In the pseudospin-$\frac{1}{2}$ honeycomb Mott insulators with strong spin-orbit coupling, there are two types of bond-dependent exchange interactions, named Kitaev ($K$) and $\Gamma$, leading to strong frustration. While the ground state of the Kitaev model is a quantum spin liquid with fractionalized excitations, the ground state of the $\Gamma$ model remains controversial. In particular, the phase diagram of the $K\Gamma$ model with ferromagnetic $K$ and antiferromagnetic $\Gamma$ interactions has been intensively studied because of its relevance to candidate materials such as $\alpha$-RuCl$_3$. Numerical studies also included the effects of tuning the bond strengths, i.e., $z$-bond strength different from the other bonds. However, no clear consensus on the overall phase diagram has been reached yet. Here we study the classical $K\Gamma$ model with anisotropic bond strengths using Monte Carlo simulations to understand the phases that emerge out of the competition between two frustrated limits. We also address how the anisotropic bond strength affects the phase diagram and strength of quantum fluctuations. We found various large unit cell phases due to the competing frustrations, and analyzed their intrinsic degeneracy based on the symmetry of the Hamiltonian. Using the linear spin wave theory we showed that the anisotropic bond strength enhances quantum fluctuations in the $\Gamma$-dominant regime where a small reduced moment is observed. The implications of our findings in relation to the quantum model are also discussed.

I. INTRODUCTION

The Kitaev spin model on the two-dimensional honeycomb lattice serves as a fascinating example of a quantum spin liquid (QSL) [1]. In particular, the braiding statistics of fractionalized Majorana excitations in the Kitaev spin liquid (KSL) has generated intense interest in both condensed matter physics and quantum information communities due to their application in fault-tolerant quantum computation [2]. A key ingredient of the model is a particular type of bond-dependent interactions resulting in spin frustration, different from more traditional approaches based on geometrical constraints or going beyond nearest-neighbor interactions on bipartite lattices [3,6]. This intriguing model had been a pure theoretical interest until the Jackeli-Khaliullin mechanism [7,8] outlined how the Kitaev interactions are generated in the low-energy description of pseudospin $J_\text{eff} = 1/2$ moments in spin-orbit coupled Mott insulators. However, it was shown that in solid-state materials non-Kitaev interactions are inevitable, and a nearest-neighbor generic model includes another bond-dependent off-diagonal exchange term named the $\Gamma$ interaction in addition to a conventional Heisenberg ($J$) term [9]. The generic model was studied using a 24-site exact diagonalization (ED) which showed a rich phase diagram including various ordered and disordered phases, but the nature of the disordered phases near the $\Gamma$ region was not identified [9].

A considerable amount of theoretical efforts has been made to pin down the phase diagram of the extended model and to identify the potential QSL in Kitaev candidate materials such as $\alpha$-RuCl$_3$ [10,24]. While the KSL and various ordered phases are uncovered, there still remains regions of the phase space which are not well understood, with the most peculiar region being that of ferromagnetic (FM) Kitaev and antiferromagnetic (AFM) $\Gamma$ interactions ($K\Gamma$ model). Several numerical simulations of the $K\Gamma$ model have reported quantum disordered phases [25,32], but the phase diagram is still controversial [33]. The classical $K\Gamma$ model in a small phase space near the pure Kitaev [34,39] or pure $\Gamma$ region was also studied [19,30,40,43]. They revealed the macroscopic degeneracy at the pure Kitaev and $\Gamma$ limits [44,45] and the large unit cells (LUCs) that cannot be captured by small clusters used in, for example, ED on the 24-site cluster.

These studies have focused on the isotropic limit, where the exchange interactions are equivalent on each honeycomb lattice bond. In parallel, the effects of exchange anisotropy on the spin frustration have also been explored to find possible QSLs and to understand their connection to the KSL [46-49]. They suggest that the strong $z$-bond region hosts large regions of disordered phases but it is not clear whether they correspond to the isolated dimer limit [47,48] or spin liquid states such as the $\Gamma$ spin liquid (FSL) [30,43] or multi-node gapless QSLs [49]. These numerical studies may also suffer from finite-size effects and thus an investigation of the classical $K\Gamma$ model whereby the bond strength is tuned would offer an insight to the ground states of the anisotropic $K\Gamma$ quantum model.

