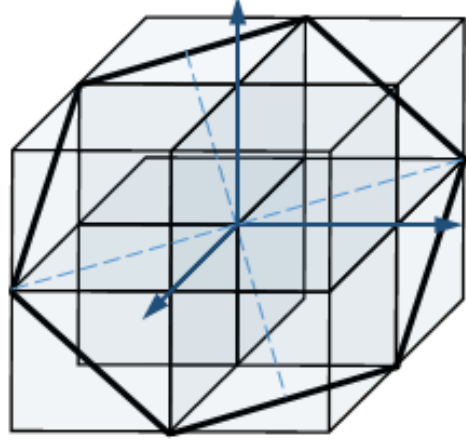


FIG. 3: The 2D honeycomb lattice formed within the 3D cubic structure of an A_2IrO_3 crystal.

A. Iridium Oxides

It would be very exciting if this carefully tuned model was realizable in a magnetic material that we can create in the lab. This would allow the direct comparison of experimental data and exact calculation. As we indicated in the last section, there has been some hope for finding a system of localized magnetic moments whose effective angular momentum corresponds to spin-1/2, with an interaction that is very closely related to that of the Kitaev model (3). The candidate materials are complex Iridium oxides of the form A_2IrO_3 . The key is spin-orbit interaction separating the $J_{\text{eff}} = 1/2$ state from the $J_{\text{eff}} = 3/2$ excited state. In the ion Ir^{4+} this interaction is very strong compared to the interactions between sites. Those orbitals (d_{xy} , d_{xz} , and d_{yz}) are degenerate containing one hole [13], and form a Kramers doublet of isospin states [14]. There are two effective momentum states, which form a local spin-1/2 degree of freedom [13].

$$|m_{\text{eff}} = \pm 1/2\rangle = \frac{1}{\sqrt{3}} (|xy, \mp\sigma\rangle \mp |yz, \mp\sigma\rangle + i|zx, \pm\sigma\rangle), \quad (4)$$

where xy and σ represent the orbital and spin states respectively, and so on. This effective spin state structure has been verified experimentally [13, 15].

The interactions between the local ‘spins’ is determined by finding the possible exchange paths [14] and the overlap integrals for the actual angular momentum states and then projecting those interactions onto the Kramer’s double doublet [13]. The primary NN terms in

this effective Hamiltonian are an anisotropic Kitaev term and Heisenberg exchange [14]

$$H = - \sum_{\langle ij \rangle^a} \left(J_1 S_i^a S_j^a + \sum_b J_2 S_i^b S_j^b \right),$$

where the label a is for the three different types of bonds that connect NN Ir atoms. These bonds form a honeycomb lattice within the cubic structure of edge-sharing octahedra with transition metal atoms in the center and oxygen at the corners. Here the parameters J_1 and J_2 are related to the hopping and potential terms in the effective Mott-Hubbard model [13].

This effective interaction is modified by a number of next-order interactions between the angular momentum states. Higher-order hopping paths, direct orbital overlaps, trigonal distortions, and spin-orbit energy splittings within the iridium two-electron propagator all contribute spin interactions other than the Kitaev term [12, 16]. Another possible issue with these materials is trigonal distortion effects [17–20].

We should immediately mention that if an Iridium-based material were found to be in a Kitaev spin liquid phase, neutron scattering may be difficult due to the large neutron cross section of Iridium ions [21–23]. However, there have been some worthwhile results using neutron scattering [24]. In addition, recent advancements in resonant inelastic X-ray scattering (RIXS) [22, 25, 26] have already been applied [23, 27, 28]. While the relationship between the RIXS cross section and the dynamic structure factor is less well-studied than that for neutron scattering, they have been shown to be closely related [29]. One may also consider electron spin resonance (ESR) to probe the dynamic structure factor and the dynamical correlation functions [3, 30]. Predictions for the Raman spectrum of the perturbative Kitaev-Heisenberg model have already been explored [31].

B. Experimental Observations and Interpretations

The candidate materials $A_2\text{IrO}_3$ with $A=\text{Na}, \text{Li}$ have not been found in a spin liquid phase. However, there are indications that the Li_2IrO_3 may be proximate to the spin liquid phase [12, 32]. X-ray scattering experiments show magnetic ordering [33] below a temperature that is low compared to the coupling strengths, indicating some frustration. This so-called zig-zag order could come from a third-nearest-neighbor exchange term [12], although other proposals have been made recently. However, the spin liquid state is not observed because of a relatively large perturbing Hamiltonian, in particular a Heisenberg exchange term ($\vec{S}_i \cdot \vec{S}_j$)

[12, 17, 18, 34]. Still the precise perturbations and the signs of their couplings are not agreed upon [34], and therefore a number of possible phase diagrams have been proposed placing Na_2IrO_3 and Li_2IrO_3 at different places with respect to the Kitaev phase [12, 34–37]. In the best case Li_2IrO_3 is near to the Kitaev spin liquid phase [12, 32].

Other theoretical proposals exist for the experimental realization/simulation of the Kitaev Hamiltonian including optical lattices [38], NMR systems [39], and by modifying the Heisenberg Hamiltonian for a short time with appropriate magnetic pulses, thereby creating a short lived Kitaev Hamiltonian [40].

III. EXACT SOLUTION OF THE PURE KITAEV MODEL

We solve the Hamiltonian as Kitaev did by representing the spins by majorana fermions in a way specific to the honeycomb lattice. Then we find a gauge degree of freedom corresponding to fermion number operators defined on the lattice links. Finally, the remaining degree of freedom is diagonalized by a reciprocal space Bogoliubov transformation.

