Kitaev quasiparticles in a proximate spin liquid: A many-body localization perspective

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We study the stability of Kitaev quasiparticles in the presence of a perturbing Heisenberg interaction as a Fock space localization phenomenon. We identify parameter regimes where Kitaev states are localized, fractal or delocalized in the Fock space of exact eigenstates, with delocalization implying quasiparticle instability. Finite temperature calculations show that a vison gap, and a nonzero plaquette Wilson loop at low temperatures, both characteristic of the deconfined Kitaev spin liquid phase, persist far into the neighboring proximate spin liquid phase that has a concomitant stripy spin-density wave order. Remarkably, Kitaev quasiparticle excitations are stable at low-energy states over a significant parameter space in the stripy phase.

The honeycomb Kitaev model describes an integrable $Z_2$ quantum spin liquid exhibiting the spin-fractionization phenomenon. The Kitaev quasiparticles consist of gapped $Z_2$ plaquette fluxes (visons) and delocalized Majorana fermions (spinons)\cite{4,9}. Considerable theoretical\cite{2,24} and experimental\cite{25,42} debate surrounds the question of Kitaev quasiparticle effects in the presence of competing spin-interactions, since in the commonly studied Kitaev materials\cite{13–17}, the ground state is magnetically ordered. Experimental observations such as the incoherent features in inelastic neutron scattering\cite{3,18} and the broad peak in THz spectroscopy\cite{27,11} at higher energies, as well as thermal conductivity\cite{25,48}, thermal Hall response\cite{22}, and high field torque response\cite{23,39,49,50} have been interpreted in both ways as evidence of Kitaev physics\cite{4,25,42,49,50} and other anisotropy effects\cite{51}. This motivates us to pose a basic question independent of material specific details: can many-body excitations of a Kitaev model over a range of energy densities have spin density wave order?

Here we study the stability of Kitaev quasiparticles for a simple $(J-K)$ model, consisting of ferromagnetic (FM) Kitaev $(K)$ and antiferromagnetic (AFM) Heisenberg $(J)$ interactions, using recently developed exact diagonalization methods, namely FEAST\cite{52} and Krylov-Schur\cite{53} algorithms for systems of up to $N = 24$ spins. The FEAST\cite{52} eigensolver algorithm is based on a contour intergation projection technique. It allows evaluation of eigenstates within an arbitrary user-specified eigenvalue range, and is able to handle degeneracies. Computing a large number of states is necessary not only to establish Fock space delocalization but also for the study of specific signatures of the Kitaev spin liquid such as the vison gap that exists only at higher energies, and would not be readily accessible from an analysis of the ground state properties such as that usually computed using Lanczos or density matrix renormalization group methods\cite{54}. For the higher system sizes ($N = 20 – 24$), because of large memory requirements of FEAST, we instead use the Krylov-Schur algorithm that gives us significant numbers of eigenstates, including degeneracies, near the extreme ends of the spectrum ($\sim 2 \times 10^3$ for $N = 24$), and works better than Lanczos algorithms.

The ground state of our model is known\cite{5,20} to be a paramagnetic Kitaev spin liquid (KSL) in the parameter range $0 \leq J/K \lesssim 0.12$, exhibiting a stripy AFM order for $0.12 \lesssim J/K \lesssim 0.75$, and Néel AFM order for larger $J/K$. There is also a special point, $J/K = 0.5$, where stripy AFM order peaks, and where, upon a sublattice transformation\cite{5}, the $J – K$ model in the transformed basis maps exactly to an isotropic Heisenberg ferromagnet implying the stripy AFM is an exact ground state at this point. The regime $0.12 \lesssim J/K \lesssim 0.5$ is our proximate spin liquid phase (PSL) where the ground state shows magnetic order but the proximity to the KSL phase implies significant Kitaev correlations.

We find that low-energy states over a significant range of the interaction parameter in the PSL corresponding to $0.12 \lesssim J/K \lesssim 0.5$, Kitaev quasiparticles corresponding to the $J/K = 0$ limit are stable, and in the vicinity of the KSL-PSL phase boundary, better describe the exact eigenstates than the stripy wavefunctions corresponding to $J/K = 0.5$. On the average, states with comparable energy densities have comparable stabilities. We obtain energy density windows where Kitaev quasiparticles are stable for $J/K \gtrsim 0.12$. At high enough energy densities comparable to the stripy AFM ordering scale, the PSL states resemble neither Kitaev nor stripy AFM quasiparticles. Our finite temperature calculations show the presence of a vison gap, and at low temperatures, a nonzero value of the Kitaev plaquette fluxes, both signatures of the deconfined KSL phase, persisting in the PSL all the way to $J/K = 0.5$, despite the simultaneous presence of stripy AFM order.