In this paper, we tackle this problem by addressing the following questions. What types of magnetic orderings appear via the competition between two extreme frustrated limits, i.e., Kitaev and $\Gamma$ limits? How does the exchange anisotropy affect the classical ground states of
the KT model, and which regions of the anisotropic phase space may exhibit a quantum-disordered ground state? Using classical Monte Carlo simulations, we found various LUCs with intriguing fourfold or eightfold degeneracy except for a few special points with macroscopic degeneracy. It is likely that LUCs are results of the generic except for a few special points with macroscopic degeneracy associated with each ordered phase independent of the bond anisotropy.

We then discuss the effects of quantum fluctuations leading to a complete destruction of the magnetic moment suggesting possible QSLs in this region.

The rest of the paper is organized as follows. In Sec. II we briefly discuss the physics of an isolated z-bond before introducing x- and y-bond interactions, and then present the phase diagram of the two-dimensional model obtained via classical Monte Carlo simulations. In Sec. III we introduce three symmetry operations that map each bond Hamiltonian to itself, which reveals the degeneracy of each ordered phase independent of the bond anisotropy. In Sec. IV we focus on the phases near the Γ-dominant region, which arise from freezing the Ising degrees of freedom that form the classical ΓSL. In Sec. V we discuss the effects of quantum fluctuations using linear spin wave theory (LSWT). We then summarize our results and discuss implications of our findings on the quantum model in the last section.

II. DIMER HAMILTONIAN AND CLASSICAL PHASE DIAGRAM

We study the KT model on the honeycomb lattice with bond anisotropy, where the Hamiltonian is given by

$$H = \sum_{(ij)\gamma} K_{ij}^\gamma S_i^\gamma S_j^\gamma + \Gamma^\gamma \left( S_i^x S_j^y + S_i^y S_j^x \right),$$

where $\gamma \in \{x, y, z\}$, $\alpha, \beta \in \{x, y, z\} \setminus \gamma$ label the interaction along a particular bond. Here the spin direction $\vec{S}_i$ is defined in the local octahedral $xyz$ basis as shown in Fig. 1. The crystallographic $XYZ$ basis is also shown, where $\vec{Z}$ is perpendicular to the honeycomb plane, and $\vec{X}, \vec{Y}$ are perpendicular and parallel to the $z$-bonds, respectively. These will be used when we describe the magnetic ordering moment directions in Sec. III. Near the $\Gamma$-dominant region, the bond energy is minimized by setting $\theta_0 = \theta_1$ and $\phi_1 + \phi_2 = -\pi/2$, and the moments can be written as $\vec{S}_1 = S (a, b, c)$, $\vec{S}_2 = S (-b, -a, c)$ where $a, b, c \in \mathbb{R}$ satisfy $a^2 + b^2 + c^2 = 1$. The bond energy for this configuration is then

$$E_{(12)_a}/S^2 = -\Gamma - (K - \Gamma) c^2.$$  

Note that when $K = \Gamma$ ($\psi = \pi/4$) each of the $N/2$ isolated z-bonds retain an $O(3)$ symmetry, where $N$ is the number of sites. Away from this point the $O(3)$ symmetry is lifted and one of two states may stabilize, while the macroscopic degeneracy associated with each z-bond remains. When $K > \Gamma$ the energy is minimized by setting $c = 1$ and the moments form FM dimers pinned along the $\hat{z}$ direction with a twofold Ising degeneracy. On the other hand, when $\Gamma > K$ the bond energy is minimized by placing the moments in the $xy$-plane. In this case the moments retain a continuous $O(2)$ degeneracy with the restriction that $\phi_1 + \phi_2 = -\pi/2$. The transition between the two phases is thus a first-order spin-flop transition. Introducing interactions along the $x-$ and $y$-bonds when
We distinguish the phases that share the same ordering pattern but with a different moment orientation using a subscript of $i = x, y, z$. For example, the ZZ$_x$ and ZZ$_y$ both have four sites in the magnetic unit cell, but the zigzag chains repeat along the $z$-bond direction in the former and the $y$-bond direction in the latter. There is also a ZZ$_x$ orientation that is degenerate with ZZ$_y$ and can be obtained by a $C_2$ rotation about the $z$-bond direction $Y$, but it is omitted in Fig. 2 for simplicity.

