

Proximate Tomonaga-Luttinger liquid in an anisotropic Kitaev-Gamma model

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The characterization of quantum spin liquid phases in Kitaev materials has been a subject of intensive studies over the recent years, both theoretically and experimentally. Most theoretical studies have focused on an isotropically interacting model with its coupling strength being equivalent on each bond in an attempt to simplify the problem. In this Letter, we study an extended spin-1/2 Kitaev- Γ model on a honeycomb lattice with an additional tuning parameter that controls the coupling strength on one of the bonds: We connect the limit of isolated Kitaev- Γ chains, which is known to exhibit an emergent $SU(2)_1$ Tomonaga-Luttinger liquid phase [Yang *et al.*, *Phys. Rev. Lett.* **124**, 147205 (2020)], to the two-dimensional model. We report on an instance, in which properties of the Tomonaga-Luttinger liquid persist for finite interchain coupling forming a phase we call the proximate Tomonaga-Luttinger liquid (pTLL). This pTLL is strongly anisotropic in character analogous to *sliding Luttinger liquids*, and features spinon-like excitations similar to those of the antiferromagnetic Heisenberg chain. We use numerical exact diagonalization and density matrix renormalization group on various cluster geometries in a complementary way to overcome finite-size limitations.

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Introduction. Following the “More is different” philosophy by Anderson [1], competing interactions—or frustrations—can give rise to emergent features: fractional excitations, topological order, emergent gauge fields, anyonic exchange statistics, etc. [2–4]. Kitaev’s honeycomb model [5] is a paradigmatic spin-1/2 model in this context, due to being exactly solvable and featuring a quantum spin liquid (QSL) ground state composed of itinerant Majorana fermions and a static $\mathbb{Z}_2$ gauge field. The bond-dependent Kitaev spin exchange is realized in certain magnets with strong spin-orbit coupling [6]. This mechanism, however, introduces additional spin exchanges [6,7] that spoil the exact solvability of the Kitaev model. Many candidate materials have been proposed [8–12] among which α - RuCl_3 [13] has gained much attention due to a putative QSL phase in an in-plane magnetic field [14,15]. Even more so, since the measurement of a nearly half-quantized thermal Hall effect due to emergent Majorana fermions has been reported [16–18], although its origin remains disputed [19–25].

The spin-1/2 Kitaev- Γ ($\text{K}\Gamma$) model on the honeycomb lattice with ferromagnetic Kitaev exchange and positive symmetric off-diagonal Γ exchange has been proposed as a minimal model for α - RuCl_3 [26–29]. Many methods have been applied, yet no clear understanding of its ground-state phase diagram has emerged. Among the suggested states are magnetically ordered ones, such as zigzag [30], ferromagnet

[30–32], six-sublattice [31], or incommensurate spiral order [7,30,32], but also quantum paramagnetic states such as a putative gapped QSL [33], a lattice-nematic paramagnet [31,34], or a gapless QSL with multiple Majorana-Dirac nodes [30].

We like to change the perspective and focus on an aspect rarely included in theoretical works on Kitaev materials: We additionally tune the strength of the spin exchange spatially, ranging from a limit of uncoupled chains to spatially equal, yet still strongly anisotropic, spin exchange. In fact, such spatial anisotropy may either be intrinsic due to a reduced symmetry of the underlying lattice, such as $C2/m$ [35–38] instead of a full C_3 rotational symmetry, or spatial anisotropy can be induced by applying external pressure or strain [39], which possibly realizes various different QSL [40].

The one-dimensional limit features an emergent Tomonaga-Luttinger liquid (TLL) with critical properties similar to the antiferromagnetic Heisenberg (AFH) chain [41]. Since the TLL is a critical state, most TLLs are unstable when small interchain coupling is added [42,43]. An exception is *sliding TLLs* [44–46] that occur if the interchain coupling competes with the dominant correlations along the chains. As a consequence, the formation of long-range order is suppressed and the excitations can be described mostly by the TLL due to a dimensional reduction [47–52]. A perturbative treatment of coupled $\text{K}\Gamma$ chains, however, appears to be challenging [53].

