Discovery of novel topological phases in the anisotropic Kitaev model in a field

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The Kitaev model with bond dependent Ising interactions of strengths $K_x, K_y$ and $K_z$ on the three bonds of a honeycomb lattice offers an exactly solvable model for $\mathbb{Z}_2$ quantum spin liquids with gapped $\mathbb{Z}_2$ fluxes and gapless linearly dispersing majorana fermions in the isotropic limit ($K_x = K_y = K_z$). The majorana fermions get gapped out in the anisotropic Toric code limit when one of the coupling strengths is much larger than the other two, leading to a gapped $\mathbb{Z}_2$ QSL where the $\mathbb{Z}_2$ fluxes form the low energy excitations – bosonic Ising electric ($e$) and magnetic ($m$) charges with their bound state $\epsilon = e \times m$ being a fermion. The transition between the gapless and the gapped QSLs occurs at $K_z = 2K$ where $K_x = K_y \equiv K$. The effect of an external magnetic field, $h$, in the [111] direction is remarkably different on the gapless and the gapped $\mathbb{Z}_2$ QSL. While the former shows transitions to a gapped chiral QSL (CSL) and a gapless U(1) QSL before the polarized paramagnet sets in, the latter gives way to a valance bond solid (VBS) phase with dimers on z bonds. Key to understanding this rich phenomenology is the Zeeman field induced hybridization between the $e$ and majorana fermions resulting in a $\psi$ fermion that leads to a gapped $\mathbb{Z}_2$ QSL at intermediate magnetic field and anisotropy – dubbed the Primordial Fractionalized (PF) phase. All the other phases in the $(h, K)$ plane are naturally obtained from this primodial soup: the gapped primodial liquid is continuously connected to the TC limit by a cross-over; through continuous phase transitions to the CSL via a change in the topological invariant of the band structure of the $\psi$ fermions, which reduces to the usual majoranas in the weak field limit; to a gapless U(1) QSL with a Fermi surface via loss of $(\psi \bar{\psi})$ pairing; and to the VBS phase with a dimer order parameter via confinement. Our analysis is based on susceptibilities, (topological) entanglement entropy, and excitation dynamics obtained via exact diagonalization and density matrix renormalization group calculations.

I. INTRODUCTION

Quantum spin liquids (QSLs) are long-range entangled states of matter that develop in a Mott insulator, an insulator with an odd number of electrons in a unit cell formed because of strong local repulsive interactions [1–4]. The resulting local moments interact with neighboring moments on a specified lattice. The fate of the interacting moments can progress along two paths as the temperature is lowered: the moments can undergo long range ordering, spontaneously breaking the continuous rotational symmetry, leading to a magnetic phase; or the moments can remain disordered but get quantum mechanically entangled with their bound state $\epsilon = e \times m$ being a fermion. The possibility of obtaining QSL phases is enhanced by having a low spin and enhanced quantum fluctuations, and frustration arising from the lattice geometry and/or competing spin-spin interactions.

The Kitaev model is a paradigmatic model of $S=1/2$ local moments or qubits on a honeycomb lattice with very specific bond-dependent Ising interactions [7–9], to which we add an external magnetic field perpendicular to the honeycomb plane along the [111] direction, given by:

$$\mathcal{H} = \sum_{\langle i,j \rangle, \alpha} K_{\alpha} \sigma_i^\alpha \sigma_j^\alpha - h \sum_{i=1} (\sigma_i^x + \sigma_i^y + \sigma_i^z) \quad (1)$$

where $\alpha = x, y, z$ refers to the three bonds of the honeycomb lattice. For the purposes of this paper, $K_x = K_y = K$ are set to unity, while we vary $K_z > 0$ and $h$.

In absence of time reversal (TR) symmetry breaking perturbations, i.e., for $h = 0$, the Kitaev model is integrable due to the extensive number of conserved $\mathbb{Z}_2$ gauge fluxes resulting in an effective quadratic hopping problem for the majorana fermions in each flux sector with the ground state belonging to the zero flux sector in accordance with Lieb’s theorem [7]. For $1 < K_z/K \leq 2$ the majorana fermions are gapless, while in the highly anisotropic regime $K_z/K > 2$ they are gapped. This exact solution is easily obtained following Kitaev’s original prescription [7] of representing the spin degrees of freedom in terms of majorana fermions. The nature of the lowest energy excitations in the gapless and gapped $\mathbb{Z}_2$ liquid are very different: For $K_z \approx K$, the majorana fermions form linearly dispersing gapless excitations, similar to graphene. However, deep inside the anisotropic phase, $K_z/K \gg 2$ the model approaches the Toric code (TC) limit since the effective Hamiltonian can be written in terms of mutually commuting Ising stabilizers [10]. In this regime the lowest energy excitations are gapped $\mathbb{Z}_2$ fluxes of the honeycomb model which now form bosonic Ising electric and magnetic charges with mutual semionic statistics [7, 10, 11] while the majorana fermions have a gap much larger than the fluxes.