A. Majoranas

The Kitaev majorana basis has 4 majorana fermions at each site c^μ , $\mu = 0, 1, 2, 3$, which are defined by their fermionic (anti)commutation relations

$$\{c_i^\mu, c_j^\nu\} = 2\delta^{\mu\nu}\delta_{ij}. \quad (5)$$

The 4 majoranas at each site make a 4D Hilbert space of states while the spin Hamiltonian has a 2D manifold of states per site. That is, this basis is overcomplete. The spin algebra in the $SU(2)$ Hilbert space can be represented by a subspace of the extended Hilbert space as long as this space is preserved by our representations of the physical space operators S_i^a , and those representations obey the $SU(2)$ commutation relations. We define the physical Hilbert space at site i as the stabilizer of the operator $D_i = c_i c_i^x c_i^y c_i^z$, $D_i |\Psi\rangle_{\text{phys}} = |\Psi\rangle_{\text{phys}}$ [2, 41].

If we represent spins as a product of these majoranas $S_j^a = ic_j c_j^a$ the $SU(2)$ commutation relations $[S_i^a, S_j^b] = i\varepsilon^{abc} S_i^c \delta_{ij}$ are preserved in the physical Hilbert space. Moreover, the constraint operators D_j do commute with the spin operators so that we have a working representation of the spin algebra with unique spin operators [2].

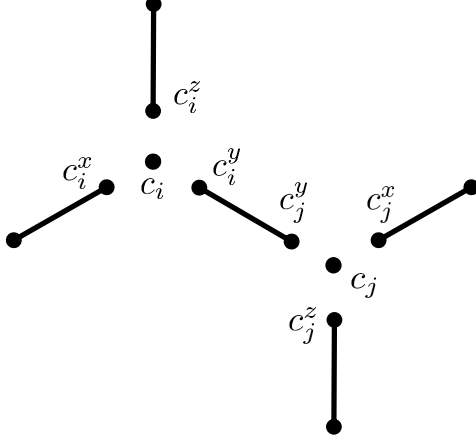


FIG. 4: A graphic representation of the majorana representation on the lattice sites.

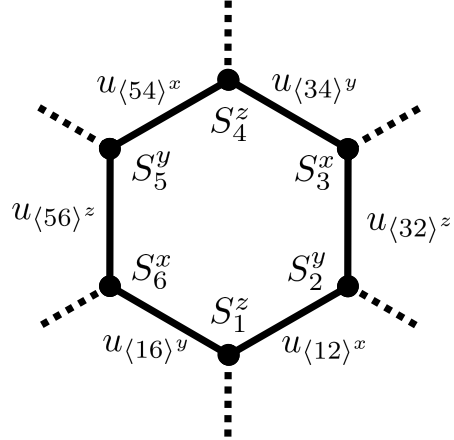


FIG. 5: The two representations of the plaquette operator.

Majorana fermions can be paired as the Hermitian and anti-Hermitian parts of a Dirac fermion. We choose to pair the c_j^a fermions across the a -bond from the site j as in Figure 4 so that three bond fermions are

$$\chi_{\langle ij \rangle^a} = \frac{1}{2} (c_i^a + i c_j^a) \quad \chi_{\langle ij \rangle^a}^\dagger = \frac{1}{2} (c_i^a - i c_j^a), \quad (6)$$

where we choose a convention for $\langle ij \rangle^a$ such that the index on the left is in the A sublattice and the index on the right is in the B sublattice. We point out that the link identifier $\langle ij \rangle^a$ requires only two of i , j , and a to specify a lattice link. Switching the sublattices switches $\chi_{\langle ij \rangle^a}$ and $\chi_{\langle ij \rangle^a}^\dagger$. We write then

$$\begin{aligned} H_K &= \sum_{\langle ij \rangle^a} J^a c_i c_i^a c_j c_j^a \\ &= i \sum_{\langle ij \rangle^a} c_i c_j \left(2 \chi_{\langle ij \rangle^a}^\dagger \chi_{\langle ij \rangle^a} - 1 \right) \\ &= \sum_{\langle ij \rangle^a} J^a u_{\langle ij \rangle^a} i c_i c_j, \end{aligned} \quad (7)$$

which conserves the link-fermions since they appear only as a number operator (They commute with the Hamiltonian, as well as each other). The most interesting choice for $u_{\langle ij \rangle^a} = 2 \chi_{\langle ij \rangle^a}^\dagger \chi_{\langle ij \rangle^a} - 1$ is the one that gives the ground state [2]. It follows from a theorem by Lieb [2, 42] that the ground state has zero flux, where the flux is defined by the operator

(see Figure 5)

$$W_p = S_1^z S_2^y S_3^x S_4^z S_5^y S_6^x = -u_{\langle 12 \rangle^x} u_{\langle 32 \rangle^z} u_{\langle 34 \rangle^y} u_{\langle 54 \rangle^x} u_{\langle 56 \rangle^z} u_{\langle 16 \rangle^y}. \quad (8)$$

That is, we should think of $u_{\langle ij \rangle^a}$ as a gauge degree of freedom, with the fermionic representation redundant. However, this representation is useful for the calculation of correlation functions so we keep it below [41]. The gauge choice simply fixes our representation and we can perform the remaining calculations in any gauge [2, 41]. We choose $u_{\langle ij \rangle^a} = 1$ so that $\chi_{\langle ij \rangle^a}^\dagger |0\rangle = 0$.

B. Diagonalization

The remaining Hamiltonian is simply one for the fermions c_j . We can diagonalize this one-particle Hamiltonian by a Bogoliubov transformation in reciprocal space. Kitaev diagonalized this Hamiltonian in terms of majoranas [2]. We follow Knolle [3] and choose to first write the dispersive majoranas in terms of a single complex fermion. We pair them by combining the A and B fermions in each unit cell, so that the resulting complex fermions is associated with a unit cell μ [3].

$$f_\mu = \frac{1}{2} (c_{\mu A} + i c_{\mu B}) \quad f_\mu^\dagger = \frac{1}{2} (c_{\mu A} - i c_{\mu B}). \quad (9)$$

Note that the choice of unit cell and hence f_μ distinguishes the bond connecting the two sites in the cell.