Here, we argue that a similar mechanism arises in the anisotropic $\text{K}\Gamma$ model: The TLL phase of the $\text{K}\Gamma$ chain turns into an extended quantum paramagnetic phase retaining some of the TLL properties, i.e., algebraic correlations along chains. In the remainder, we refer to this phase as the proximate Tomonaga-Luttinger liquid (pTLL). Remarkably,

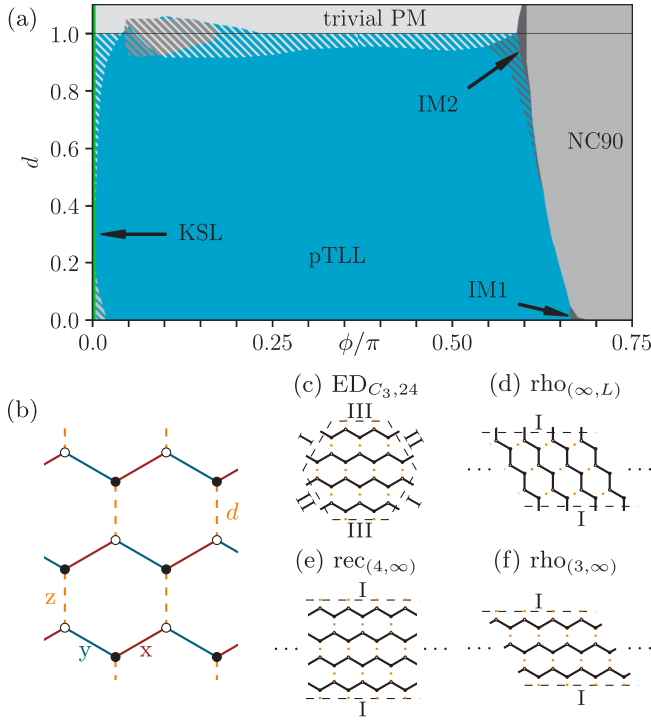


FIG. 1. (a) Schematic ground-state phase diagram of the anisotropic K Γ model. pTLL is highlighted in blue. KSL exist only in a small range next to $\phi = 0$. NC90 refers to a magnetically ordered phase with noncoplanar 90° order. Hatched areas illustrate where DMRG and ED differ. (b) Honeycomb lattice with bond-dependent interactions and modification of the coupling along z by a factor d [see Eq. (1)]. We use various geometries: (c) C_3 -symmetric 24-site cluster within ED, (d) rhombic unit cell with finite K Γ chains ($L = \{6, 12, 18\}$) coupled along the infinite direction, (e) rectangular unit cell with four infinite K Γ chains, and (f) rhombic unit cell with three infinite K Γ chains. Geometries (d)–(f) are employed within DMRG. Roman literals visualize periodic boundaries.

we find pTLL to extend within a wide range of $\Gamma > 0$ with ferromagnetic Kitaev exchange, and up to the C_3 -symmetric K Γ model with spatially equal spin-exchange strength (C_3 limit), see Fig. 1(a). We make the following key observations about the pTLL: (i) continuously connected to the TLL of the K Γ chain, (ii) absence of an excitation gap, (iii) suppression of the effective interchain coupling resulting in exponentially decaying transverse and algebraically decaying longitudinal correlations, and (iv) the dynamical spin-structure factor (DSF) exhibits a linear dispersion at low energies and an excitation continuum similar to the AFH chain [54–57].