In this background, it is rather interesting to understand the effect of either of the $\mathbb{Z}_2$ QSLs to the simplest experimental probe of spin systems— an external magnetic field— represented by the second term in Eq. 1. Given the fractionalised nature of the low energy excitations and
FIG. 1. (a,b) A schematic of the phase diagram in the bond strength anisotropy $K_z/K$ vs. magnetic field $h$ along the [111] direction. We identify the generic gapped $\mathbb{Z}_2$ fractionalized phase in the central region, dubbed the Primordial Fractionalized (PF) phase (yellow color), from which all the other phases around originate. The key low energy excitation of the PF phase comprises of a gapped fermion, $\psi$, that carries $\mathbb{Z}_2$ gauge charge and is obtained via magnetic field mediated hybridization of the majorana fermion, $c$, of the Kitaev QSL and the $\epsilon = e \times m$ fermion obtained in the TC limit where $e$ and $m$ are the Ising electric and magnetic charges of gapped $\mathbb{Z}_2$ QSL obtained in the TC limit. As we look toward the four quadrants, from the PF phase, for large $K_z$ and small $h$, there is a cross over to the $\mathbb{Z}_2$ Abelian phase as the $c$ fermion gap increases beyond the flux gap with a concomitant reduction in the magnetic field induced hybridization, approaching the pure TC gauge theory as $K_z/K \rightarrow \infty$. For large $K_z$ and large $h$ there is a first order phase transition to a $z$-bond dimer or valence bond state (VBS) (shown in blue) reflected by the order parameter via confinement of the gauge theory. The VBS is smoothly connected to the polarized state at large magnetic field at lower anisotropy. In the lower left region for small $K_z$ and small $h$, the flux sector has a larger gap while the majorana sector is gapless at $h = 0$ and a finite smaller gap for small $h$. In this region, the majorana fermions form a gapped non-Abelian CSL (shown in green) equivalent to a gapped $p+ip$ superconductor. With increasing field the pairs break forming a gapless QSL with spinon fermi surfaces (shown in pink) and ultimately a polarized phase for large $h$ (shown in grey). (c) Mapping of the anisotropic Kitaev model of $\sigma$ qubits on a honeycomb lattice to an effective square lattice with $\tau$ qubits on links made out of the two $\sigma^\alpha$ spins on the $z$-bond.

II. PHASE DIAGRAM

For large anisotropy of the bond strengths, i.e., $K_z/K \gg 2$, the gapped Kitaev QSL can be mapped to the TC defined on an underlying square lattice as shown in Fig. 1(c) [24], where the ground state manifold...
for large $K_z/K$ is given by $\{|\uparrow\rangle, |\downarrow\rangle\}$; and the excited states by $\{|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle\}$. The fourth order perturbation in this ground state manifold gives the four-point interaction between these new degrees of freedom $\tau^z = (\sigma^z_A - \sigma^z_B)/2$ which is equivalent to the TC model [24].

The quantum phase transition between the gapless and the gapped QSLs arises due to a modification of the majorana band structure at $K_z/K = 2$ in the zero flux sector. At the isotropic point $K_z/K = 1$ the majorana band has Dirac-like gapless modes located at $K$ and $K’$ points of the Brillouin zone (BZ) similar to electrons in graphene. As is shown in Fig.1(b), upon increasing the anisotropy, the two Dirac points move toward each other, which ultimately combine into a single semi-Dirac gapless mode at the M point when $K_z/K = 2$ is reached; and furthermore the bands get gapped out immediately after the transition point with a gap that continues to increase monotonically with $K_z$ in the zero flux sector and is $O(K_z)$ for $K_z/K \gg 2$ while the flux energy scale is $\sim K^4/K_z^2$ in the same limit. These low energy fluxes in the TC limit are canonically best described in terms of a deconfined Ising gauge theory of which they form electric and magnetic charges [24].

Thus the primary effect of a small [111] external magnetic field is to couple the gapless majorana fermions in the zero flux sector near the isotropic limit to the low energy Ising gauge charges in the TC limit. This opens up the window for interplay and selective tunability of the different fractionalised excitations which, as we shall show is best understood in terms of a generic primordial $Z_2$ QSL of which the exactly solvable model is a special limit. This primordial fractionalised (PF) liquid allows for instabilities along different channels as a function of bond anisotropy and magnetic field well beyond the currently known small field perturbative regimes—the CSL at low magnetic field in the isotropic regime obtained by the gapping out the linearly dispersing majoranas via a chern mass while the flux still remains gapped [7], and, a dimerised short range entangled phase out of the TC topological order in the anisotropic limit via a first order transition owing to the confinement of the $Z_2$ gauge charges.

