

Triangular J_1 - J_2 Heisenberg antiferromagnet in a magnetic field

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The behavior of the paradigmatic J_1 - J_2 triangular lattice Heisenberg antiferromagnet in a magnetic field remains unsettled despite decades of study. We map out the phase diagram using three complementary approaches, including self-consistent nonlinear spin-wave theory, density-matrix renormalization group, and variational Monte Carlo. This combined analysis resolves the competition among different field-induced magnetic orders and magnetization plateaus across the classically frustrated parameter range. In particular, there is a finite range in the parameter regime around $J_2/J_1 = \frac{1}{8}$ in which (i) upon the application of the external field, the gapless quantum spin liquid acquires a finite density of monopoles, and (ii) by further increasing the field, two plateaus are clearly obtained at $m = \frac{1}{3}$ and $m = \frac{1}{2}$. We discuss the experimental importance of the consecutive magnetization plateau transitions as a signature of an underlying quantum spin-liquid phase.

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Introduction. Triangular lattice antiferromagnets (TrAFMs) are not only widely used illustrations of geometrically frustrated magnets, but arguably the founding examples of an entire research field [1]. Famously, Wannier showed that the triangular Ising model realizes a critical liquid with an extensive classical ground state degeneracy [2] and the frustration is also manifest as an unusual steplike magnetization process of the model as a function of an applied magnetic field. Early on, it was shown that the magnetization jumps from zero to a plateau value $m = \frac{1}{3}$ and then to full saturation [3]. Adding further next-nearest-neighbor (NNN) interactions J_2 in addition to the standard nearest-neighbor (NN) J_1 one enables a new magnetization plateau at $m = \frac{1}{2}$ [4,5] from the interplay between geometric and exchange frustration. Beyond Ising models, the phase diagram is even richer for triangular Heisenberg-like systems with quantum fluctuations [6,7] and thermal fluctuations stabilizing collinear plateau phases [8–10]. In general, the study of magnetization plateaus has a long history [11–13] and is a telltale experimental signature of magnetic frustration [14,15].

The interest in the TrAFM has significantly increased in recent years because their competing interactions can stabilize sought-after quantum spin liquids (QSLs) [16–18] in a number of candidate materials [19–25]. Since Anderson’s original proposal [26], the $S = \frac{1}{2}$ Heisenberg TrAFM has been a prominent theoretical candidate for realizing a QSL ground state. Indeed, upon the addition of NNN Heisenberg

exchange of strength $0.07 \lesssim J_2/J_1 \lesssim 0.16$ a QSL is by now well established numerically [27–30]. Recent progress on the experimental side has suggested that the Yb-based delafossites are expected to be accurately modeled by this type of Heisenberg model [24,31,32] but finding unambiguous signatures of QSL behavior remains a challenge [17,33]. In this context, studying the phase diagram of TrAFM models beyond the QSL regime is important to gain theoretical insights into their stability and the degree to which basic models resemble physical materials.

In this Letter we study the phase diagram of the spin- $\frac{1}{2}$ Heisenberg TrAFM in a magnetic field described by the Hamiltonian

$$\mathcal{H} = J_1 \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \vec{S}_i \cdot \vec{S}_j - H \sum_i S_i^z, \quad (1)$$

and concentrate on $0 \leq J_2/J_1 \leq 1$. The classical limit exhibits a three-sublattice phase for $0 \leq J_2/J_1 \leq \frac{1}{8}$, a four-sublattice phase for $\frac{1}{8} \leq J_2/J_1 \leq 1$, and a fully polarized phase for $H \geq \max\{4.5J_1, 4(J_1 + J_2)\}$, yet the ground state is infinitely degenerate in the former two (see Supplemental Material [34]). Quantum fluctuations lift the degeneracy, which has been extensively studied and verified in the zero-field limit [35–37]. Furthermore, the phase diagram for small and large J_2 including a magnetic field has been studied in linear spin-wave theory (LSWT) with self-consistent nonlinear spin-wave theory (NLSWT) applied to the plateaus and Ginzburg-Landau theory on condensates [38–40].