Anisotropic K Γ model. We consider the spin-1/2 K Γ model on the honeycomb lattice with x , y , and z bonds [see Fig. 1(b)]. Its spin exchange is described by the Hamiltonian

$$\mathcal{H} = -K \sum_{\langle i,j \rangle_{\gamma=x,y}} S_i^\gamma S_j^\gamma + \Gamma \sum_{\langle i,j \rangle_{\gamma=z}, \alpha, \beta \neq \gamma} [S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha] - dK \sum_{\langle i,j \rangle_{\gamma=z}} S_i^\gamma S_j^\gamma + d\Gamma \sum_{\langle i,j \rangle_{\gamma=z}, \alpha, \beta \neq \gamma} [S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha], \quad (1)$$

where d determines the strength of the K Γ exchange on the z bond; $d = 1$ refers to equal exchange strength along each bond restoring the C_3 lattice-rotation symmetry, while $d = 0$ refers to the chain limit. Here, we are interested in the range $0 \leq d \lesssim 1$ connecting both limits. We set $K = \cos \phi$ and $\Gamma = \sin \phi$, focusing on the range $0 \leq \phi/\pi \leq 3/4$.

Yang *et al.* [41,58] have extensively studied the K Γ -chain limit and identified two relevant sublattice transformations: a six-sublattice transformation mapping the K Γ chain to either the ferromagnetic Heisenberg (FMH) chain at $\phi/\pi = 3/4$ or the AFH chain at $\phi/\pi = -1/4$, and a three-sublattice transformation mapping $\Gamma \mapsto -\Gamma$ such that the phase diagram is symmetric about the Kitaev limits, $\phi \mapsto -\phi$. An emergent $SU(2)_1$ TLL phase stabilizes in a wide range, $0 < \phi/\pi < \pm 0.66$ [41], around the dual AFH points, $\phi/\pi = \pm 1/4$. While the $SU(2)$ symmetry is a property of the Hamiltonian at the dual points, the system retains the $SU(2)$ symmetry as an emergent property at any other ϕ within the TLL phase.

Methods. We make use of different numerical techniques and their respective cluster geometries [Figs. 1(c)–1(f)] in a complementary way. Exact diagonalization (ED) enables us to study the K Γ model on a C_3 -symmetric cluster with 24 sites. In the chain limit, the 24-site cluster decomposes into two chains with 12 sites each implying finite-size gaps. With density matrix renormalization group (DMRG) [59] and the infinite matrix product state (iMPS) [60,61] framework we can access two complementary limits: a finite number of chains infinite in length eliminating their finite-size gap, and an infinite number of finite length chains. In the remainder of the text, we will refer to each geometry by the label given in Figs. 1(c)–1(f). In addition to the ground-state properties, we compute the DSF employing a time evolution of matrix product states [62,63] on $\rho_{(3,\infty)}$ containing three coupled chains (see the Supplemental Material, SM [64]).

Ground state. We start with the ground-state properties at $\phi/\pi = 1/4$, see Fig. 2. Near the chain limit, ED $_{C_3,24}$ obtains a lower ground-state energy in agreement with the finite-chain geometry $\rho_{(\infty,12)}$ in DMRG. The finite-size gap is sizable for both geometries. Shortly before approaching the C_3 limit, $\text{rec}_{(4,\infty)}$ with infinite chains obtains a lower ground-state energy until eventually all geometries converge to a single line for $d \gtrsim 1.1$ and finite-size effects become negligible.

The second derivative $\partial_d^2 E$ features a single phase transition at $d_{c,1}^{ED} = 1$ for ED $_{C_3,24}$ and at $d_{c,1}^{12} = 1.025$ for $\rho_{(\infty,12)}$. The results on $\text{rec}_{(4,\infty)}$ exhibit two features: A kink originating from a first-order transition near $d_{c,1}^\infty = 0.92$ and a broad peak around $d_{c,2}^\infty \approx 0.99$. The entanglement entropy of a bipartition S_E is particularly enhanced for $d < d_{c,1}^\infty$ connecting to the chain limit. Here, S_E depends on the bond dimension χ in a way that is consistent with a gapless phase; $S_E(\chi)$ follows equidistant lines if χ is increased exponentially, $\chi = \{1000, 1414, 2000\} \approx 2^{\frac{n}{2}} \times 1000$ with $n = 0, 1, 2$. S_E drops off upon increasing d beyond $d_{c,1}^\infty$ and ceases to depend on χ implying a gapped phase. An excitation gap is expected for $d > 1$ due to an adiabatic connection to a product state of triplet-dimer states with quadrupole moments [65], which we refer to as trivial paramagnet (trivial PM). In the case of $\text{rec}_{(4,\infty)}$, finite-size effects are most pronounced for $d \approx 1$, likely resulting in a finite-size gap for $d \sim 1$ and shifting the transition.