The effective Hamiltonian is one of hopping and superconductivity of these unit-cell fermions f_μ .

$$\begin{aligned} H &= \sum_{\langle ij \rangle^a} J^a i c_i c_j \\ &= \sum_{\mu} i \left[J^z c_\mu^A c_\mu^B + J_x c_\mu^A c_{\mu+n_1}^B + J_y c_\mu^A c_{\mu+n_2}^B \right] \\ &= \sum_k \left[2 f_k^\dagger f_k (J^z + J^x \cos(n_1 k) + J^y \cos(n_2 k)) - J^z + f_k f_{-k} (J^x e^{-i n_1 k} + J^y e^{-i n_2 k}) + \text{h.c.} \right] \\ &= \sum_k \left[f_k^\dagger f_k 2 \text{Re} \Gamma_k - J_z + (f_k f_{-k} - f_{-k}^\dagger f_k^\dagger) i \text{Im} \Gamma_k \right], \end{aligned} \quad (10)$$

where we exchanged site indices (i, j) with indices for the unit cell μ and sublattice A/B . In the last step we used that the operator $f_k f_{-k}$ is odd under $k \rightarrow -k$, which can be

switched in the summation, so that it only couples to part of $(J^x e^{-in_1 k} + J^y e^{-in_2 k})$ that is odd in k , and similarly for the Hermitian conjugate (the term $odd \times even$ sums to zero since the BZ limits of integration are symmetric in k). We have also defined the function $\Gamma_k = J^z + J^x e^{in_1 k} + J^y e^{in_2 k}$. The reciprocal space Hamiltonian is easily diagonalized by a Bogoliubov transformation.

$$H = \sum_k \begin{pmatrix} f_k^\dagger \\ f_{-k} \end{pmatrix}^T \begin{pmatrix} 2 \operatorname{Re} \Gamma_k & i \operatorname{Im} \Gamma_k \\ -i \operatorname{Im} \Gamma_k & 0 \end{pmatrix} \begin{pmatrix} f_k \\ f_{-k}^\dagger \end{pmatrix} - \sum_k J_z \quad (11)$$

$$= \sum_k \begin{pmatrix} a_k^\dagger \\ a_{-k} \end{pmatrix}^T \begin{pmatrix} |\Gamma_k| & 0 \\ 0 & -|\Gamma_k| \end{pmatrix} \begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix} + \sum_k [J^x \cos(n_1 k) + J^y \cos(n_2 k)], \quad (12)$$

where the Bogoliubov quasiparticles are related by a unitary matrix [3]

$$\begin{pmatrix} f_k \\ f_{-k}^\dagger \end{pmatrix} = \begin{pmatrix} \cos \theta_k & i \sin \theta_k \\ i \sin \theta_k & \cos \theta_k \end{pmatrix} \begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix} \quad (13)$$

$$\sin 2\theta_k = -\frac{\operatorname{Im} \Gamma_k}{|\Gamma_k|} \quad \cos 2\theta_k = \frac{\operatorname{Re} \Gamma_k}{|\Gamma_k|}, \quad (14)$$

as can be checked by acting with this unitary matrix on the Hamiltonian matrix.

IV. DYNAMICS CALCULATIONS

We begin by reviewing the work that has been done in calculating dynamic correlation functions of the Kitav model.

A. Previous work

In addition to being able to diagonalize the Hamiltonian exactly in terms of the single f -fermions, the commutation properties of the link fermions with the Hamiltonian allow for the simplification of spin-spin correlation functions in terms of the ones for the f -fermions [41]. Recall that the spin operators $S_j^a = ic_j c_j^a$ are the product of a dispersive majorana c_i (a linear combination of f -fermions) and the majoranas c_i^a which we write in terms of the link fermions $\chi_{\langle ij \rangle}^{(\dagger)a}$. Also, our gauge choice $\langle \chi_{\langle ij \rangle}^{(\dagger)a} \chi_{\langle ij \rangle}^a \rangle = 1$ is such that $\chi_{\langle ij \rangle}^{(\dagger)a} |0\rangle = 0$. Therefore, since the c_i fermions do not affect the gauge structure the link fermion operators coming from the spin operators must destroy the same link fermions that it creates. For the

two spin correlation function $\langle S_i^a S_j^b \rangle$ this implies that the spins must be nearest neighbors (or same site) operators of like components. Therefore we find [41]

$$\begin{aligned}\langle S_i^a S_j^b \rangle &= i \langle c_i \chi_{\langle ij \rangle^a}^\dagger c_j \chi_{\langle ij \rangle^a} \rangle \delta^{ab} \delta_{\langle ij \rangle^a} \\ &= -i \langle c_i c_j \rangle \delta^{ab} \delta_{\langle ij \rangle^a} \\ &= - \left(2 \langle f_\mu^\dagger f_\mu \rangle - 1 \right) \delta^{ab} \delta_{\langle ij \rangle^a},\end{aligned}\tag{15}$$

As shown in ref. 41, the dynamic correlation function can also be written in terms of a propagator for the f -fermions, but the link fermions in the spin operators change the background gauge $u_{\langle ij \rangle^a}$ that the f -fermions requiring the introduction of a time dependent potential [41]. This result can be achieved by commuting the link fermion operators with the time evolution operator e^{iHt} and re-exponentiating an effective Hamiltonian [41].

$$\langle T S_i^a(t) S_j^b(0) \rangle = i \langle c_i \chi_{\langle ij \rangle^a}^\dagger e^{iHt} c_j \chi_{\langle ij \rangle^a} \rangle \delta^{ab} \delta_{\langle ij \rangle^a} \tag{16}$$

$$= -i \langle T c_i e^{i(H + \hat{V}_{\langle ij \rangle^a})t} c_j \rangle \delta^{ab} \delta_{\langle ij \rangle^a}, \tag{17}$$

where $A(t) = e^{-iHt} A e^{iHt}$, T is the time-ordering operator, and $\hat{V}_{\langle ij \rangle^a} = -2J^a i c_i c_j$. The resulting problem for the f -fermions is equivalent to an X-ray edge problem [3, 41], for which there exists extensive literature [43–47].