Despite the long research history, several open questions remain: (i) the precise location of phase boundaries; (ii) the extent of the magnetization plateaus around the interesting classical frustration point $J_2/J_1 = \frac{1}{8}$; (iii) the validity of semiclassical approaches; and, most importantly, (iv) the

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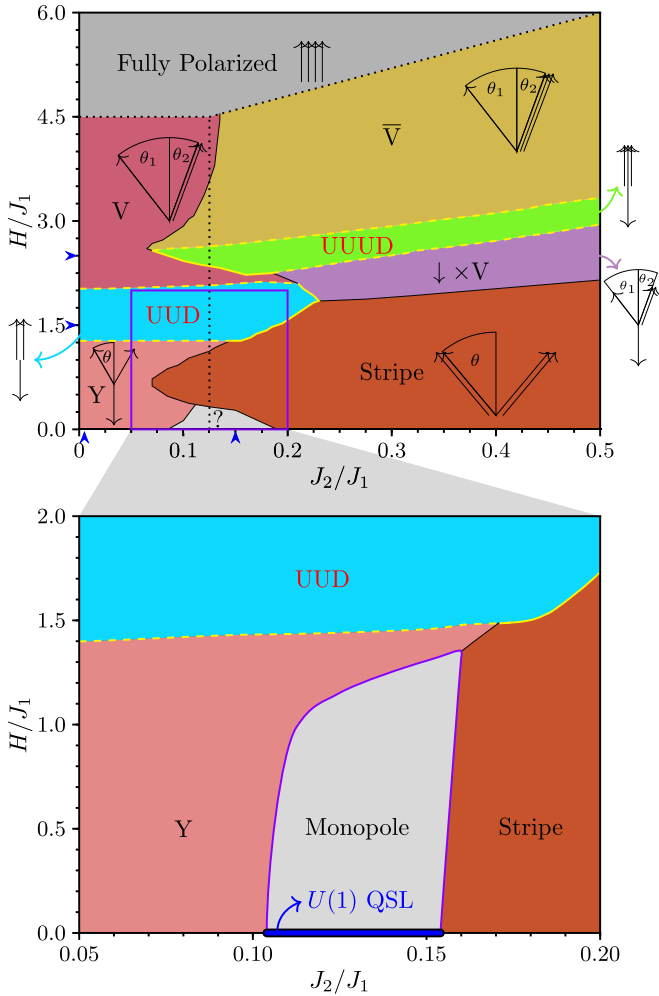


FIG. 1. Top: Phase diagram of the J_1 - J_2 - H model determined from self-consistent NLSWT on a 30×30 triangular lattice with PBC. Dotted lines indicate classical phase boundaries between three- and four-sublattice and fully polarized phases. Solid (dashed) lines indicate first- (second-) order phase transitions. The light gray area denotes the expected breakdown of semiclassical configurations as predicted from LSWT and mode condensation. The $m = \frac{1}{3}$ (UUD) and $m = \frac{1}{2}$ (UUUD) magnetization plateaus are highlighted in light blue and green, with their phase boundaries highlighted in yellow. The purple box contains a region beyond the reach of the semiclassical theory. Bottom: The low-field phase diagram of the J_1 - J_2 - H model in the vicinity of QSL obtained from VMC on an 18×18 triangular lattice.

fate of the critical QSL when switching on a magnetic field. Here, we determine the phase diagram by combining NLSWT, density-matrix renormalization group (DMRG) [41,42], and variational Monte Carlo (VMC) [43] analyses. Within NLSWT, we implement the Holstein-Primakoff (HP) transformation and extract self-consistent solutions including quantum corrections up to second order (S^{-2}) across the full range of J_2 and H under study. We place these results alongside independent DMRG and VMC calculations on representative cuts through the phase space, using these complementary approaches to cross-validate one another and thereby establish the phase diagram shown in Fig. 1.

Remarkably, we find overlapping $m = \frac{1}{3}$ and $m = \frac{1}{2}$ magnetization plateaus above the zero-field QSL regime. Thus, the experimental observation of such consecutive plateaus is a strong indication that the Hamiltonian is in a parameter regime allowing for a zero-field QSL. In addition, we show that applying a field to the critical QSL leads to a ground state with a finite density of monopoles; see Fig. 1 for a quantitative estimate of the phase diagram in vicinity of the QSL regime.