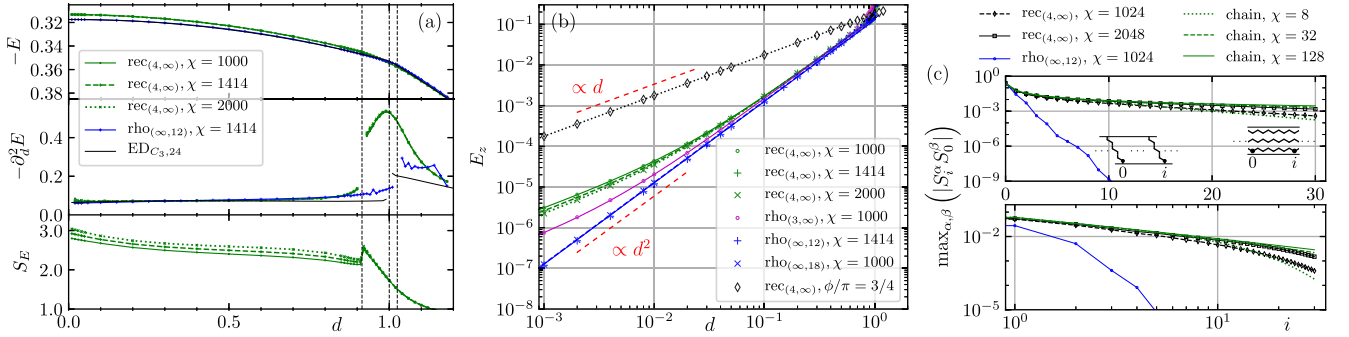


FIG. 2. (a) Representative cut of the phase diagram (Fig. 1) at $\phi/\pi = 1/4$ varying interchain coupling d . $\text{ED}_{C_3,24}$ features a single transition at $d_c^{ED} = 1$ close to $d_c^{12} = 1.025$ of $\text{rec}_{(\infty,12)}$, whereas $\text{rec}_{(4,\infty)}$ exhibits two transitions at $d_{c,1}^\infty \approx 0.92$ and $d_{c,2}^\infty \approx 0.99$. For $d < d_{c,1}^\infty$, $\text{rec}_{(4,\infty)}$ features a χ dependence of the entanglement entropy S_E , suggesting a gapless phase. (b) The energy at the z bond E_z scales as $E_z \propto d^2$ within pTLL, while E_z scales linearly, $E_z \propto d$, at $\phi/\pi = 3/4$ within NC90. Lines in (b) are fits to a quadratic function. (c) Spin-spin correlations along the cylinder axis at $\phi/\pi = 1/4$ and $d = 0.5$ illustrating exponentially decaying transverse correlations for $\text{rho}_{(\infty,12)}$ and algebraically decaying longitudinal correlations for $\text{rec}_{(4,\infty)}$. Since the Γ exchange introduces off-diagonal components in $C_{i,j}^{\alpha\beta} = \langle S_i^\alpha S_j^\beta \rangle$, we plot the largest element $\max_{\alpha\beta} (C_{i,j}^{\alpha\beta})$ for each pair (i,j) . Correlations in a single chain are included for comparison and illustrate the χ dependence.

Turning to small interchain coupling, $d \rightarrow 0$, Fig. 2(b) shows the local energy at the interchain bond E_z as a function of d . In fitting the quadratic function $f(d) = c_1 d^2 + c_2 d$, we find $E_z \propto d^2$ at $\phi/\pi = 1/4$ within pTLL. This is most evident for finite-chain geometries $\text{rho}_{(\infty,L)}$ with $L = \{12, 18\}$, while infinite-chain geometries, $\text{rho}_{(3,\infty)}$ and $\text{rec}_{(4,\infty)}$, have small linear corrections $c_2 \lesssim 0.02c_1$, which reduce further upon increasing χ . In contrast, a linear scaling is expected for NC90 at $\phi/\pi = 3/4$, as confirmed in Fig. 2(b).