The above perturbative limits completely misses the physics of intermediate anisotropy and magnetic field—the central topic of this work. Central to our observation is—while the TC is traditionally described in terms of the bosonic Ising electric, $e$, and magnetic charges, $m$, an equally valid description is in terms of the fermion $e = e \times m$ and either $e$ or $m$. Notably the $e$ fermion lies in the same super-selection sector as the majorana [7] and hence can hybridize with it via local spin operators. As we show, the two complementary effects of the [111] magnetic field—(1) it preferentially leads to the dispersion of $e$ fermions, and, (2) fosters hybridization of the $e$ fermions and the majoranas due to the Zeeman term—directly lead to the emergence of a low energy hybridized fermion, the $\psi$ fermion, carrying a $Z_2$ gauge charge whose dynamics determines the fate of the system in the intermediate regime—far from the perturbative limits.

It is useful to consider the analogy of the Anderson model in context of heavy fermion system where there are two species of fermions (electrons)—one almost localised and the other itinerant—that hybridizes via the Anderson coupling. The situation is somewhat similar except for the fact that both the bandwidth of the localised fermions and the magnitude of the hybridization are fostered by the magnetic field. The PF liquid is therefore the analog of the heavy fermion phase, albeit in this case, it is gapped. From such point of view, the Kitaev model is the exactly solvable limit where the hybridization goes to zero concomitantly with the gapping of the $\epsilon$ fermion, while the majorana fermions form a gapped or gapless spectrum depending on the anisotropy.

A. Diagnostics of the Phases and Phase Transitions

As the [111] magnetic field is turned on, there emerges a far richer phase diagram as a function of both $K_z$ and $h$ than known previously. Figure 2 summarises various diagnostic calculations, which together determine the phase boundaries and crossovers shown in the schematic diagram Fig.1.

Our new discovery lies in the novel behavior of the gapped $Z_2$ abelian phase in a finite magnetic field obtained by making the coupling $K_z$ larger compared to the other two. For $K_z \gg K$ in the TC limit, the $Z_2$ abelian QSL undergoes a first order transition to a confined short range entangled dimerised phase discussed in greater detail in next section, which, in turn gives way to a polarised phase at even larger fields $h \sim K_z$. However, we find that there exists a remarkably richer physics between the integrable $Z_2$ Abelian phase at zero field and the polarized phase at large field as already indicated schematically in Fig. 1(b). This includes—(1) a CSL phase at small magnetic field, (2) a $U(1)$ liquid at intermediate magnetic field and almost isotropic limit, and, (3) centrally, a gapped $Z_2$ QSL at intermediate magnetic field and anisotropy that we dub the primordial fractionalized (PF) phase.

We first calculate the susceptibilities as the conventional measure of quantum phases and phase transitions:

$$
\chi_h = \frac{\partial^2 E_{gs}(K_z, h)}{\partial h^2}, \quad \chi_z = \frac{\partial^2 E_{gs}(K_z, h)}{\partial K_z^2}
$$

The results are shown in Fig.2(a,b) and their cuts on the right side of the contours. Figure 2(a) shows the zero-temperature isothermal magnetic susceptibility $\chi_h$, which marks out several boundaries highlighted in the schematic phase diagram. At finite field in the range $0.22 < h/K < 0.35$ and for near-isotropic interaction, there is a gapless QSL sandwiched between two singularities of $\chi_h$, reported in our previous works [25–27] as well as others [28–35]. For even larger $h$ the system becomes partially polarized, whose phase boundary is also clearly visible in Fig.2 as singularities in different measures (see below). $\chi_h$ marks out the four phases: the CSL in the lower left region, the Abelian
$Z_2$ QSL at high anisotropy and finite field, the gapless QSL and the VBS/polarized phase; while in $\chi_z$ (Fig. 2(b)) the boundary between Abelian $Z_2$ QSL and the VBS/polarized phase are not as clear, since the transition is being driven by the field.

The distinction between the VBS and the polarized state is not revealed by the susceptibility measurements. To characterize the emergence of the VBS phase we calculate the von-Neumann entropies $S_{vN}^y$ and $S_{vN}^z$ for subsystems obtained by cutting along $y$ bonds or $z$ bonds respectively. These are shown in Fig. 2(d) and (f). While $S_{vN}^y$ drops off once the QSL is destroyed, $S_{vN}^z$ persists in the VBS phase indicating the presence of dimers on them, which finally gives away to the polarised phase at even larger magnetic fields whence $S_{vN}^z$ falls off to zero. The entanglement entropies are also generically sensitive to all gap-closing transitions such as the one out of the CSL and hence indicating the transition out of it.