The pure classical Kitaev model exhibits an extensive ground-state degeneracy, and when $g > 0$ the moments form disconnected FM dimers along the $z$-bond, which point in the $\pm \hat{z}$ direction $[34, 35]$. This is denoted by the solid gray line in Fig. 2. When $\Gamma$ is turned on the magnetic order is stabilized and a FM is formed with moments pinned near the $\hat{z}$ axis. The 120° order, which is degenerate with the FM, can be obtained by a symmetry operation to be discussed in the next section. In a small region between the $(ZZ + 12)_y$ and $6 + 18$ regions we find 16 + 48 and 24-site orders which may arise from further moment frustration. Below we will focus our attention on the $(ZZ + 12)_y$, 6 + 18, 18°, and 18°' orders which occupy the major part of the phase space extending from the $K = \Gamma$ dimer point at $(\psi, g) = (0, 0.25\pi, 1)$ to the isotropic limit. The $(ZZ + 12)$ and 6 + 18 orders are stabilized in the Kitaev-dominant region and are sensitive to anisotropy since a particular orientation is selected based on the values of $g$ and $\Gamma/K$. On the other hand, the 18° and 18°' phases remain eightfold-degenerate throughout their respective phase regions. In the next two sections we present the patterns of each magnetic order and the symmetries related to their degeneracy, and in Sec. V we will discuss the quantum effects on the magnetically ordered states using LSWT.

III. CLASSICAL K"{A} DEGENERATE MANIFOLDS

The degeneracy of the classical orders exhibited in Fig. 2 originates from a symmetry of the Hamiltonian Eq. (1). This can be seen by considering the dual honeycomb lattice, i.e., a triangular network with sites at the center of each hexagon labeled by the three plaquette sublattices.
\(\mathcal{A}, \mathcal{B}, \mathcal{C}\) in Fig. 1. For a sublattice \(\bar{\sigma} \in \{\mathcal{A}, \mathcal{B}, \mathcal{C}\}\), we define the operation
\[ R_\bar{\sigma} = \prod_{p \in \bar{\sigma}} \prod_{s \in \partial p} C^{\text{out}(i)}, \]  
(5)

where \(C^{\bar{\sigma}}\) is a \(\pi\) rotation about the cubic \(\alpha\)-axis and \(\text{out}(i) = x, y, z\) refers to the bond which extends outwards from the plaquette \(p \in \bar{\sigma}\) at site \(i\). The notation \(\partial p\) refers to the boundary of the plaquette \(p\), which consists of six bonds. For example, the \((12)_z\) bond Hamiltonian \(H_{(12)}\) is
\[ H_{(12)} = K^z S_i^z S_j^z + \Gamma^z (S_i^x S_j^x + S_i^y S_j^y). \]

(6)

If we apply this operation to the remaining sites of the honeycomb lattice, the total Hamiltonian Eq. (1) maps to itself. This is the case for the \(R_{\mathcal{B}}, R_{\mathcal{C}}\) operators defined for the plaquette sublattices \(\mathcal{B}, \mathcal{C}\), respectively. Thus the Hamiltonian is intact under the three \(R_{\bar{\sigma}}\) symmetry operations of Eq. (5). Since \((R_{\mathcal{A}})^2 = R_{\mathcal{A}} R_{\mathcal{B}} R_{\mathcal{C}} = 1\), the set \(\{1, R_{\mathcal{A}}, R_{\mathcal{B}}, R_{\mathcal{C}}\}\) is isomorphic to the Klein four-group \(\mathbb{Z}_2 \times \mathbb{Z}_2\). This group leads to the degeneracy in all the phases shown in Fig. 2.

We note that the \(R_{\bar{\sigma}}\) transformations were first introduced in the context of the pure isotropic \(\Gamma\) model \([10]\). In this work we show that these operations continue to be symmetries of the \(K\Gamma\) model with finite \(g\).

Let us now explore the action of \(R_{\bar{\sigma}}\) on the phases shown in Fig. 2 using the \((ZZ + 12)_z\) orientation as an example. The \(ZZ_2\) orientation shown in Fig. 3(a) is given by FM chains of moments \(\vec{S}_i = S(-a,-a,+c), \vec{S}_{i'} = S(+a,+a,-c)\) separated by \(z\)-bonds, where \(|S_{i,i'}^z| = \sqrt{S^2_i + S^2_{i'}} = S\) and \(2a^2 + c^2 = 1\). These moments lie in the crystallographic \(XZ\) plane and \(a \gg c\) due to the proximity to the \(\Gamma\) dimer limit, which favours moments lying in the \(xy\)-plane. Now we apply the symmetry operation \(R_{\mathcal{A}}\) on this configuration where \(\mathcal{A}\) is the plaquette sublattice shown in dark gray in Fig. 3. Explicitly we perform \(C^{\bar{\sigma}}_2\) rotation on sites \(1, 6, 1', 6', 3', 3''\) and \(C^{\bar{\sigma}}_2\) on sites \(2, 5, 2', 5'\) which results in the 12-site order shown in Fig. 3(b) given by
\[ \vec{S}_1 = S(-a,+a,-c), \quad \vec{S}_{1'} = S(-a,+a,+c), \]
\[ \vec{S}_2 = S(+a,+a,+c), \quad \vec{S}_{2'} = S(-a,-a,-c), \]
\[ \vec{S}_3 = S(+a,-a,-c), \quad \vec{S}_{3'} = S(+a,-a,+c), \]
\[ \vec{S}_4 = S(+a,-a,-c), \quad \vec{S}_{4'} = S(+a,+a,+c), \]
\[ \vec{S}_5 = S(+a,+a,+c), \quad \vec{S}_{5'} = S(-a,-a,-c), \]
\[ \vec{S}_6 = S(-a,+a,-c), \quad \vec{S}_{6'} = S(-a,+a,+c). \]  
(7)