Finding a quadratic—rather than linear—dependence on d suggests that the dominant correlations along the chains compete with the interchain coupling. While successive application of the six- and three-sublattice rotations maps $\text{K}\Gamma$ chains along the xy bonds to AFH chains [41], the exchange along the z bond maps to a Heisenberg-like diagonal exchange with a peculiar, positionally dependent modulation of the signs for each diagonal component. This modulation is not compatible with the dominant, Néel-like correlations along the chain [66]. As a consequence, spin-spin correlations retain a strongly anisotropic character [Fig. 2(c)] reminiscent of sliding TLLs; correlations decay exponentially transverse to the chains, while longitudinal algebraic correlations remain. In particular, we find a correlation length of $\xi \approx 0.6$ for transverse correlations, which is smaller than the distance 1 between neighboring chains indicating a very fast decay and (almost) vanishing interchain coupling.

Extent of the pTLL phase. Based on the ground-state energy $E = E(d, \phi)$ for the Hamiltonian, Eq. (1), its first derivative $\partial_d E$ ($\partial_\phi E$), and its second derivative $\partial_d^2 E$ ($\partial_\phi^2 E$) against d (ϕ), we map out the extent of pTLL, see Fig. 1(a). The ferromagnetic KSL at $\phi = 0$ is very fragile against the Γ exchange, which is consistent with earlier results at $d = 1$ [7,33,67]. Results for $\text{ED}_{C_3,24}$ suggest a direct transition between KSL and pTLL for $0 < d < 1$ at $\phi_c(d) < 0.005$ (see the SM [64]), while for $\text{rec}_{(4,\infty)}$ a phase exists with a dimerization along the x and y bonds for $\phi/\pi < 0.02$ at small $d \lesssim 0.2$, as well as a trivial PM for $0.3 \lesssim d \lesssim 1$ and $\phi/\pi < 0.05$.

In the chain limit, $d = 0$, the TLL phase appears for $0 < \phi/\pi < 0.66$ in ED (DMRG). A long-range-ordered

phase with D_4 symmetry (D4FM) stabilizes at $0.69 \lesssim \phi/\pi < 0.88$ around the FMH dual point [41] that extends to $d > 0$ forming noncoplanar 90° order (NC90). In contrast to Refs. [41,58], we find an intermediate region (IM1) with strong incommensurate correlations between TLL and D4FM that survives small $d \lesssim 0.05$. For $0.05 \lesssim d < d_{c,\text{IM2}} \approx 0.8$ (0.5), $\text{ED}_{C_3,24}$ ($\text{rec}_{(4,\infty)}$) shows a direct first-order transition between pTLL and NC90. Another intermediate phase (IM2) stabilizes for $d > d_{c,\text{IM2}}$, that is characterized by the absence of local magnetic moments and signatures of incommensurate correlations [66].

Near the C_3 limit, $d = 1$, ED and DMRG results show qualitative differences. $\text{ED}_{C_3,24}$ features a single transition between pTLL and a trivial PM at $d = 1$ in a wide range $0.2 \lesssim \phi/\pi \lesssim 0.6$ (see the SM [64]). On the other hand, $\text{rec}_{(4,\infty)}$ features two transitions: a kink in $\partial_d^2 E$ at $d \approx 0.9$ to 0.95 , and a broad feature near $d \approx 1$. Both transitions merge into a single kink at $d \approx 0.95$ for $\phi/\pi \gtrsim 0.3$.