The problem of quasiparticle stability in interacting systems has a deep connection to the many-body localization (MBL) phenomenon\cite{55}. To see this, we represent individual Kitaev eigenstates as linear superpositions of the exact eigenstates of the $(J-K)$ model in the parameter space $J/K \in [0, \infty]$. In the basis of exact eigenstates, the scaling of the support size $\xi$ of the Kitaev states with the dimensionality $D = 2^N$ of the Fock space in accordance with the law $\xi \sim D$ implies a
fully many-body delocalized state or a decaying quasiparticle, while $\xi \sim D^0$ corresponds to a localized state where the quasiparticle does not decay. A third possibility, $\xi \sim 2^{cN} = D^c$, with $c < 1$, represents a fractal delocalized state and still corresponds to a long-lived quasiparticle excitation since $\xi/D \to 0$ as $D \to \infty$.

We begin our analysis with the following nearest-neighbour $J - K$ model:

$$H = -K \sum_{\langle ij \rangle, \gamma} \sigma_i^\gamma \sigma_j^\gamma + J \sum_{\langle ij \rangle} \sigma_i \cdot \sigma_j,$$

where $K, J > 0$, $\gamma = x, y, z$ labels an axis in spin space and a bond direction of the honeycomb lattice and $\sigma_i^\gamma$ represent Pauli spin matrices at the site labeled $i$. We consider clusters with (even) number $N$ of spins ranging from 10 to 24, and subjected to periodic boundary conditions.

We use the FEAST eigensolver algorithm\cite{52} to compute the large numbers of eigenvectors in arbitrarily specified energy ranges for different values of the ratio $J/K$ for $N$ up to 18 spins. Unlike the usual projection methods such as Lanczos and Jacobi-Davidson that are based on the Krylov subspaces, the FEAST algorithm implements projection using the contour integration based projector,

$$\frac{1}{2\pi i} \oint_C \frac{dE}{EI - H} |v\rangle = \sum_{n \in C} \langle n |v\rangle |n\rangle,$$

where $|v\rangle$ is in general some random vector defined on the entire Fock space of dimension $D = 2^N$, and $\{|n\rangle\}$ are the eigenvectors corresponding to, say, $m$ eigenvalues lying within the user-defined contour $C$. By choosing a number $p \geq m$, of these random vectors (in general linearly-independent), we end up with a set of $m$ linearly-independent vectors spanning the eigenspace enclosed in $C$. Among the advantages this method offers are suitability for parallelization and the ability to obtain large numbers of eigenvectors in user-specified energy ranges, including degeneracies. For $N = 20$ to 24, memory requirements restrict our usage of FEAST, and for that we employed the Krylov-Schur algorithm\cite{53} which yields a significant number of levels (around 1500 for $N = 24$ on our machine) reckoned from the extreme ends of the excitation spectrum. While this does not yield information about states in the middle of the spectrum, it is sufficient to demonstrate Fock space localization of Kitaev states in the $J - K$ model.

To study the resemblance of a given Kitaev state $|\alpha_k\rangle$ with the exact eigenstates $|\psi_i\rangle$ of the $J - K$ model, we expand it as a linear superposition,

$$|\alpha_k\rangle = \sum_{i=1}^D a_{ki} |\psi_i\rangle,$$

and obtain the inverse participation ratio (IPR),

$$P_k = \sum_{i=1}^D |a_{ki}|^4.$$
$J/K \lesssim 0.12$, the support $\xi$ is small, shows fluctuations as a function of $N$, but does not increase exponentially at least up to $N = 24$. For $0.12 \lesssim J/K \lesssim 0.5$, the increase is exponential, $\xi \sim 2^{cN}$, with the exponent $c < 0.71 \pm 0.16$, signifying a fractal delocalized phase. Beyond $J/K = 0.5$, the exponent sharply increases, within numerical accuracy, to $c \approx 1$, and remains near this value for larger $J/K$. This regime corresponds to fully delocalized low-lying Kitaev states. These MBL transitions respectively occur in the vicinity of the Kitaev-stripy AFM transition point ($J/K \approx 0.12$) and the special point $J/K = 0.5$ where the stripy SDW order peaks. We also studied the scaling behavior of the entanglement entropy $S_k$,

$$S_k = -\sum_{i=1}^{D} |a_{ki}|^2 \log_2 |a_{ki}|^2,$$

and found it in agreement (see Appendix) with conclusions drawn from the scaling of $\xi$. We conclude that for $J/K \gtrsim 0.5$, this two-flux Kitaev state is completely delocalized in the Fock space ($\xi \approx fD$) and consequently decays, while for smaller $J/K$, it is either fractal or many-body localized and consequently infinitely long-lived.