These results were extended to n -point correlations functions in 5, finding that n -spin correlation functions are non-vanishing only for correlation functions involving strings of an even number of NN and same-site spins. In the same paper they use Wicks theorem in the fermionic language to reduce the n -spin problem to the calculation of propagators in the presence of the time-dependent potentials. In ref. 5 the effects of a perturbing magnetic field were considered by solving for the propagators in the limit of large t and large r [5].

More recently, the exact calculation two point function, and therefore the dynamic spin structure factor (and not just the effects of a magnetic field) was performed in ref. 3. They solve for the propagator in the presence of a time-dependent potential using Dyson's equation, which they solve numerically using integrals transformations that are used in the study of integral equations. The non-interacting propagator is calculated using the diagonalization presented above and the numerical analysis can be improved by trading the reciprocal space integrals above for integrals over the density of states (DOS) and another spectral function, both of which are calculated exactly in Appendix E.

B. New contributions

The author has begun the calculation of n -spin correlation functions for the Kitaev model. Unlike the work of ref. 5, we are interested in the result for all t and all r so that we can predict the types of spectra that could be found in an inelastic scattering experiment. Although the spatially short correlations imply that the large r results reflect effects of the perturbation, they cannot account for the changes in the dynamic structure factor. Rather, as the Fourier transform of the 2-spin correlation function, the structure factor depends on the the propagators at all t and all r . A calculation of the Fourier transform of the n -spin correlation functions would allow us to develop a similar perturbative framework in which to study the Kitaev model under any relevant perturbations, and in particular the ones in the iridates such as Heisenberg exchange, as well as in the presence of a magnetic field.

The dynamic structure factor for the Heisenberg-Kitaev model has recently been calculated numerically by exact diagonalization in ref. 4. The results show new features in the spectrum that are not present in the pure Kitaev model, even for very small perturbations [4]. This result suggest that if we knew the signatures of various possible perturbing Hamiltonians, the dynamic structure factor may help distinguish which proposed terms appear in the underlying Hamiltonian. If an Iridium compound were found to realize a Kitaev spin liquid phase, a measurement of the dynamic structure factor along with this calculation could help clarify the Hamiltonian, as well as offering a test of our understanding of the observed fractional excitations.

The extension of previous work on exact propagators [3] requires the solution of Dyson's equation for a more complicated time-dependent potential. If we take $g_{\mu\mu'}(t, 0)$ to be the propagator without the potential $V_{\nu\nu'}(\tau)$, and $G_{\mu\mu'}(t, 0)$ the interacting propagator, then this equation reads

$$G_{\mu\mu'}(t, 0) = g_{\mu\mu'}(t) + \sum_{\nu\nu'} \int_0^t d\tau g_{\mu\nu}(t - \tau) V_{\nu\nu'}(\tau) G_{\nu'\mu'}(\tau, 0), \quad (18)$$

where we have used that the free propagator $g_{\mu\mu'}(t)$ is time-translation invariant. This was solved numerically in ref. 3 for the NN 2-spin case. The integral equation becomes more complicated for higher spin correlation functions because then the integral in (18) involves multiple piece-wise constant terms in the potential. However, after recognizing that (18) is of the form of a Laplace-type convolution the author has found that this equation can be

solved exactly using integral transforms. This type of equation is special to the case where the support of the potential in time is slave to the times at which the fermion operators are taken. We have solved the general equation (18) directly by breaking the Green's function (the propagator) into its two distinct parts that come from time ordering. that is, solving it for $t > 0$ and $t < 0$ separately. This type of decomposition of the Green function is similar to that of advanced and retarded Green's functions [48, 49] but is well-suited to the exact solution of an integral equation with a Laplace-type convolution. The result is a simple algebraic relation in reciprocal between the interacting Green function and the Fourier transform of the appropriate kernel $K_{r,R}(t - \tau) = \sum_{R'} g_{r-R'}(t - \tau) \tilde{V}_{R',R}(t - \tau)$.

$$G_{r,r'}^{\pm}(\omega) = [\delta_{r,r'} - K_{r,R}^{\pm}(\omega)]^{-1} g_{r-r'}^{\pm}(\omega), \quad (19)$$

where $g^{+}(t) = \Theta(t)g(t)$ and similarly for the other operators, which leads to $G_{r,r'}(\omega) = G_{r,r'}^{+}(\omega) + G_{r,r'}^{-}(\omega)$.

The author hopes that this result along with some of the technical calculations outlined in the appendices will be enough to allow for the characterization of important 4- and 6-spin correlation functions, or at least their Fourier transform, allowing for a calculation of the contributions of important perturbations to the dynamic structure factor. A result like this for the exactly solvable Kitaev model could help us identify such a system if it were to be found, and provides a framework for the calculation of dynamic structure factors near a relatively simple point in the phase diagram, which may be extendable to other spin liquids whose ground state is only calculable at some mean field approximation.

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Appendix A: Effective potential

Here we complete the calculation of the effective f -fermion potential for the 2-point spin-spin correlation function. The calculation of n -spin correlation functions is similar with more fluxes turning on and off at different times corresponding to the times that the spin operators are created [5].

The necessary commutators are

$$\begin{aligned} [\chi_{\langle ij \rangle^a}^\dagger, H] &= J^a i c_i c_j [\chi_{\langle ij \rangle^a}^\dagger, (2\chi_{\langle ij \rangle^a}^\dagger \chi_{\langle ij \rangle^a} - 1)] \\ &\equiv \hat{V}_{\langle ij \rangle^a} \chi_{\langle ij \rangle^a}^\dagger, \end{aligned} \quad (\text{A1})$$

where $\hat{V}_{\langle ij \rangle^a} = -2J^a i c_i c_j$. Then

$$\chi_{\langle ij \rangle^a}^\dagger e^{itH} = e^{it(H + \hat{V}_{\langle ij \rangle^a})} \chi_{\langle ij \rangle^a}^\dagger. \quad (\text{A2})$$