Semiclassical theory. We begin by outlining details of the well-known HP transformation to obtain quantum corrections to classical ground states. The states considered are not collinear, hence the transformation is applied in a rotated frame $\tilde{S}'$, chosen such that the z axis is aligned with the respective classical spin direction. The spin inside the Hamiltonian is obtained using a standard rotation matrix R such that $\tilde{S} = R\tilde{S}'$. The transformation itself is given as

$$S'^+ = \sqrt{2S - a^\dagger a} a, \quad S'^z = S - a^\dagger a, \quad (2)$$

which we then expand for large S .

To compute the ground state energy, we include up to quartic terms in the expansion of the full Hamiltonian, and treat quartic and cubic terms self-consistently. Since the ground state is (not always) collinear, we need to additionally consider terms linear in the operators. For classical ground states, the leading order vanishes; however, higher orders require a renormalization of angles such that any term linear in the bosonic creation and annihilation operators vanishes. For this work, we need the renormalized set of angles θ up to order S^{-1} , which is generally determined from the requirement

$$\mathcal{H}^{(1)}(\theta) + \frac{1}{S} \overline{\mathcal{H}}^{(3)}(\theta) = 0 + O(S^{-2}), \quad (3)$$

combined with preserving the classical limit $\theta = \theta_{cl} + O(S^{-1})$. The overline ($\overline{\mathcal{H}}$) indicates that terms have been contracted to scalar, linear, and quadratic order in the boson operators. Solving this equation for θ yields the proper set of renormalized angles. We use the angle determined from these equations inside the Hamiltonian and perform the expansion thereof. In doing so, we do not expand the angle in S^{-1} but rather treat it akin to a variational parameter

$$\begin{aligned} \mathcal{H}(\theta) &= \mathcal{H}_{cl}(\theta) + \frac{1}{S} \mathcal{H}^{(2)}(\theta) + \frac{1}{S^2} \overline{\mathcal{H}}^{(4)}(\theta) \\ &= N E_{cl}(\theta) + \frac{1}{2S} \sum_{\mathbf{k}} [a_{\mathbf{k}}^\dagger M_{\mathbf{k}}(\theta) a_{\mathbf{k}} - \Delta_{\mathbf{k}}], \end{aligned} \quad (4)$$

where N is the total number of lattice sites and the sum runs over all accessible points in the Brillouin zone. The ground state (GS) energy is then obtained by diagonalizing the Hamiltonian under periodic boundary conditions (PBCs) using a standard Bogoliubov transformation.

To obtain a self-consistent solution, we make use of complementary two algorithms: The *local algorithm* works at a single point in parameter space. At every step, it uses a linear combination of mean-field parameters from the previous two steps at some mixing angle and computes the ground state energy from Eq. (4) and new mean-field parameters from the eigenvalues thereof. This process is repeated until the energy has converged within bounds of 10^{-9} for ten consecutive steps. Since this algorithm is prone to runaway effects and