We call this particular orientation \(12_z\) due to the two-site periodicity along the \(z\)-bond as shown in Fig. 3(b). This shows that the two orders are degenerate. The two other operations \(R_{\mathcal{B}, \mathcal{C}}\) applied on \(ZZ_z\) give the \(12_z\) order up to translations of the magnetic unit cell, so that the total degeneracy due to \(R_{\bar{\sigma}}\) and time reversal \(T : S_i^z \to -S_i^z\) is four. Similarly, the \((ZZ + 12)_y\) orientation is four-fold degenerate but cannot be mapped to the \((ZZ + 12)_z\) orientations when \(g \neq 0\) and a first order transition separates the two. This analysis applies to the three orientations of the \(\mathcal{F} + 120^\circ, 6 + 18\), and \(16 + 48\) orders as well: the \((6 + 18)_z\) orientation is shown in Fig. 4.

From Eq. 7 we note that the moments in the \(12_z\) configuration alternate in a six-site pattern ABCBCBA along the \(xy\)-chain. This is also the case for the \(6 + 18\) phases as indicated in Fig. 4. This pattern is referred to as a counterrotating spiral as the moments alternate as ABC along one site sublattice and ACB along the other, forming two FM dimers serving as inversion centers. This pattern has appeared in previous models of hyperhoneycomb materials \([55, 58]\) suggesting a relation between the \(12_z\) and \(6 + 18\) phases to the so-called \(K\) states of Ref. \([57]\).
IV. FREEZING THE Γ SPIN LIQUID: 18° AND 18' PHASES

In this section we focus on the 18° and 18' phases, where there are four degenerate spin patterns (excluding time-reversal partners) with the same size of magnetic unit cell. One vortex pattern is denoted by 18°C (called 18-C3 in Ref. 25) and three patterns as 18°i for i ∈ {x, y, z}, see Fig. 4. Crucially, the four orientations are connected by the three Rσ operations.

To discuss the appearance of the 18° and 18' phases in the Γ-dominant limit, and the difference between the two, we first review the physics of the isotropic Γ model. There it was found that the classical ground state is the Γ spin liquid (ΓSL), which contains an extensive degeneracy due to free Ising degrees of freedom ηp = ±1 that reside on each plaquette p in addition to a continuous O(3) degeneracy [40]. This can be seen by separating the sign and magnitude of the spin components as

$$\vec{S}_i = \begin{cases} +S(\eta_i^p a_i, \eta_i^p b_i, \eta_i^p c_i), & i \in A \text{ sublattice,} \\ -S(\eta_i^p a_i, \eta_i^p b_i, \eta_i^p c_i), & i \in B \text{ sublattice,} \end{cases} \quad (8)$$

where A and B are the honeycomb site sublattices and 

$$(a_i, b_i, c_i) = (|S_i^x|, |S_i^y|, |S_i^z|)/S$$

satisfies $a_i^2 + b_i^2 + c_i^2 = 1$ and $\eta_i^p = \pm 1, \alpha \in \{x, y, z\}$. We introduce a visual guide where each site is represented by a triangle with each corner corresponding to one of the three $\eta_i^p$.