Using this identity Eq. (16) becomes

$$\begin{aligned} \langle i c_i(t) \chi_{\langle ij \rangle^z}^\dagger(t) c_j(t') \chi_{\langle ij \rangle^a}(t') \rangle &= \langle i c_i \chi_{\langle ij \rangle^z}^\dagger e^{iH(t'-t)} c_j \chi_{\langle ij \rangle^a} \rangle \\ &= - \langle i c_i e^{i(H + \hat{V}_{\langle ij \rangle^a})(t'-t)} c_j \chi_{\langle ij \rangle^z}^\dagger \chi_{\langle ij \rangle^a} \rangle \\ &= - \langle i c_i(t) c_j(t') \rangle_{H + \hat{V}_{\langle ij \rangle^a}}, \end{aligned} \quad (\text{A3})$$

where in the last line we have expressed that the expectation value is taken for the effective time-dependent Hamiltonian $H'(\tau) = H + \hat{V}_{\langle ij \rangle^z}(\tau; t, t')$ [41]. The time-ordered result becomes

$$\begin{aligned} \langle T S_i^z(t) S_j^z(t') \rangle &= \Theta(t - t') \langle -i c_i(t) c_j(t') \rangle_{H + \hat{V}_{\langle ij \rangle^a}} - (t' \leftrightarrow t) \\ &= - \langle T i c_i(t) c_j(t') \rangle_{H + \hat{V}_{\langle ij \rangle^z}(\tau; t, t')}, \end{aligned} \quad (\text{A4})$$

which is precisely the result in eq. (17) of the text. The effective potential here is

$$\begin{aligned} \hat{V}_{\langle ij \rangle^z}(\tau; t, t') &= \hat{V}_{\langle ij \rangle^z} \chi(\tau; t, t') \\ \chi(\tau; t, t') &= \Theta(\tau - t') \Theta(t - \tau) + \Theta(t' - \tau) \Theta(\tau - t), \end{aligned} \quad (\text{A5})$$

where the function $\chi(\tau; t, t')$ here simply ensures that τ is in the interval created by t and t' . It is convenient to define [3] $v^a = -4J^a$ and to specify links by their unit cell and direction $\langle ij \rangle^z \rightarrow \mu, a$ so that

$$\hat{V}_{\mu, z} = \frac{1}{2} v^z i c_\mu^A c_\mu^B = v^z \left(f_\mu^\dagger f_\mu - \frac{1}{2} \right). \quad (\text{A6})$$

Appendix B: Dyson's equation

Here we derive the Dyson equation used in the text from the equation of motion of the fermionic operators following the work of [50] on the X-ray edge problem [45]. We start with

the equation of motion for the f^\dagger .

$$-i\partial_t f_k^\dagger(t) = \left[H', f_k^\dagger \right] (t),$$

where we have taken the time-dependent effective Hamiltonian $H'(\tau) = H + \hat{V}(\tau; t, t')$. The initial Hamiltonian H was given in Eq. (10) and the effective potential is a piecewise constant function of time $V(\tau) = \sum_R \chi_R(\tau) V_R$ which turns on and off potentials at positions R that share a unit cell with a spin operator in the correlation function under consideration. The locality of the potential in space breaks translational symmetry making the potential non-diagonal in reciprocal space.

$$\hat{V}(\tau) = \sum_R \chi_R(\tau) (f_R^\dagger f_R - 1) = \sum_{k,k'} V_{k,k'}(\tau) f_k^\dagger f_{k'}' - N_R, \quad (\text{B1})$$

where $N_R = \sum_R 1$ is a constant.

Since f^\dagger commutes with the superconducting term $(f_k f_{-k} - f^\dagger_{-k} f_k^\dagger)$ in H the Heisenberg equation of motion is closed in terms of the operator f_k^\dagger ,

$$-i\partial_t f_k^\dagger(t) = 2\text{Re}\Gamma_k f_k^\dagger(t) + \sum_q V_{k,q}(t) f_q^\dagger(t). \quad (\text{B2})$$

Now we can use the chain rule to evaluate the time derivative of the interacting green function,

$$\begin{aligned} -i\partial_t G_{k,k'}(t, t') &= -i\partial_t \left\langle T f_k^\dagger(t) f(t')_{k'} \right\rangle \\ &= \left\langle T \partial_t f_k^\dagger(t) f(t')_{k'} \right\rangle - i\delta(t - t') \left[f_k^\dagger(t) f(t)_{k'} + f(t)_{k'} f_k^\dagger(t) \right] \\ &= 2\text{Re}\Gamma_k G_{k,k'}(t, t') + \sum_q V_{k,q}(t) G_{q,k'}(t, t') - i\delta(t - t') \delta_{k,k'}. \end{aligned} \quad (\text{B3})$$

Or,

$$[\partial_\tau - 2i \text{Re} \Gamma_k] G_{k,k'}(\tau - t') = \delta(\tau - t') \delta_{k,k'} + i \sum_q V_{k,q}(\tau) G_{q,k'}(\tau, t'). \quad (\text{B4})$$

The only difference for the non-interacting propagator EOM is that we set $V_{k,q} = 0$. That is,

$$[\partial_t - 2i \text{Re} \Gamma_k] g_{k,k'}(t - t') = \delta(t - t') \delta_{k,k'}. \quad (\text{B5})$$

We find that without fluxes the spinon momentum is conserved $g_{k,k'}(t-t') = \delta_{k,k'}g_k(t-t')$. For a given k the equation of motion is solved by

$$g_k(t-t') = \frac{1}{2} [\text{sgn}(t-t') + 2g_k(0)] e^{2i \text{Re} \Gamma_k t}. \quad (\text{B6})$$

We can use the EOM for $g_k(t-t')$ to simplify the equation for $G_{k,k'}(t, t')$. We simply multiply Eq. (B4) by $g_k(t-\tau)$ and integrate over τ ,

$$\begin{aligned} \delta_{k,k'}g_k(t-t') + \int d\tau \sum_q g_k(t-\tau)V_{k,q}(\tau)G_{q,k'}(\tau, t') &= \int dt g_k(t-\tau) [\partial_\tau - 2i \text{Re} \Gamma_k] G_{k,k'}(\tau, t') \\ &= \int dt G_{k,k'}(\tau, t') [-\partial_\tau - 2i \text{Re} \Gamma_k] g_k(t-\tau) \\ &= \int dt G_{k,k'}(\tau, t') [\partial_t - 2i \text{Re} \Gamma_k] g_k(t-\tau) \\ &= \int dt G_{k,k'}(\tau, t') \delta(\tau-t) \\ &= G_{k,k'}(t, t'). \end{aligned} \quad (\text{B7})$$

Changing back to a spatial representation,

$$G_{r,r'}(t, t') = g_{r-r'}(t-t') + \int d\tau \sum_{R,R'} g_{r-R}(t-\tau)V_{R,R'}(\tau)G_{R,r'}(\tau, t') \quad (\text{B8})$$

This is the Dyson equation used in the text [3].