We also define the following operator that is sensitive to the dimerization:

$$\hat{Q}^{\alpha\beta}_{pp'} = \left(\frac{\sigma_\alpha^p\sigma_\beta^{p'}}{2} + \frac{\sigma_\beta^p\sigma_\alpha^{p'}}{2} - \delta_\alpha\beta\sigma_p\sigma_p'\right)$$

where $pp'$ stands for the $p$-bond and $\alpha, \beta \in \{x, y, z\}$. The behavior of the order parameter is discussed in more detail in the next section. These measure, as is shown in Fig. 2(c) and (e), marks out the distinction between VBS and polarized phase as schematically shown in Fig. 1(b).
The PF phase is not visible in standard measurements based on two-point correlations, e.g. $\chi_z$ and $\chi_h$ shown in Fig.2(a,b), however, its nature is explicitly revealed in the third order mutual information $I_3$ :

$$I_3(A_1 : A_2 : A_3) = I(A_1 : A_2) - I(A_1 : A_2|A_3)$$

where $I(A_1 : A_2|A_3)$ is the conditional quantum mutual information [36]. The physical meaning of $I_3$ converges to the topological entanglement entropy $\gamma$ [37, 38]:

$$I_3 \rightarrow -\gamma = S(A_1) + S(A_2) + S(A_3) - S(A_1 A_2) - S(A_1 A_3) - S(A_2 A_3) + S(A_1 A_2 A_3)$$

when the correlation length satisfies $\xi/|\partial A_i| \rightarrow 0$ and $A_i$ are chosen such that they share boundaries with each other. In particular, at small but finite $h$ whereby fluxes are approximately conserved, we retrieve the exact $I_3 = -\gamma = -2 \log 2$ in both CSL and Abelian $Z_2$ QSL as is shown in the white area of Fig.2(g). Indeed, at small $h$ the $x$ is extremely small such that it is possible to retrieve the topological entanglement entropy locally [39]. At $1 < K_z/K < 2$ the very large $|I_3|$ marks out a gapless QSL phase with large $\xi$. Interestingly, at a larger $h$ inside the Abelian $Z_2$ QSL, $|I_3|$ also increases to $|I_3| \approx 2 \log 2$, indicating strong non-local physics and synergistic information inherent in frustration and quantum entanglement [40]. This is the region dubbed PF phase connected to the topological entanglement entropy locally [39]. This is the region dubbed PF phase connected to the topological entanglement entropy locally [39]. This is the region dubbed PF phase connected to the topological entanglement entropy locally [39]. This is the region dubbed PF phase connected to the topological entanglement entropy locally [39]. This is the region dubbed PF phase connected to the topological entanglement entropy locally [39].

It is useful to understand the above physics in terms of the $\sigma$ spins. For instance the TC ground state is given by

$$|\text{GS}\rangle = \prod_i \left( \frac{1 + W_i}{2} \right) \otimes \uparrow$$

where $W_i$ (see Eq.6) flips both the spins on two consecutive $z$ bonds albeit with a decorated sign structure that depends on the other $z$ bonds. This highly entanglement state leads to a finite topological entanglement entropy, and the existence of fractionalized excitations and anyonic statistics. The flux excitations correspond to the states where $(W_i) = -1$ that are static in the absence of a field but gain field-dependent dispersions. The instability of these excitations lead to various phase transitions.

We now perform a unitary transformation such that on the horizontal bonds $\{ \tau^x, \tau^y, \tau^z \} \rightarrow \{ \tau^y, \tau^z, -\tau^x \}$; and on the vertical bonds $\{ \tau^x, \tau^y, \tau^z \} \rightarrow \{ \tau^y, \tau^z, \tau^x \}$. The transformed Hamiltonian is given by

$$\hat{H} = -J_{TC} \sum_i A_s + \sum_p B_p - \sum_i \frac{2h^2}{K_z} \tau_i^y$$

where $A_s$ and $B_p$ are the star and the plaquette operators in the standard TC perturbed with a Zeeman field in the $y$ direction and $J_{TC} = \frac{K^4}{16I_3}$. The exactly solvable $h = 0$, $Z_2$ QSL phase of the TC is gapped and hence stable to small magnetic fields. While the excitations of this gapped QSL are usually described in terms of the bosonic Ising electric charge $e$ on the vertices, and the magnetic charge $m$ on the plaquettes, of the square lattice in Fig.1(c) arising from $A_s(B_p) = -1$ [10], we find an alternate, but equivalent, description of this Ising gauge theory in terms of the fermion, $\epsilon = e \times m$, and the bosonic electric or magnetic charge, that allows for a transparent understanding of the effect of the magnetic field. The description in terms of the $\epsilon$ fermion and boson can also be successfully extended to the near isotropic limit (see below).
This is because while all $e, m$ and $\epsilon$ have a gapped flat band for $\hbar = 0$, the second term in Eq.8, provides, to the leading order, dispersions in $\epsilon$, rather than individual $e$ and $m$ charges along the diagonal directions $d_1$ or $d_2$ as shown in Fig.3(d). To the leading order, the one dimensional dispersions of $\epsilon$ fermions are given by

$$\varepsilon_x(\overline{K}) = 4J_T\cos\left(\frac{\sqrt{3}}{2}k_x + \frac{3}{2}k_y\right)$$