We refer to this as the $\eta$-representation of the moments $\vec{S}_i$, which allows us to easily extract the role of the spin component signs $\eta_i^p$ in the energy minimization process. For example, the signs of the two energy contributions from $\Gamma^z$ along the $\langle 12 \rangle_z$ bond in Fig. 1 are $\mathrm{sgn} (\Gamma^z S_i^z S_j^z) = -\eta_i^p \eta_j^p$ and $\mathrm{sgn} (\Gamma^z S_i^z S_j^z) = -\eta_i^p \eta_j^p$, which are minimized for general $a_i, b_i$ when $\eta_i^p \eta_j^p = \eta_i^p \eta_j^p = 1$. In the pure $\Gamma$ limit all $\eta$-constraints may be minimized by fixing the signs of an arbitrary site $i$ as $(\eta_i^p, \eta_i^p, \eta_i^p) \equiv (\eta_1, \eta_2, \eta_3)$ and distributing the signs by satisfying the $\eta$-constraints bond by bond, introducing new $\eta$'s as necessary to parametrize the signs of any leftover spin components. One may see that each plaquette $p$ may be assigned an Ising variable $\eta_p$ by satisfying the $\eta$-constraints along the plaquette’s boundary. Furthermore, the energy is insensitive to the value of $\eta_p$ as each contribution squares to unity, so that the pure $\Gamma$ limit is equivalent to an Ising gas on the triangular superlattice and exhibits an extensive ground-state degeneracy [40]. The combination of time-reversal and one of the three global $R_\sigma$ transformations on the TSL corresponds to flipping the signs of all $\eta_p$ which live on one of the plaquette sublattices $\sigma \in \{A, B, C\}$ [40] [41]. For example, for the plaquettes shown in Fig. 6 applying $T \cdot R_A$ on each moment gives

$$\vec{S}_1 \rightarrow (-\eta_0|S_1^0|, S_1^y, S_1^z), \quad \vec{S}_4 \rightarrow (S_4^x, +\eta_0|S_4^y|, S_4^z), \quad \vec{S}_2 \rightarrow (S_2^x, S_2^y, +\eta_0|S_2^z|), \quad \vec{S}_5 \rightarrow (S_5^x, S_5^y, -\eta_0|S_5^z|), \quad \vec{S}_3 \rightarrow (S_3^x, -\eta_0|S_3^y|, S_3^z), \quad \vec{S}_6 \rightarrow (+\eta_0|S_6^x|, S_6^y, S_6^z),$$

and similarly for the i' and i'' moments which will flip the signs of $\eta_{i'}$ and $\eta_{i''}$, respectively.

We add a finite Kitaev term and investigate the stability of the TSL. For the $(61')_x, (4'3'')_y,$ and $(2'5')_z$ bonds shown in Fig. 5 the Kitaev contributions to the energy come with sign

$$\mathrm{sgn} E^K_{(61')_x} = -\mathrm{sgn} K \eta_0^x \eta_{1'}^y = \eta_0 \eta_{1'}, \quad \mathrm{sgn} E^K_{(4'3'')_y} = -\mathrm{sgn} K \eta_0^x \eta_{3'}^y \eta_{5'}^z = \eta_0 \eta_{3'} \eta_{5'}, \quad \mathrm{sgn} E^K_{(2'5')_z} = -\mathrm{sgn} K \eta_2^x \eta_5^z = \eta_c \eta_{a},$$

(11)
and thus are minimized when \( \eta_a \eta_b = \eta_b \eta_c = \eta_c \eta_a = -1 \). The three \( \eta_{a,b,c} \) cannot be fixed simultaneously without violating one of the \( \eta \)-constraints, which shows that perturbing the GS with Kitaev interactions is identical to the triangular Ising antiferromagnet with interactions between next-nearest neighbor \( \eta \)-variables [3, 59, 60]. It also presents a clear demonstration of the competition present between Kitaev and \( \Gamma \) interactions of opposite signs [44].

The ground state is obtained when two-thirds of all \( \eta_p \) carry one sign while the remaining third carry the opposite sign [3]. For next-nearest neighbor interactions only, there are several configurations of \( \eta_p \) that minimize the energy [60]. However including the spin magnitude \( |S_i^\alpha| \) lifts this degeneracy and selects the state with nine \( \eta_p \), or 18 sites, in the magnetic unit cell. This is precisely the 18\( ^0 \) phase, which is a subset of the classical degenerate ground states of the GS that is selected by FM \( K \). Similar to the GS the 18\( ^0 \) phase exhibits well-defined plaquette fluxes \( W_p = 2^6 \prod_{i \in \partial p} S_i^{\text{out}}(i) \neq 0 \), see Fig. [7](a).