In Fig. 2 we show the support sizes for the Kitaev ($J/K = 0$) and stripy AFM ($J/K = 0.5$) states in the Fock space of the exact eigenstates of the $J-K$ model as a function of the normalized energy density for three representative values of $J/K$ in the PSL phase for an 18-site cluster [56]. The choice of normalized energy density for characterizing the support sizes of the quasiparticles is based on our empirical observation that states with comparable energies have comparable support sizes (see Appendix). For $J/K = 0.15$, in the PSL phase close to the KSL phase boundary (Fig. 2(a)), the Kitaev states clearly have smaller support sizes compared to stripy SDW. Furthermore, we have performed a finite-size scaling analysis at fixed energy density to determine the nature of Fock space localization of the states. The blue shaded region refers to the fractal phase of Kitaev states, beyond which the fully delocalized phase appears where Kitaev quasiparticles decay. The numbers on the Kitaev curve denote the calculated scaling exponent $c$. Finite-size scaling analysis of the support of stripy SDW states for $J/K = 0.15$ shows that they delocalize at lower energy densities than the corresponding Kitaev states, and have larger values of $c$ (not shown in the Figure). The case $J/K = 0.2$ (Fig. 2(b)) is deeper in the PSL phase. At the lowest energy densities, the Kitaev states have still have smaller support sizes than stripy SDW, and finite size scaling analysis shows that they are also more localized. Beyond the lowest energy densities, the Kitaev and stripy SDW states show similar scaling behavior, and the phase boundaries separating fractal and completely delocalized phases occur at comparable energy densities for the two. Further away (Fig. 2(c)), for $J/K = 0.3$ that is also in the PSL phase, there is only a very small region of low energy density where Kitaev states have a smaller support than stripy SDW, and are stable. For this value of $J/K$, the stripy SDW states continue to show fractal scaling (stability) to much higher energy densities ($\sim -0.7$). We conclude that in the PSL phase, the exact eigenstates may be approximated as Kitaev states only for the lowest energy densities, and beyond a sufficiently high energy density that depends on $J/K$, both Kitaev and stripy SDW descriptions are not appropriate.

Figure 3 shows the phase diagram of the Kitaev states according to their finite size scaling behavior in the $J/K$ vs. energy density plane. Low energy Kitaev states are clearly more robust against delocalization compared to the high energy states by a Heisenberg perturbation. As one approaches the middle of the spectrum, where the energy density is zero, Kitaev states get delocalized even by small perturbations. We also found that this behav-
Our findings may also be relevant to the Kitaev materials $\alpha$-RuCl$_3$ and Na$_2$IrO$_3$, that are believed to be in...
a PSL phase, although the ground state order is of the zigzag SDW type owing to somewhat different competing interactions. Our study suggests that probing low-energy excitations is more likely to reveal Kitaev quasiparticle effects than excited states above the zigzag SDW ordering scale. This view is supported, for example in the observation of quantized thermal Hall conductivity at low temperatures in \( \alpha \)-RuCl\(_3\) (but not at higher temperatures), and the field-induced quantum spin liquid state inferred from high-field magnetometry at low temperatures in Na\(_2\)IrO\(_3\). Similarly, the incoherent features seen in inelastic neutron scattering measurements at higher energy scales, while supporting the case that magnons may not be good quasiparticles here, do not necessarily imply that the excitations instead resemble Kitaev quasiparticles. Recent numerical studies of realistic spin models for \( \alpha \)-RuCl\(_3\) suggest that the ground state at intermediate magnetic fields is a Kitaev spin liquid based on the appearance of field induced \( Z_2 \) flux states. It would be interesting to make a direct comparison with the Kitaev wavefunctions in this regime.

We end with some comments on the relevance of our findings in the general context of MBL transitions. Disorder, a common cause of MBL, is absent in our model; however, it is not strictly necessary for localization – recent developments show that MBL transitions are also possible in disorder-free systems. A distinguishing feature of such disorder-free models is that the many-body localized and delocalized phases are both nonergodic. Interestingly, we find that the level-spacing distribution remains Poisson-like in the entire parameter space (see SI), so that our model is always nonergodic, and yet exhibits the above MBL transitions. Another feature of the MBL transition in disordered interacting systems is the presence of a mobility edge, which has not been studied in the disorder-free context in Refs. Our finite size scaling analysis of the support size of Kitaev quasiparticles indicates the presence of two energy scales (mobility edges) separating many-body localized, fractal and delocalized phases.