$$\varepsilon_y(\overline{K}) = 4J_T\cos\left(\frac{\sqrt{3}}{2}k_x - \frac{3}{2}k_y\right)$$

where $4J_T$ is the gap to an e-m excitation in absence of the magnetic field. This e-m composite fermion has extremely anisotropic dispersion as shown in Fig.3(d) and hosts zero modes at $\sqrt{3}k_x \pm 3k_y = 4n\pi$ for $4J_T = \frac{4\hbar^2}{K_z}$. Interestingly it is known that given the duality in the system [43, 44], a $\gamma$ perturbation to the TC leads to a first order transition at $K_z = 2k_x$ i.e. at $h_c = K_z/\sqrt{3}$ as shown in Fig.2(a) for $Q^{xx})_{VBS} = 2/3$. This state, even when being a short range entangled product (over the $z$-bonds), is however distinct from a completely polarized state found as $h \gg K_z$, where all the spins are polarized in the [111] direction. In this state the magnetisation is finite but $\langle Q^{xx}\rangle_{PM} = 0$. For the dimerized VBS and polarized states, the order parameter Eq.3 evaluates respectively to:

$$\langle Q^\alpha_{pp'}\rangle_{VBS} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

$$\langle Q^\alpha_{pp'}\rangle_{PM} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

Note however that these phases are smoothly connected and unlike a symmetry broken state, here time-reversal, spin-rotation and lattice symmetries are explicitly broken due to a $K_z$ anisotropy and a field.

Notably the fully polarized state is a direct product state in terms of the individual $\sigma$-spins such that the bipartite entanglement between any subsystem bipartition is zero. On the other hand, the dimer state, $|\Psi_{VBS}\rangle$, is a product state over the $z$-bonds and hence any bipartition cutting a $z$-bond would contribute $\log 2$ per $z$- bond to the von-Neumann entanglement entropy. Such Bell-pair contribution is absent when the bipartition is made across the $y$-bonds. This is shown in Fig. 2(d) and (f).

Therefore in the strong $K_z$ limit, as a function of $h$, we can expect a transition to a VBS state at $h_c \sim K_z^2$ and smooth transforms to a polarized state at $h \sim K_z$. This analysis provides a detailed understanding of the nature of the phase diagram in the strong $K_z$ limit as shown in Fig.1.

### C. The isotropic limit: $1 < K_z/K < 2$

The isotropic point $(K_x = K_y = K_z = 1)$, is most naturally described in terms of fractionalized degrees of freedom ($c_i, b^\dagger_i$) where $\sigma_0^\alpha = i c_i b_i^{\dagger}$ [7] and $c_i, b_i^\dagger$ are majorana fermions. The sublattice character of the honeycomb lattice allows these majoranas to be combined into canonical fermions [45]

$$c_i \equiv f_i + f_i^{\dagger}, \quad c_{i+\hat{z}} \equiv i(f_i - f_i^{\dagger})$$

where $c_i$ denotes the majorana operator on the $A$ sublattice of the $i$-th site of the Bravais lattice; and $c_{i+\hat{z}}$ denotes that of $B$ sublattice thereof. Similarly for the bond fermions [46]

$$b_i^\dagger = \chi_{i\alpha} + \chi_{i\alpha}^{\dagger}, \quad b_i^{\dagger} = i(\chi_{i\alpha} - \chi_{i\alpha}^{\dagger})$$

This maps the Ising exchange on the $z$ bonds as

$$K_z \sigma_i^z \sigma_{i+\hat{z}} = -K_z(2n_i^{\dagger} - 1)(2n_i^{\dagger} - 1)$$

thereby mapping the spin states on the sites $i$ and $i + \hat{z}$ (labelled by $|\sigma_i^z,\sigma_{i+\hat{z}}^z\rangle$) to a basis $|n_i^{\dagger}, n_i^{\dagger}\rangle$ on every $z$-bond. The spin configurations $|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle$ map to $|00\rangle, |11\rangle$ and $|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle$ map to $|01\rangle, |10\rangle$ states similarly. The other Kitaev exchanges $K_z \sigma_i^z \sigma_{i+\alpha}$ are transformed to $-K_z c_i c_{i+\alpha}$, for $n_\alpha = 1$. The static flux sector, which corresponds to $n_\alpha = 1$, then leads to a free fermionic description for the $f, \phi$ fermions that at $K_z = 1$ describes a $p + ip$ superconductor with Dirac cones at the $\pm K$ point [7, 47]. Increasing $K_z$ displaces the Dirac cones, merging them via a semi-Dirac dispersion at $K_z = 2$. Increasing $K_z$ further opens up a gapped phase which is smoothly connected to the TC phase as detailed above. The operator correspondence between various ways of describing the excitations of the Kitaev model is illuminating. A two-spin flip operator $\sim \sigma_i^z \sigma_{i+\hat{z}}$ on $|\sigma_i^z\rangle$ state corresponds to a two fermion excitation $\sim f_i^{\dagger} \chi_{i\alpha}^{\dagger} + f_i \chi_{i\alpha}$, in terms of $f$ and $\chi_z$ fermions, which in turn correspond to four flux excitations (two $e$-m pairs) in terms of the $\tau^y$ operator acting on the ground state of the TC (see Eq.8).
D. Excitations in the Abelian phase