Appendix C: Interacting solution

We follow Ref. 3 to compute the two-point functions of the f -fermions in under the influence of $H'(\tau)$ in terms of the interaction under H using Dyson's equation. We define the free and interacting Green's functions for the f -fermions,

$$g_{\mu\mu'}(t, t') = i \langle T f_\mu^\dagger(t) f_\mu(t') \rangle_H, \quad G_{\mu\mu'}(t, t') = i \langle T f_\mu^\dagger(t) f_\mu(t') \rangle_{H+V}. \quad (\text{C1})$$

Dyson's equation for the interacting Green's function follows directly from the equation of motion [50]. The result is the following integral equation

$$G_{\mu\mu'}(t, 0) = g_{\mu\mu'}(t) + \sum_{\nu\nu'} \int_0^t d\tau g_{\mu\nu}(t-\tau)V_{\nu\nu'}(\tau)G_{\nu'\mu'}(\tau, 0), \quad (\text{C2})$$

where we have used that the free Green's function $g_{\mu\mu'}(t)$ is time-translation invariant. Also, we have written down a general potential $V_{\nu\nu'}(\tau)$, which accounts for general fluxes turning

on and off. For the case we were considering above $V_{\nu\nu'} = \delta_{\nu 0} \delta_{\nu' 0} v^z \chi(\tau; 0, t)$. In general, we are interested in higher order correlation functions that can be written in terms of products of two point-functions with different fluxes turning on and off based on the χ operators, coming directly from spins. The interaction term $V_{\nu\nu'}(\tau)$ knows the times when the fluxes turn on and off. Moreover, in space it has components only across NN unit cells, or the same cell.

The solution of the Dyson equation (C2) was obtained in Ref. 3 for the case of the NN two-point function by numerically solving an equivalent integral equation. We have solved the general equation (C2) directly by breaking the Green's function into its two distinct parts that come from time ordering, solving for $t > 0$ and $t < 0$ separately. This type of decomposition of the Green function is similar to that of advanced and retarded Green's functions [48, 49] but is well-suited to the exact solution of an integral equation with a Laplace-type convolution.

The potential $\hat{V} = \sum_{R,R'} V_{R,R'}(\tau) f_R^\dagger f_{R'}$ is actually slave to the spin-spin correlation function being considered. Therefore, the potential $V_{R,R'}(\tau)$ must only depend on the difference $(t - t')$ and differences $(t_i - t)$ or $(t_i - t')$, where the times t_i mark when background fluxes turn on and off. Further, if the integration bounds are set to $\int_t^{t'} d\tau$, then the effective potential $V_{R,R'}(\tau)$ can be replaced by a function $\tilde{V}_{R,R'}(t - \tau)$ that does not turn off at $\tau = t'$, and is therefore constant out to $\tau = \infty$. Similarly $\tilde{V}_{R,R'}(t - \tau)$ can be made continuous at $\tau = t$ by turning on the fluxes from $\tau = -\text{inf}$. In any case $\tilde{V}_{R,R'}(t - \tau)$ is independent of the difference $(t - t')$ and only a function of $t - t_i$ for $t_i \in (t, t')$, the time differences at which the potential changes value in between. In this case we can write the time integral in Dyson's equation as a convolution.

$$\sum_{R,R'} \int d\tau g_{r-R}(t - \tau) V_{R,R'}(\tau) G_{R,r'}(\tau, t') = \int d\tau \sum_R K_{r,R}(t - \tau) G_{R,r'}(\tau, t'), \quad (\text{C3})$$

where the Kernel is $K_{r,R}(t - \tau) = \sum_{R'} g_{r-R'}(t - \tau) \tilde{V}_{R',R}(t - \tau)$. This is the Volterra integral equation, which can be solved by Laplace transform [51] for functions on $(0, \infty)$. Define $g_{r-r'}^+(t - t') = \Theta(t - t') g_{r-r'}(t - t')$, and similarly $G_{r,r'}^+(t, t')$. If we multiply equation (C2) by $\Theta(t - t')$ and set $t' = 0$, we get

$$G_{r,r'}^+(t, 0) = g_{r-r'}^+(t) + \int_0^t d\tau \sum_R K_{r,R}^+(t - \tau) G_{R,r'}^+(\tau, 0), \quad (\text{C4})$$

where the integration bounds allow us to replace integrands with their half-line counterparts. In this case we can use the Fourier transform in place of the Laplace transform by letting the integration bounds go to infinity since the integrand is zero there. Similarly, multiply Eq. (C2) by $\Theta(-t)$ leads to an identical equation for $G_{r,r'}^-(t, 0) = \Theta(-t)G_{r,r'}(t, 0)$. The solutions are

$$G_{r,r'}^\pm(\omega) = [\delta_{r,r'} - K_{r,R}^\pm(\omega)]^{-1} g_{r-r'}^\pm(\omega), \quad (\text{C5})$$

where the matrix $K_{r,R}^\pm(\omega)$ is nonzero only for r, R that are at the site of, or NN of, a spin operator in the n -point functions under consideration. Therefore, the necessary matrix inversion in Eq. (C5) is a computationally trivial algebraic operation. Finally, the ‘interacting’ solution follows from $G_{r,r'}(t, 0) = G_{r,r'}^+(t, 0) + G_{r,r'}^-(t, 0)$. The decomposition is not well-behaved at $t = 0$ similar to the case for advanced and retarded Green’s functions. Therefore we get $G_{r,r'}(\omega) = G_{r,r'}^+(\omega) + G_{r,r'}^-(\omega)$

In the case for the 2-point function the only times in the problem are 0 and t so that $\tilde{V}_{R,r}$ can be taken to be a constant. If we choose the orientation of the unit cell to contain the two sites involved, then the potential is localized $\tilde{V}_{R,r} = \delta_{R,0}\delta_{R,r}v$. The solution reduces to

$$G_{0,0}^\pm(\omega) = \frac{g_{0,0}^\pm(\omega)}{1 - v g_{0,0}^\pm(\omega)}. \quad (\text{C6})$$

This is enough to specify the 2-point spin correlation function.