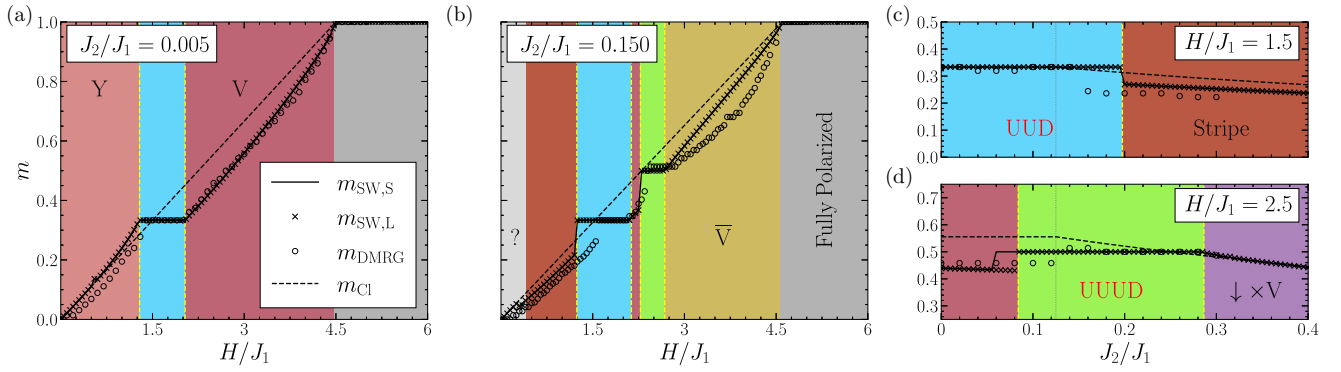


FIG. 2. Magnetization cuts marked by the blue arrowheads on the axes of Fig. 1 (top), obtained from different methods; phases are colored according to the results from self-consistent stable ($m_{\text{SW,S}}$) and local NLSWT ($m_{\text{SW,L}}$). The crosses are obtained from the local algorithm, the continuous line from the stable algorithm, and the DMRG data obtained on a 6×24 cylinder is shown using circles. Both NLSWT algorithms run on a 30×30 lattice using PBC. The dashed line shows the classical magnetization. (a), (b) Plots as a function of H/J_1 at fixed J_2/J_1 . (c), (d) Plots of magnetization as a function of J_2/J_1 at different fixed magnetic fields $H = 1.5$ and $H = 2.5$. The horizontal dashed line indicates the classical phase transition.

lattice-size-dependent instabilities, we use the *stable algorithm* as a cross-check. In this case, the local algorithm is performed at a point $J_2^{(0)}, H^{(0)}$ in parameter space, for which the ground state is well defined. The mean-field parameters of this solution are then used analogous to the local algorithm, however additionally modifying the parameters J_2 and H in small increments at every step. Clearly, the stable algorithm is preferable for computing the phase diagram (in the sense of computational cost) if the state is stable and adiabatically connected to the previous state. In contrast, the local algorithm is able to capture self-consistent ground states that may not be adiabatically connected to neighboring states in the sense of the MF parameters.

Phase diagram and magnetization plateaus. The semiclassical analysis outlined above predicts the rich phase structure shown in the top panel of Fig. 1, obtained from the local algorithm, evaluating the energy of all plausible states on a grid of steps $\Delta J_2 = 0.005$, $\Delta H = 0.1$ and choosing the state of minimal energy. At $H = 0$, LSWT predicts a breakdown of the Y state, and hence any 120° ordered state, at $J_2/J_1 \gtrsim 0.085$ while the Stripe phase has no self-consistent solution without condensates below $J_2/J_1 \lesssim 0.16$, in agreement with the current literature. We thus find a finite region in parameter space connected to the QSL regime in which none of the classical states investigated are stable, as denoted by the purple box in the top panel of Fig. 1. The low-field phase diagram near the QMC regime is instead given by the VMC approach shown in the bottom panel of Fig. 1, whose details are to be discussed in the next section. Note, contrary to previous works [39,40], we find that the stripe state is not the ground state close to the fully polarized phase for $J_2/J_1 \gtrsim \frac{1}{8}$ in self-consistent NLSWT. We attribute this tension to our method leading to a gapped spectrum for any $H \neq 4(J_1 + J_2)$, implying the condensation in the aforementioned work does not occur. We also verified that the umbrella state, defined as an in-plane 120° order with all spins canted along the direction of the magnetic field, is never the self-consistent solution in the phase diagram with lowest energy within our NLSWT.

We now obtain a complete semiclassical characterization of the magnetic phases for $H \neq 0$ and variable

next-nearest-neighbor exchange. In addition to the well-known field-induced Up-Up-Down (UUD) phase at small J_2 , we find two consecutive magnetization plateaus at distinct magnetic fields: the UUD plateau with $m = \frac{1}{3}$ for small-to-moderate NNN exchange $0 < J_2/J_1 \lesssim \frac{1}{4}$ at moderate fields [blue area in Fig. 2(a)], and the (Up-Up-Up-Down) UUUD plateau with $m = \frac{1}{2}$ for $J_2/J_1 \gtrsim 0.08$ at slightly higher fields [green area in Fig. 2(b)]. Both plateaus remain stable beyond the classical regime in H and J_2 once nonlinear corrections are included. Remarkably, as clearly shown in Fig. 2(b), there is an overlapping window around $J_2/J_1 \sim \frac{1}{8}$ in which both UUD and UUUD phases appear successively upon increasing the field, while a QSL is expected in the zero-field limit. This two-plateau structure therefore provides a useful diagnostic of the range of NNN Heisenberg couplings where a Dirac QSL is likely to occur at low fields, albeit its robustness against anisotropies remains an open question for future work.