In the strong $K_z$ limit, given the mapping to the TC, it is natural to describe the excitations in terms of just $e$, and $m$ charges or the flux excitations, or their bound state $e = e \times m$ which is a fermion. However, as $K_z$ is reduced, we must include the effect of the itinerant majoranas $(f)$ which becomes gapless at $K_z/K = 2$ and remain gapless for $1 < K_z/K < 2$. Given that the $e$ particles and the $f$ fermions belong to the same super-selection sector they can, in general, hybridize via local spin-operators and hence the strength of the hybridization can be tuned via local interactions in the spin Hamiltonian such as the magnetic field. It is useful to interpret these in light of the emergent degrees discussed in Eq.13 and Eq.14. A magnetic field of the form $= \chi \chi$ leads to hybridization between $\chi_a$ and $f$ fermions, however their behavior at low energies is crucially different.

A term of the form $h^2 \sigma_i^a \sim h^2 (i \eta_i^a c_i) \sim i h^a (\chi_{i\alpha} + \chi_{i\alpha}^\dagger) (f_i + f_i^\dagger)$ (where $i$ belongs to A sublattice) – indicates that $h^a$ mediates hybridization between $f$ fermions and $\chi_a$. Including such contributions from both the sublattice leads to hybridization,

$$ih[(e^{ikd_1} - 1) \chi_{kz} f_{-k} - (e^{ikd_1} + 1) \chi_{kz} f_k^\dagger] + h.c$$ (16)

and similarly for $y$ ($x \rightarrow y$, $d_1 \rightarrow d_2$). For $1 < K_z/K \leq 2$, the $f$ fermions are gapless and easily hybridize with the low energy $\chi_a$ fermions via the above mechanism in presence of the magnetic field.

With reducing bond anisotropy, the gap of the $f$ fermions closes at the M point in the BZ and reopens at finite magnetic field through a change in the Chern number of the band. Under the static flux approximation [7], even at a finite field, the transition between the CSL and the TC state occurs via a Dirac closing at the M point. In particular near $M = \{0, \pi, \pi\}$ where $f$ are low-lying near $K_z/K \sim 2$, the hybridization leads to

$$-2ih(\chi_{kz} f_{-k} - f_{-k}^\dagger \chi_{kz}^\dagger) + (x \leftrightarrow y)$$ (17)

which implies instead of considering $\chi_x/y$ and $f$ fermions separately (as near $h \sim 0$), we should instead consider

$$\psi \sim \frac{1}{\sqrt{2}} (\chi_{kz}^\dagger + \chi_{kz}^\dagger + if_{-k})$$ (18)

as the low energy excitations of the $Z_2$ liquid in intermediate fields and $K_z \sim 2$. It is this regime of the phase diagram we call the PF phase. Thus the PF phase we find is a generic $Z_2$ liquid, whose more specific cases correspond to various $Z_2$ spin liquid realized in the Kitaev model. This qualitatively explains the fan-like shape of the PF phase which emanates from $K_z/K \sim 2$ shown in Fig.1(b) and Fig.2(g). To further investigate the nature of such excitations we now look at their dynamical signatures.

For large $K_z$, the single particle excitations for both $\chi_x$ and $f$ fermions are gapped at the $K_z$ scale, which can be integrated out, consistent with Eq.15. The low energy excitations are however the $\chi_x$ and $\chi_y$ fermions gain an independent dispersion due to the quadratic perturbation in $(h^x)^2$ and $(h^y)^2$. In fact a quadratic perturbation in $(h^x)^2$ gives $(h^x)^2 \sigma_i^x \sigma_j^z$

$$\sim (h^x)^2 (2n_i^x - 1) (\chi_{i\alpha}^x \chi_{i+z\alpha}^x \chi_{i+z\alpha}^x \chi_{i+z\alpha}^x + \chi_{i+z\alpha}^x \chi_{i+z\alpha}^x)$$ (19)

which when acting on a single-fermion sector corresponds to the dispersion for the bond fermions albeit normalized by the occupancy of $f$ fermions within mean-field. The dispersion of $\chi_x$ fermions is of the form $\sim 2(h^x)^2 \cos(k \cdot d_1)$ which is indeed the dispersion shown in Eq.9. An equivalent picture emerges when $x \rightarrow y$, $d_1 \rightarrow d_2$. Thus the composite (e-m) pairs distilled in the large $K_z$ limit and the TC mapping in the previous subsection are in fact describable in the $\chi_x$ and $\chi_y$ fermions as discussed in Eq.14. These excitations are energetically low lying close to the VBS phase at large $K_z$ when perturbed by $h$. Note that in this regime, $f$ fermions behave as spectators and do not mix with $\chi_a$ fermions, and therefore do not affect the low energy physics albeit when confinement leads to VBS phase.