iMPS χ scaling. We utilize the procedure outlined in the SM [64] and Refs. [68,69] to extract the excitation gap from the iMPS transfer matrix (TM), which contains full information about equal-time correlations in the ground state [70,71]. For Hamiltonians with local interactions, equal-time correlations are related to the excitation gap [72], $\xi(\mathbf{k}) \sim 1/\Delta(\mathbf{k})$ near momentum $\mathbf{k}$ [64,70]. If translational symmetry is not broken, TM eigenvalues λ_i can be sorted by their longitudinal and transverse momenta, $k_x = \arg \lambda_i$ and $k_y = 2\pi n/L_y$ with $n \in \mathbb{Z}$. Here, we select λ_i for $k_x \approx 2\pi/3$ and $k_y = 0$, where we obtain the smallest excitation gap $\epsilon_k = \epsilon_{0,k} = 1/\lambda_1$, corresponding to the dominant correlation. We find $\epsilon_k(\chi)$ to decrease as a function of the spacing between the inverse eigenvalues, $\delta_k(\chi) = \sum_i c_i \epsilon_{i,k}$ where $\sum_i c_i = 0$, see Fig. 3(a). Upon fitting $f(\delta) = c_1 \delta^2 + c_0$, $\epsilon_k(\chi)$ is almost linear with $c_2 = 1.0(1)$ and $c_0 = 0.00(3)$ consistent with pTLL being gapless. For comparison, we include data for a $\text{K}\Gamma$ chain whose ground state is the gapless $SU(2)_1$ TLL with a well-defined scaling form. Moreover, we confirm that local magnetic moments vanish as $\chi \rightarrow \infty$, ruling out long-range magnetic order. Details are presented within the SM [64].

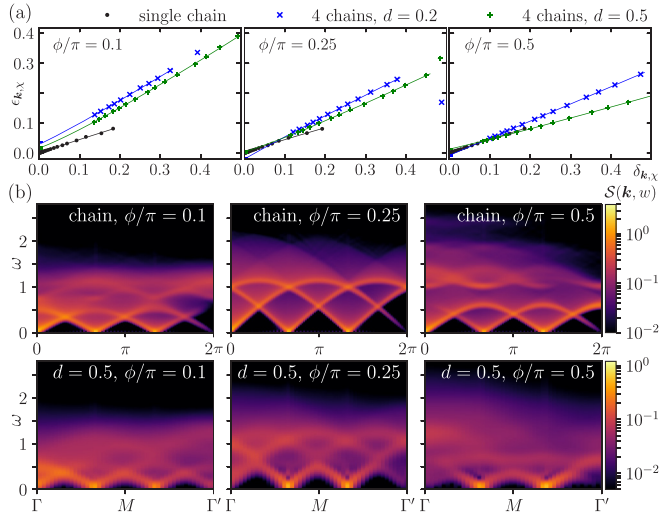


FIG. 3. (a) Excitation gap $\epsilon_k(\chi)$ at $\mathbf{k} = (2\pi/3, 0)$ extracted from the ground-state iMPS transfer matrix vanishing linearly with $\delta_k(\chi)$ as $\chi \rightarrow \infty$ similar to the $\text{K}\Gamma$ chain (black). We confirm these results at $\phi/\pi = \{0.1, 0.25, 0.5\}$ using $\text{rec}_{(4,\infty)}$ at $d = 0.2$ (blue) and 0.5 (green). Solid lines represent fits to $f(\delta) = c_1 \delta^{c_2} + c_0$. (b) Dynamical spin-structure factor $S(\mathbf{k}, \omega)$ for the $\text{K}\Gamma$ chain (top), and $\rho_{(3,\infty)}$ at $d = 0.5$ (bottom). At $\phi/\pi = 1/4$ the $\text{K}\Gamma$ chain is equivalent to the AFH chain with its characteristic spinon continuum shifted by $\delta k_x = \pm 2\pi/3$. Within the resolution limit ($\sigma_\omega = 0.080$), the linear gapless modes and the continuum persist for finite d .