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**Appendix A: localization of two-vortex states in Fock space**

1. **Overlap of two-vortex Kitaev state with exact eigenstates of \( J - K \) model**

As the Heisenberg perturbation is increased, the Kitaev states begin overlapping significantly with an increasing number of exact many-body states of the \( J - K \) model. Here we show how the support size of a two-vortex state, lying close to the ground state of the Kitaev model, increases with the ratio \( J/K \). Figure 3 shows a plot of the squares of the overlap, \( |a_{ki}|^2 \), of a two-vortex state of the Kitaev model with exact many-body states corresponding to two different values of \( J/K \), where \( |k\rangle = \sum_i a_{ki}|i\rangle \) is the two-vortex Kitaev state and \( \{ |i\rangle \} \) are the exact eigenstates of the \( J - K \) model. For \( J/K = 0.03 \), the two-vortex state has a very small support size in the Fock space, while for \( J/K = 0.7 \), the support size is large. Finite size scaling behaviors of the support sizes (Figure 1 in main text) tells us about the localization of these states. For \( J/K = 0.03 \), this two-vortex state is localized in Fock space while for \( J/K = 0.7 \), the state is delocalized.

2. **Finite size scaling of entanglement entropy**

Apart from the inverse participation ratio, we also analyzed the scaling behavior of the entanglement entropy \( S_k \), of the \( k^{th} \) Kitaev state with the exact eigenstates, \( |i\rangle \), of the \( J - K \) model:

\[
S_k = - \sum_{i=1}^D |a_{ki}|^2 \log_2 |a_{ki}|^2, \tag{A1}
\]

The entanglement entropy shows a very similar scaling behavior as that of the support size, \( \xi_k \). In Fig. 8 we show the scaling of the entanglement entropy of the two-flux state with \( N \) for different values of \( J/K \). In the localized regime, \( J/K \lesssim 0.12 \), the slope of \( S_k/N \) vs. \( 1/N \) is negative, while it is positive in the fractal and delocalized regimes. In the completely delocalized regime, \( J/K \gtrsim 0.5 \), the entropy increases linearly with \( N \) with approximately unit slope.

**Appendix B: Support sizes of higher Kitaev states**

Figure 7 shows that the Kitaev states with comparable energies have comparable support sizes. The flat regions correspond to nearly degenerate Kitaev states. Some rare states appear to have anomalously low support sizes - these form a small fraction of the total, and do not affect the average trend of increasing support size with energy. This justifies regarding the energy density as an appropriate parameter for describing Fock space localization of Kitaev states.
Appendix C: Energy level statistics

Figure 5 shows the distribution $P(s)$ of energy level spacings $s$, measured in units of the mean level spacing $\delta$, for an 18-site cluster, for $J/K = 1$ corresponding to the fully delocalized regime for the Kitaev states. The distribution fits well to a Poisson law and not Wigner-Dyson, showing that the model is nonergodic in this fully delocalized regime. We found that the level statistics remains Poisson like through the localized, fractal and delocalized regimes, supporting the view [61] that in disorder-free models, many-body localization transitions are possible without an accompanying ergodic-nonergodic transition. For $s = 0$ (not shown in the plot), $P(s)$ takes a rather large value \(\sim 0.82\) owing to the large number of degenerate or nearly degenerate states near the middle of the spectrum.

Figure 6. Plot describing finite size scaling of the entanglement entropy, $S$, of the lowest two-vortex Kitaev state for different values of $J/K$. The fits are to a volume law, $S/N = c + \frac{1}{2} \ln_2(1/f)$, where $f < 1$ and scales slower than exponential. Lines with negative (positive) slopes correspond to many-body delocalized (localized) phases. The numbers on the solid lines indicate the value of $J/K$.

Figure 8. Plot showing the distribution $P(s)$ of energy level spacings $s$ (in units of the mean level spacing $\delta$) obtained for an $N = 18$ cluster, for $J/K = 1$ that corresponds to the fully delocalized regime for the Kitaev states. The fit is to a Poisson distribution, $P(s) = A \exp(-bs)$, where $A = 0.00152$ and $b = 0.16432$. The Poissonian level statistics is seen throughout the parameter space corresponding to localized, fractal and delocalized regimes. The Fock space transitions to fractal and completely delocalized phases occur completely within the nonergodic regime in our disorder-free model.
Figure 7. Figure showing the support sizes of the lowest Kitaev states in the Fock space of exact eigenstates of the $J - K$ model, for two different values of $J/K$. The data is for an 18-site cluster, and support sizes of the lowest 12,000 states are shown. The flat regions correspond to nearly degenerate Kitaev states. Barring some rare exceptions, Kitaev states with comparable energies have comparable support sizes. Also note the overall increase of the support size of the excited states with increasing $J/K$.

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