Equation (C6) should be compared with equation the approximate result in Fourier space obtained in Ref. 3 using the advanced Green’s function.

$$G_{0,0}^a(\omega) = \frac{g_0^a(\omega)}{1 - v g_0^a(\omega)}. \quad (\text{C7})$$

Appendix D: f -fermion propagators

The f -fermion correlation functions follow from the dynamics of the diagonalized fermions. Consider the dynamic two-point function $\langle a(t)a^\dagger(t') \rangle$. The ground state is defined as the state that is destroyed by a_k , and is constant in time. For $t' < t$ this creates an excitation into the excited eigenstate, whose energy is $|\Gamma_k|$ above the ground state. Therefore, by the Schroedinger equation for an eigenstate $i\partial_t\Psi = E\Psi$, we find that the wave function’s phase evolves by the dynamic action $-E(t - t')$. Finally, it is brought back to the ground state.

$$\langle T a_k(t) a_k^\dagger(t') \rangle = \Theta(t - t') e^{-i2|\Gamma_k|(t-t')}, \quad (\text{D1})$$

where $E_k = 2\Gamma_k$ is the energy of the k th excited stated. The corresponding result for the f -fermions is

$$\begin{aligned}
\langle T f_k^\dagger(t) f_k(t') \rangle &= \Theta(t - t') \langle f_k^\dagger(t) f_k(t') \rangle - \Theta(t' - t) \langle f_k(t') f_k^\dagger(t) \rangle \\
&= \Theta(t - t') \sin^2 \theta_k \langle a_k(t) a_k^\dagger(t') \rangle - \Theta(t' - t) \cos^2 \theta_k \langle a_k(t') a_k^\dagger(t) \rangle \\
&= \Theta(t - t') \frac{1}{2} \left(1 - \frac{\text{Re } \Gamma_k}{|\Gamma_k|} \right) e^{-i2|\Gamma_k|(t-t')} - \Theta(t' - t) \frac{1}{2} \left(1 + \frac{\text{Re } \Gamma_k}{|\Gamma_k|} \right) e^{i2|\Gamma_k|(t-t')} \\
&= \frac{1}{2} \left[\text{sgn}(t - t') - \frac{\text{Re } \Gamma_k}{|\Gamma_k|} \right] e^{-i2|\Gamma_k||t-t'|}.
\end{aligned} \tag{D2}$$

Appendix E: DOS

The calculation of density of states allows for the exchange of a multidimensional reciprocal space integral for a one dimensional integral, in this case over energy, of the product of the integrand and the density of states, or more generally some spectral function if the integrand cannot be completely written in terms of the energy. Moreover, there is physical information to be gotten from the density of states and the spectral weight. For calculation of the spinon Green function the two relevant reciprocal space integrals are

$$\int_{BZ} d^2k \frac{1}{\omega - E_k} = \int dE \frac{\rho(E)}{\omega - E} \tag{E1}$$

$$\int_{BZ} d^2k \frac{\text{Re } \Gamma_k / |\Gamma_k|}{\omega - E_k} = \int dE \frac{\rho_R(E)}{\omega - E}, \tag{E2}$$

where $E_k = 2|\Gamma_k|$ is the energy of the excited state with reciprocal lattice vector k , and we have exchanged each integral for relevant ones over energy space. The density of states and the chosen spectral weight are

$$\rho(E) = \int_{BZ} d^2k \delta(E - 2|\Gamma_k|) = \int_{BZ} \frac{E}{2} \delta((E/2)^2 - |\Gamma_k|^2) \tag{E3}$$

$$\rho_R(E) = \int_{BZ} d^2k \delta(E - 2|\Gamma_k|) \frac{\text{Re } \Gamma_k}{|\Gamma_k|} = \int_{BZ} \delta((E/2)^2 - |\Gamma_k|^2) \text{Re } \Gamma_k, \tag{E4}$$

where we have written the delta function in a more convenient form involving the square of the energy by using the appropriate delta function relation,

$$\delta[f(x)] = \sum_{x_0 \in f^{-1}(0)} \frac{\delta(x - x_0)}{|f'(x_0)|}. \tag{E5}$$

Here evaluate $\rho(E)$ and $\rho_R(E)$ exactly. Using x and y in place of k_x and k_y for convenience we get

$$|\Gamma_k| = 1 + 4 \cos^2 \frac{\sqrt{3}x}{2} + 4 \cos \frac{\sqrt{3}x}{2} \cos \frac{3y}{2} = 1 + 4u(u+v)$$

$$\text{Re } \Gamma_k = 2 \cos \frac{\sqrt{3}x}{2} + \cos \frac{3y}{2} = 2u + v,$$

where we have anticipated a change of variables to exchange trigonometric functions for rational functions of square roots. The simplest unit cell for integration is the diamond. The corners are the turning points of $\cos \frac{\sqrt{3}x}{2}$ and $\cos \frac{3y}{2}$. Reflection symmetry of the integrands allows us to integrate over a single quadrant (a quarter of the diamond),

$$\int_{BZ} d^2k = 2 \frac{\sqrt{3}}{2\pi} \frac{3}{2\pi} \int_0^{\frac{2\pi}{\sqrt{3}}} dx \int_0^{\frac{2\pi}{\sqrt{3}} - x/\sqrt{3}} dy = \int_{-1}^1 \frac{du}{\sqrt{1-u^2}} \int_{-u}^1 \frac{dv}{1-v^2}. \quad (\text{E6})$$