The 18\( ^1 \) phase is separated from 18\( ^0 \) phase via a second order transition. It is similar to the 18\( ^0 \) phase with eightfold-degeneracy but the spin patterns respect inversion symmetry. We label the orientations of 18\( ^1 \) as \( i = x, y, z_1, z_2 \) and we note that inversion maps each of 18\( ^1 \) to itself, whereas 18\( ^1 \) maps to 18\( ^1 \) and vice versa. The 18\( ^1 \) phase contains an “idle” plaquette with vanishing flux as shown in Fig. [7](b), and the six surrounding moments are pinned near the [100], [011], and [110] axes. Note that these moments lie in the \( xy \) plane, which reflects the increasing influence of the \( \Gamma \) dimer’s \( O(2) \) degeneracy discussed earlier as bond anisotropy is increased. Thus the 18\( ^0 \) and 18\( ^1 \) phases result from the competing physics of the dimer and isotropic \( \Gamma \) limits in the presence of Kitaev interactions.

V. EFFECTS OF QUANTUM FLUCTUATIONS

In this section we discuss the effects of quantum fluctuations on the classical ground states by measuring the zero-point motion about the ordered states. Using LSWT the magnon gap is defined as \( \Delta_0 = \min \omega_k^s \) > 0 where \( \omega_k^s \) are the magnon dispersions and \( s \) labels the sites of the magnetic unit cell. Increased quantum fluctuations lead to a reduction of the moment magnitude

\[
\langle M \rangle = S - \frac{1}{N} \sum_i \langle a_i^\dagger a_i \rangle ,
\]

where \( \langle a_i^\dagger a_i \rangle \) is the number of magnons per site in the ground state \( |0 \rangle \) at \( T = 0 \).

In Fig. [8] we show two cuts where the bond anisotropy is varied at fixed \( \Gamma/K \) in the Kitaev dominant limit \( \psi = 0.2\pi \) (\( \Gamma/K \) \( \sim \) 0.73) and the \( \Gamma \)-dominant limit \( \psi = 0.4\pi \) (\( \Gamma/K \) \( \sim \) 3.08). We indicate the magnon gap \( \Delta_0 \) and the reduced moment \( \langle M \rangle/S \) in blue and red, respectively. \( \langle M \rangle/S \sim 0 \) indicates that the classical order is unstable due to quantum fluctuations. Throughout both cuts the moment is reduced by more than 50% indicating strong quantum effects in all phases. However, the effects of anisotropy are qualitatively different between the \( \Gamma \) and \( \Gamma \) regimes. In the Kitaev dominant region increased anisotropy leads to a decrease in moment reduction, and the gap increases due to the stability of the Ising easy-axis at the pure dimer limit. On the other hand, in the \( \Gamma \)-dominant limit the gap goes to zero as anisotropy is increased. This is due to the proximity of the \( O(2) \) symmetric \( \Gamma \) dimer, which exhibits gapless excitations within the \( xy \)-plane as discussed in Sec. [4].

Interestingly, while the magnons are gapped away from this limit, the reduced moment indicates that quantum fluctuations become strong enough to completely destroy the magnetic order within LSWT.
The degeneracy related to this symmetry in all the magnetic orders shown in this study is lifted in the presence of an incommensurate spiral order along the KT line using a single-Q variational ansatz. Further studies of the KT line go beyond this approximation using classical Monte Carlo techniques. More recently it was found that the incommensurate spiral order is stabilized at low temperatures $T \sim 0.1 - 0.2$ as exhibited by the magnetic susceptibility and heat capacity. In contrast, we obtain the LUC orders in this region of $g = 0$ when $T \sim 10^{-9}$ where thermal fluctuations are minuscule compared to the average interaction scale. We determine the energy of each phase to a high precision using the algorithm given in Ref. [38], i.e., by annealing the cluster to this ultra-low temperature and then performing sweeps of the cluster where the moments are aligned with their local molecular fields, see Appendix A for details.

Numerical studies of the quantum model in the isotropic limit $g = 0$ report various quantum-disordered phases including a proximate KSL (PKSL) [27, 31, 49], a TSL [30, 43], and a nematic paramagnet [28, 29]. Away from $g = 0$, a disordered region between the isotropic limit and the dimer phase, which rapidly expands when $\Gamma > K$, was also reported [48]. However, it is not clear whether this is a true phase boundary or simply a crossover region connecting two phases. A series of multinode gapped QSLs before entering a dimer phase at larger $g$ was found using variational MC (VMC) [49]. A further VMC simulation including the multi-Q orders around the $\Gamma$ region with finite $g$ (i.e., $18^\circ$ and $18^\prime$) would extend our current knowledge on possible QSLs and their nature in this region.