Figure 3(a) presents excitations created by Pauli matrices, where the shaded plaquette denotes the flux excitation and black dot denotes the itinerant majorana. Note that in the ground state (at $h = 0$) the occupation number of bond fermions $\chi_{a}$, $n_a$ is unity across the whole lattice, so that an on-site Pauli matrix (generated by $h$) creates both $f$ and $\chi$ excitations renormalizing their values.

To investigate into the nature of the low energy excitations, we focus on two excitations: (i) created by $\hat{O}_i = \sigma_i^x \sigma_{i+z}^x$, which near $h = 0$ is equivalent to the composite particle consisting of both occupancies of canonical $f$ fermion and a creation of a pair of $\epsilon$ particles ($\chi_x$ here) (Eq. 19); and (ii) created by $\hat{O}_i = \sigma_i^x \sigma_{i+z}^z$, equivalent to just a product of number operators for both $f$ fermion and $\chi_z$ fermion (see Eq. 15). However while this operator content is effective near the exactly-solvable limit ($h = 0$), in intermediate fields these particles hybridize as discussed near eqn. (16). The response of these hybridized particles to an external field is revealed by the dynamical structure factor and the spectral function excluding the ground state contribution:

$$S(k, \omega) = -\frac{1}{\pi} \Im \left[ \langle \Psi | \hat{O}_k \hat{\sigma}_+^- | \Psi \rangle \right]$$ (20)

$$S(\omega) = -\frac{1}{\pi} \Im \sum_k \left[ \langle \Psi | \hat{O}_k \hat{\sigma}_+^- | \Psi \rangle \right]$$ (21)

where operator $\hat{O}$s are the spin operators defined above, $\hat{H}$ is the Hamiltonian shown in eqn. (1) and $\eta$ is a small number (tending to zero) used for spectral widening.

The spectral weights $S(\omega)$ for the two operators are shown in Fig.3(b,c). For small but non-zero $h$, $\sigma_i^x \sigma_{i+z}^x$ gives a large spectral peak on the order of $J_{TC}$, indicating that the composite object consisting of $n_f$ fermion and
FIG. 3. (a) Identifying spin operators that create specific fractionalized excitations. (b) Excitation spectrum $S(\omega)$ for the operator $\sigma_j^x \sigma_{j+\pi}^z$ at $K_z = 2.5$ for different values of $h$. (c) Excitation spectrum $S(\omega)$ for the operator $\sigma_j^z \sigma_{j+\pi}^z$. (b,c) are rescaled in magnitude so as to make peaks clear; while the intensity shown in (b) is in fact much stronger than that in (c) by the order of 10^3. (d) The composite particle consisting of one $\epsilon$ and one $c$ majorana created by $\sigma_j^x$ or $\sigma_j^y$; the $\epsilon = e \times m$ particle only disperses along the direction defined by the arrows, giving 1D dispersion defined by Eq.9 and Eq.10. (e) Dynamical structure factor $S(\vec{k}, \omega)$ of $\sigma_j^x \sigma_{j+\pi}^z$ at $h = 0.10$ for the energy $\omega$ of the first peak shown by a red circle in (b). The stripy nature of the intensity reflects the 1D dispersion of $\epsilon$ particles. (f) The same structure factor for the energy $\omega$ of the second peak shown by a green circle in (b).

two $\chi_x$ particles, disperses at low energy even though the a single $f$ excitation are gapped out on the order of $O(K_z/K)$. On the other hand, $S(\omega)$ for $\sigma_j^x \sigma_{j+\pi}^z$ has non-zero weight only at $\omega \sim O(K_z/K)$ for small $h$ and therefore gives no signal for $\omega \sim J_{TC}$, as shown in Fig.3(c). However, for higher $h$ as the PF phase is approached, the peak in $S(\omega)$ of $\sigma_j^x \sigma_{j+\pi}^z$ splits into several smaller peaks, that is, the composite particles consisting of the bound state of $f$ fermions and two $\chi^\alpha$ further fractionalizes into its constituent parts. A similar signal can be seen in the $S(\omega)$ for $\sigma_j^y \sigma_{j+\pi}^z$. As shown in Fig.3(c), in contrast to having spectral weight at $\omega \sim O(K_z/K)$, non-zero intensity begins to develop at $h \geq 0.08$, indicative of the $\psi$ fermion formed from the hybridization of $f - \epsilon$ by the [111] magnetic field (see eqn. (18)).