Dynamical properties. At $\phi/\pi = 1/4$, where the $\text{K}\Gamma$ chain is equivalent to the AFH chain, the excitations are spin-1/2 spinons with the characteristic continuum in the DSF bounded by a double arc and linear dispersion at the gapless points [55,56,73,74]. As shown in Fig. 3(b), the $\text{K}\Gamma$ chain features three copies of the AFH chain spectrum due to a tripling of the unit cell by the six-sublattice transformation [41]. For coupled infinite chains—we use $\rho_{(3,\infty)}$ at $d = 0.5$ —the DSF retains these features. Within bounds set by the resolution (see the SM [64]), the DSF remains gapless with linear dispersion at $\mathbf{k} = \{\Gamma, \frac{2}{3}\mathbf{M}, \frac{4}{3}\mathbf{M}, \Gamma'\}$. The broad continuum is mostly unchanged apart from a shift of spectral weight to low energies at Γ' . Upon tuning away from $\phi/\pi = 1/4$ towards either $\Gamma \rightarrow 0$ or $K \rightarrow 0$, the lower edge of the spectrum flattens, while maintaining the same arc-like lower boundary with linear gapless modes. At $\phi/\pi = 0.1$, the upper edge of the continuum moves towards lower energies ($\omega_{\max} \approx 2$) approaching the upper cutoff known for the KSL [75,76]. At $\phi/\pi = 0.5$, on the other hand, the upper edge moves to higher energies, and a second dispersive feature develops at $1 < \omega < 1.4$.

We like to remark on the nature of the spinon excitations when $d > 0$: As worked out by Kohno *et al.* [49] in the context of the anisotropic triangular Heisenberg model, the finite interchain coupling can induce an effective interaction between spinons in two neighboring chains. In case of attractive interactions, two spinons pair to a sharp triplon mode below the spinon continuum, while for repulsive interactions the triplon mode overlaps with the continuum. Then, decay into two spinons becomes kinetically allowed, the triplon acquires

a finite lifetime and mainly causes a shift in the spectral weight within the continuum. On the basis of our numerics and limitations in the computationally achievable resolution, we cannot draw any conclusion regarding the effective interaction between spinons. However, from our ground-state numerical data we can exclude a scenario in which the condensation of triplons formed by an attractive interaction stabilizes a magnetically ordered state. Moreover, the continuum formed by the independent spinons of each individual chain remains largely unaffected by finite interchain coupling.

Discussion. We have provided numerical evidence for the existence of an extended quantum paramagnetic phase (pTLL) born out of the emergent TLL phase in the one-dimensional limit. The interchain coupling leads to frustration suppressing correlations between chains and long-range magnetic order. The quasi-1D nature of pTLL manifests itself in algebraic spin-spin correlations along the chains and exponential decay along the interchain direction. The DSF of the anisotropic $\text{K}\Gamma$ model at $d = 0.5$ closely resembles that of the $\text{K}\Gamma$ chain with its characteristic spinon continuum, indicating a dimensional reduction scenario [49]. Remarkably, pTLL extends up to the C_3 limit. The previously much studied $\text{K}\Gamma$ model is, for a wide range in ϕ/π , situated at a phase transition line providing a reason for the vastly different results in the literature. Moreover, using a non- C_3 -symmetric geometry results in significant deviations from $d = 1$ (see the SM [64]).

Additional exchanges, such as Heisenberg, off-diagonal Γ' , or further-neighbor exchanges, will act as a singular perturbation and stabilize long-range magnetic order [53]. However, we want to highlight the relation of pTLL with the lattice-nematic paramagnet (NP) found in a $\text{K}\Gamma\Gamma'$ model in an applied magnetic field along the [111] axis [31,34]. There, upon adding a negative Γ' , the NP (pTLL) phase gives way to zigzag magnetic order, while NP reappears once the applied magnetic field suppresses the magnetic order. This has important implications on possible realisations in materials: (i) pTLL exists in a wide region of mostly ferromagnetic Kitaev and antiferro-like Γ exchange and in an applied external magnetic field. When the crystal symmetry includes C_3 , applying a magnetic field along the [111] axis (or c^* axis) and tuning the tilting angle appropriately can select the NP state related to pTLL [34]. (ii) pTLL may exist in Kitaev materials with a from C_3 down to C_2 reduced lattice-rotation symmetry. Such a reduction may be intrinsic to a reduced point-group symmetry. Alternatively, applying a uniaxial strain or an external magnetic field will alter the spin-exchange via magnetoelastic coupling [38,39].

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