Upon evaluation of the inside integral we find $v_u = \frac{(E/2)^2 - 1}{4u} - u$, and

$$\int_{BZ} d^2k f(u, v) = \frac{1}{2\pi^2} \int_{u: -1 < -u < v_u < 1} du \frac{I(u, v_u)}{\sqrt{(1-u^2)(\alpha^2 - u^2)(u^2 - \beta^2)}},$$

where $\alpha = \frac{E/2+1}{2}$ and $\beta = \frac{E/2-1}{2}$. We take this integral over $I(u, v_u) = 1$ and $I(u, v_u) = 2u + v_u$ for ρ and ρ_R respectively. In each case the integrand will be an *elliptic integral* [52]. That is, a rational function of polynomials of u and the square root of a polynomial of u (without repeated zeros). Integrals of this type can always be written in terms of the three elliptic functions, whose properties are well known [52]. The evaluation of such integrals in terms of these functions can be done using a table of integrals such as Ref. 52.

The inequalities $-1 < -u < v_u < 1$ can be written as $-\alpha < u < \beta < 0$ for $E/2 < 1$ and $0 < \beta < u < 1$ for $E/2 > 1$. We find it convenient to first change variables to $t = u^2$ so that

$$\int_{BZ} d^2k I(u, v) = \frac{1}{4\pi^2} \int_c^b dt \frac{1}{\sqrt{t}} \frac{I(\pm \sqrt{t}, \pm v_{\sqrt{t}})}{\sqrt{(a-t)(b-t)(t-c)}}, \quad (\text{E7})$$

where $a = \begin{cases} 1 & E < 2 \\ \alpha^2 & E > 2 \end{cases}$; $b = \begin{cases} \alpha^2 & E < 2 \\ 1 & E > 2 \end{cases}$, $c = \beta^2$, and we $\pm = \text{sgn}(E/2 - 1)$. These are such that $a > b > c > 0$. We can evaluate the DOS by taking $I = 1$ and using equation (2.54.00) of Ref. 52 with $d = 0$ and $\gamma = b$. In terms of the complete elliptic function (integral) of the first kind $K[m] = \int_0^{\pi/2} d\theta (1 - m \sin^2 \theta)^{-1}$ this gives

$$\rho(E) = \frac{\sqrt{E/2}}{2\pi^2} \begin{cases} f(E) K[f(E)] & E < 2 \\ K[\frac{1}{f(E)}] & E > 2, \end{cases} \quad (\text{E8})$$

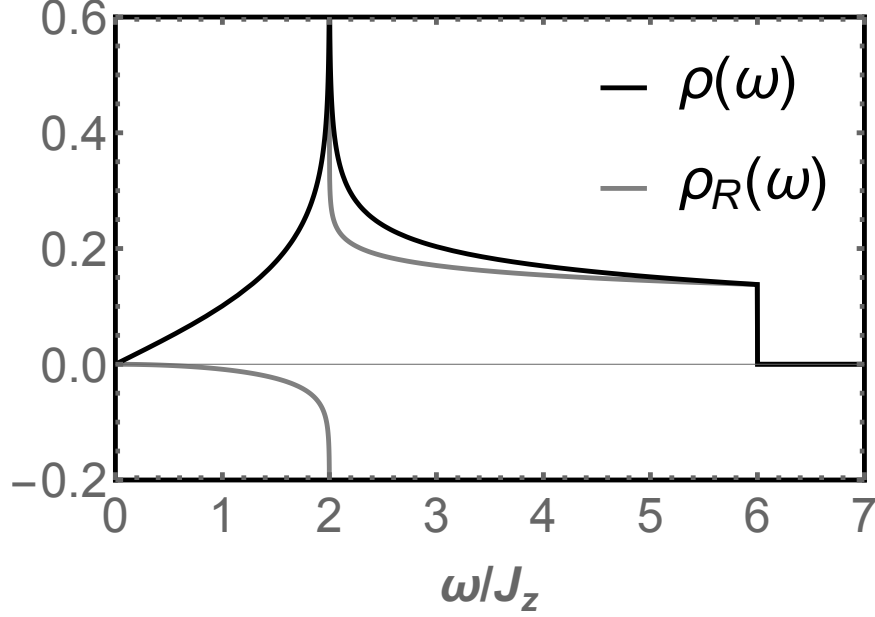


FIG. 6: The density of states (DOS) $\rho(\omega)$ and the spectral function $\rho_R(\omega)$ for the dispersive f -fermions in the pure Kitaev model.

where $f(E) = \frac{\alpha^2 - \beta^2}{\alpha^2(1 - \beta^2)} = \frac{8E}{(3 - E/2)(1 + E/2)^3}$.

For ρ_R we have $I = \pm\sqrt{t}(1 + \alpha\beta/t)$. Make use of equations (233.00) and (233.02) with $p = 0$ and $\gamma = b$ we find

$$\rho_R(E) = \frac{1}{2\pi^2\sqrt{E/2}} \begin{cases} -h(E) \left(K[h(E)] + \frac{1-E/2}{1+E/2} \Pi \left[-4 \frac{E/2}{(E/2-1)^2}, h(E) \right] \right) & E < 2 \\ \left(K\left[\frac{1}{h(E)}\right] + \frac{1-E/2}{1+E/2} \Pi \left[-4 \frac{E/2}{(E/2-1)^2} \frac{1}{h(E)}, \frac{1}{h(E)} \right] \right) & E > 2, \end{cases} \quad (\text{E9})$$

where $h(E) = \frac{\alpha^2 - \beta^2}{1 - \beta^2} = \frac{2E}{(3 - E/2)(1 + E/2)}$. Here we have introduced the complete elliptic integral of the third kind $\Pi[n, m] = \int_0^{\pi/2} d\theta [(1 - n \sin^2 \theta)(1 - m \sin^2 \theta)]^{-1}$.

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