Here, for the classical K$\Gamma$ model with $g = 0$, we find four different phases (ZZ+12, 6+18, 16+48 and 18+96) with LUCs, and the LSWT shows that, in the $\Gamma$-dominant regime, the reduced moment $\langle M \rangle / S$ for fixed $\Gamma / K$ in Fig. 8(b) decreases as $g$ increases. This supports the disordered phases reported in Refs. [48, 49]. Furthermore, if the magnetic ordering in the $18^\prime_{x,y,z}$ orientations are destroyed by quantum fluctuations but the spontaneous $C_3$ symmetry breaking survives at $g = 0$, it generates a nematic paramagnetic state. We emphasize though this broken lattice-rotational symmetry does not exclude a QSL.

Finally, an interesting proposal is a possible vison crystal spin liquid near the GSL. In fact, one feature of the GSL is significant correlations of the plaquette fluxes, which peak at the $\Gamma$ and $K, K'$ points in the reciprocal space. A vison crystal spin liquid, which is magnetically disordered yet exhibits a broken translational symmetry in the form of a long-range $(W_p W'_p)$ correlation function, may be stabilized in the $\Gamma$-dominant region with moderate $z$-bond anisotropy, which remains
FIG. 9. The two unit cells used to construct the Monte Carlo cluster, with vectors $a_1$ and $a_2$ shown along with the three bond types. From left to right: the rhombic unit cell with unit cell vectors Eq. (A1) and the rectangular unit cell with unit cell vectors Eq. (A2). The bond type $x,y,z$ are colored green, blue, and red respectively.

as a subject for future study.

In summary, we have studied the classical KT − $g$ model to understand the phases out of two competing frustrated interactions and the effects of bond anisotropy on their competition. The pure Kitaev and $\Gamma$ models have classical spin liquids with macroscopic degeneracy, but when they are both present, we found there exist several LUC phases occurring via their competition. All the phases have the intrinsic degeneracy related to a product of $\pi$ rotations around the plaquette, where a subset of degenerate states can have a smaller magnetic unit cell as a special case of a larger magnetic unit cell state. Near the $\Gamma$-dominant region, we find 18-site magnetic unit cells which retain their degeneracy in the presence of bond anisotropy unlike the $C_3$ related degeneracy appearing in the Kitaev dominant region at $g = 0$. The bond anisotropy enhances quantum fluctuations in the $\Gamma$ dominant region which suggests that this region hosts a potential QSL.

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Appendix A: Monte Carlo Simulation Details

We perform the SAMC simulation on a finite size honeycomb cluster with periodic boundary conditions. We parameterize the honeycomb sites by placing them into unit cells located at $R = \sum_i m_i T_i$, where $T_1, T_2$ define the unit cell vectors and $m_1, m_2$ are integers. The honeycomb lattice contains $s \geq 2$ sublattices within a unit cell, each forming its own sublattice: every site $i$ can be labeled by three integers $i = (m_1, m_2, t)$ where $t = 1, \ldots, s$. One choice for the geometry of the unit cell is to use the two-site rhombic unit cell with translation vectors

$$T_1 = a_1 - a_2 = (1, 0),$$
$$T_2 = a_1 = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right),$$

which is shown in Fig. 9 along with $a_{1,2}$. This choice produces a cluster that is commensurate with the 18 site phases when $m_1$ and $m_2$ are multiples of 3. We may also use the 4-site rectangular unit cell with translation vectors

$$T_1 = a_1 - a_2 = (1, 0),$$
$$T_2 = a_1 + a_2 = (0, \sqrt{3}),$$

which produces a cluster commensurate with the $(ZZ + 12)_2$ order whenever $m_1$ is a multiple of 3. Either unit cell may be used to build the cluster as long as one ensures that the ordering wavevectors of the classical states are
accessible. For our purposes we use the \( N = 288 \) site cluster with a rectangular unit cell, which accesses the \( M, K/2, \) and \( 2M/3 \) reciprocal points as shown in Fig. 10. We have also extended the cluster size to \( N = 720 \) to check whether other large unit cell orders are stabilized.

After constructing the cluster we obtain the classical ground state using the SAMC algorithm given in Ref. [38], where Monte Carlo trials are performed for a finite temperature \( T \) which is slowly tuned to zero. For our simulations we anneal according to the cooling schedule \( T_{i+1} = 0.9 T_i \) until the final temperature \( T_f = (0.9)^{200} \sim 10^{-9} \) is reached. At each temperature step \( T_i \) of the simulation, we perform \( N \times 10^5 \) Metropolis trials where we choose a random moment, “flip” it so that it points in a random direction, and accept the new configuration with probability \( \min(1, e^{-\Delta E/T}) \) where \( \Delta E \) is the energy difference between the two states. When the final temperature is reached, we further refine the energy by choosing a random moment and aligning it with its local molecular field, and then repeating this \( N \times 10^4 \) times.