The momentum-resolved $S(\vec{k}, \omega)$ for $\sigma_j^x \sigma_{j+\pi}^z$ further reveals the dispersion of the fractionalized quasiparticles. Figure.3(e,f) shows the dynamical structure factor of the lowest two peaks of the corresponding $S(\omega)$ at $h = 0.1$, $K_z/K = 2.5$, as is marked out by circles in Fig.3(b). From Fig.3(e) we can deduce that the lowest-energy dispersion is dominated by the $\epsilon$ particles, reflected in the stripy pattern of $S(\vec{k}, \omega)$ due to the 1D dispersion described in Eq.9 albeit with missing gaps due to the gapped majoranas (or $f$-fermions). These missing gaps, as shown in Fig.3(b), are pushed to a higher energy marked out by the second circle; and the intensity pattern resembles that of the $\sigma_j^y \sigma_{j+\pi}^z$ (not shown here). This suggest that itinerant majorana fermions (generated for example via $\sigma_j^x \sigma_{j+\pi}^z$) reside near the $M$ points in the Brillouin zone, which is not unexpected given that the static flux sector calculations [7] show the low energy fermions lie near the $M$ point in the presence of a field and undergo a transition via Dirac cones to the gapped TC phase when $K_z$ is increased. The energy of these excitations are lowered by the increasing magnetic field, and are low lying close to the transition to the dimerized/polarized phase. The nature of excitations in all the phases is summarized in Table.I.

**IV. CONCLUSION**

For a system with spin-orbit coupling and strong interactions, the most general magnetic interactions based
on symmetry are isotropic Heisenberg and anisotropic Kitaev and Gamma interactions. Of these, the Kitaev interactions on the honeycomb is exactly solvable to give rise to a fractionalised $\mathbb{Z}_2$ QSL phase and provides a controlled gateway to the rich world of fractionalized phases with long-range quantum many-body entanglement and topological order where the nature of the lowest energy excitations—the majorana fermions or the $\mathbb{Z}_2$ fluxes can be controlled via the coupling of the Kitaev Hamiltonian. Here we have probed this rich physics with an experimentally relevant perturbation—an external magnetic field—for various parameter regimes of the Kitaev model to reveal the structure of the underlying fractionalised excitations in terms of their response to the magnetic field and we focus on the resultant phases obtained as an interplay of bond anisotropy and the magnetic field.

The central result reported in this paper is our discovery of a gapped primordial $\mathbb{Z}_2$ fractionalized phase at intermediate bond anisotropy and magnetic field in the center of the phase diagram in the anisotropy-field plane. Key to this phase is the twin role of the magnetic field that—(1) provides dispersion to the $\mathbb{Z}_2$ fluxes which in turn selectively provides dispersion to the $\epsilon = e \times m$ fermions in the anisotropic limit, and, (2) provides hybridisation between the $\epsilon$ and the majorana fermions—to produce new hybridized fermions whose properties naturally explain the PF phase.

The significance of this finding is that all the phases surrounding this central region: the gapless Kitaev spin liquid, the gapped abelian QSL, the TC phase, the gapped chiral non-abelian QSL, the gapless U(1) QSL, the dimer or valence bond phase, and the polarized phase, emerge from the primordial fractionalized phase. We have therefore identified the essential coupled matter and $\mathbb{Z}_2$ gauge degrees of freedom in the PF phase that produce the surrounding gapped phases with topological order, gapless phases with spinon Fermi surfaces, and first order transition driven by $\epsilon$ to the VBS order. The most direct information on the nature of the PF phase has come from the dynamics and their dispersion in the Brillouin zone of different combinations of spin operators that create particular fractionalized excitations. By observing the peaks of the structure factor corresponding to these spin operators as a function of the magnetic field and anisotropy, we have been able to track their evolution across phase transitions. Since the manipulation of an anisotropy in the exchange coupling was recently proposed in the realistic materials by means of the light irradiation [48], and toric code (TC) topological phase is recently realized in cold atom setup [49], we hope our results can inspire relevant experiments on Kitaev QSLs.

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| Phase          | Hierarchy of low energy excitations                                                                 |
|---------------|-----------------------------------------------------------------------------------------------------|
| Isotropic KQSL| Gapless c majoranas, gapped flux excitations                                                         |
| CSL           | $\mathbb{Z}_2$ non-Abelian QSL with gapped $p + ip$ superconducting state of $f$ fermions            |
| TC QSL        | $\mathbb{Z}_2$ Abelian QSL; Gapped c majoranas, Gapped flux excitations $|e,\epsilon,m\epsilon|$    |
| VBS           | spin excitations (i) one gapped at energy scale $\sim h^2/K_z$, (ii) two gapped at energy $\sim K_z$ |
| Gapless QSL   | Fermi surface of $f$ fermions                                                                        |
| Polarized     | spin waves                                                                                            |
| PF            | gapped fractionalized $\mathbb{Z}_2$ QSL of $\psi$ fermions (hybridized $c$ and $\epsilon$ fermions) |

TABLE I. The summary of various phases and the nature of excitations and their associated energy scales.
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