In order to obtain the phase diagram Fig. 2 we first perform the SAMC on large clusters to resolve the possible classical ground states, and then refine the energy of each phase by either running the SAMC on small clusters or parametrizing the moments with angles \( (\phi_i, \theta_i) \) and minimizing the total energy within the unit cell with respect to each angle. To accurately obtain the \( T = 0 \) classical phase diagram it is important to determine each order’s energy to full precision as the energy difference of the competing phases is within \( \Delta E \sim \mathcal{O}(10^{-3}) \). Otherwise at higher temperatures one may stabilize a mixture of the competing phases. For example, the ZZ, 6-site, and 16-site phases, which have SSF peaks along the \( \Gamma - M \) lines in reciprocal space, are close in energy for \( \psi/\pi \sim 0.07 - 0.09 \) along \( g = 0 \). A mixture of the three phases would appear as an incommensurate order with SSF peaks that vary along \( \Gamma - M \), but such a state remains higher in energy than the true classical ground state at \( T = 0 \).

Appendix B: Magnetic Order of the K\( \Gamma \) Classical Ground States

We present in Figs. 11-16 the SSF patterns of the phases shown in the phase diagram Fig. 2. In each plot we show the first and second Brillouin zones in red and green, respectively. Different orderings, which share the same size of magnetic unit cell but with different moment orientations, are distinguished by a subscript \( i = x, y, z \). These labels are assigned by the distribution of the SSF ordering vectors about one of the three \( \Gamma - M_i \) lines in Fig. 10

![FIG. 11. SSF of the (a) ZZ\(_x\) and (b) 12\(_x\) patterns at (\(\psi, g\)) = (0.4\pi, 0.94), as well as the (c) ZZ\(_y\) and (d) 12\(_y\) patterns at (0.15\pi, 0.94) and (0.1\pi, 0.65), respectively. The ZZ peaks are located at one of the three M points, whereas the 12-site peaks are located at one of three \( \frac{1}{2}K, \frac{1}{2}K' \) pairs. The color of each ordering wavevector in Figs. 11-16 denotes the relative intensity of each peak.

![FIG. 12. SSF of the (a) 6\(_x\) and (b) 18\(_x\) patterns at (\(\psi, g\)) = (0.25\pi, 0.84), as well as the (c) 6\(_y\) and (d) 18\(_y\) patterns at (0.35\pi, 0.84). The six-site peaks are located at one of three \( \frac{1}{3}M, \frac{2}{3}M \) pairs, whereas the 18-site peaks are located at multiple \( \frac{1}{3}M, \frac{2}{3}M \) pairs.]
FIG. 13. SSF of the (a) $18^\circ_\eta_V$ and (b) $18^\circ_\eta_y$ patterns at $(0.4\pi, 0.5)$, as well as the (c) $18^\circ_{\eta_1}$ and (d) $18^\circ_{\eta_2}$ phase at $(0.4\pi, 0.71)$. The ordering vectors are located at multiple $\frac{2}{3}M$, $\frac{4}{3}M$ pairs.

FIG. 14. SSF of the (a) FM$_x$ and (b) $120^\circ_z$ phase at $(0.04\pi, 0.5)$. The dominant SSF peak is at the Γ point for the FM phase and one of three $K$, $K'$ pairs for the $120^\circ_z$ phase.

FIG. 15. SSF of the (a) $24^\circ_z$ and (b) $24^\circ_y$ patterns at $(0.125\pi, 0.57)$. The $24^\circ_z$ dominant SSF peaks are at $\frac{1}{2}M_z$ whereas for $24^\circ_y$ they are at $(\frac{1}{12}, \frac{7}{12})$, $(\frac{7}{12}, \frac{1}{12})$ in the $\{b_1, b_2\}$ basis, where $b_{1,2}$ satisfy $a_i \cdot b_j = 2\pi \delta_{ij}$.

FIG. 16. SSF of the (a) $16^\circ_y$ and (b) $48^\circ_y$ patterns at $(0.14\pi, 0.5)$. The $16^\circ_y$ dominant SSF peaks are at $\frac{3}{4}M_y$, $\frac{5}{4}M_y$, whereas for $48^\circ_y$ they are at $(-\frac{1}{3}, -\frac{1}{24})$, $(\frac{1}{3}, \frac{7}{24})$ in the $\{b_1, b_2\}$ basis, where $b_{1,2}$ satisfy $a_i \cdot b_j = 2\pi \delta_{ij}$.