The consecutive magnetization plateaus could be accessible experimentally not only through chemical tuning of the exchange ratio but also via application of pressure or strain. Similar tuning has been achieved on Kitaev and Heisenberg interactions on the honeycomb lattice [44,45]. In recent experiments on the TrAFM [24,46], the $m = \frac{1}{3}$ plateau has been observed while the $m = \frac{1}{2}$ plateau was absent for candidate materials NaYbSe₂ and TiYbSe₂ which have J_2/J_1 ratios for which we predict the $m = \frac{1}{2}$ plateau to exist. It points to the relevance of other non-Heisenberg interactions which can destabilize the plateaus. For example, an easy-plane anisotropy of the NNN exchange interaction energetically favors the canted stripe state compared to the UUUD plateau. Such XXZ-type anisotropies have been shown to persist beyond classical approximations in the $J_2 = 0$ sector [47,48]. Single-ion easy-axis anisotropies have also been shown to impact the extent of plateaus [49]. Furthermore, Dzyaloshinskii-Moriya or spin-scalar-chirality-type interactions may destabilize plateaus as well.

Although NLSWT offers a controlled semiclassical description of the competing ordered phases, we subject its predictions to a stricter test using unbiased DMRG. The DMRG calculations, while necessarily performed on finite

cylinders and therefore subject to finite-size constraints, fully incorporate quantum fluctuations and produce magnetization curves that remain consistent with the semiclassical phase structure across all accessible system sizes. Specifically, we perform grand-canonical DMRG (i.e., without fixing the total magnetization) on a 6×24 cylinder with fixed bond dimension $\chi = 1600$ and controlled truncation error $\sim 10^{-7}$, thus obtaining the optimal magnetization m for each field H . Calculations along several cuts of the phase diagram are shown in Fig. 2. The resulting magnetization curve is then directly compared to the magnetization obtained in NLSWT,

$$m = \frac{1}{SN_{\text{UC}}} \sum_{i=1}^{N_{\text{UC}}} \cos(\theta_i)(S - n_i), \quad (5)$$

where $n_i = \langle a_i^\dagger a_i \rangle$ and N_{UC} are respectively the boson occupation number and the number of sites per unit cell.

Figure 2(a) shows the cut in H with a fixed small $J_2/J_1 = 0.005$, where we find quantitative agreement between both algorithms of NLSWT and DMRG simulations in all magnetic phases. For larger $J_2/J_1 = 0.15$, shown in Fig. 2(b), a Dirac QSL is realized in the zero-field limit, where NLSWT is not applicable and the phase must be characterized by DMRG [23] or VMC (to be discussed in the next section). Note that a flux pumping through the YC6-0 DMRG cylinder is needed to stabilize the system into the odd flux sector and suppress a spurious gap in the low-field limit [20,50,51]. At higher fields, the same progression of phases is obtained in both methods; remarkably, both methods predict two successive magnetization plateaus (blue and green), albeit with minor deviations in the precise location of phase transition. It should be noted that these minor deviations lie close to the classical phase transition at $J_2/J_1 = \frac{1}{8}$, where we observe mean-field parameters such as n_i becoming larger, thus worsening the predictive power of NLSWT. This is visible in Figs. 2(c) and 2(d), cuts along J_2/J_1 at fixed magnetic fields $H = 1.5$ and $H = 2.5$, respectively, where the quantitative agreement between NLSWT and DMRG breaks down close to $J_2/J_1 = \frac{1}{8}$ [dotted lines in Figs. 2(c) and 2(d)]. Despite the perturbative nature of NLSWT and the finite-size effects of DMRG, the close agreement between these complementary methods lends strong support to the magnetic phases we identify. By contrast, in the nonmagnetic QSL regime in the zero-field limit (purple box in Fig. 1), NLSWT breaks down completely.

VMC analysis in the vicinity of QSL phase. To probe the frustrated regime near $J_2/J_1 = \frac{1}{8}$, we employ a VMC approach based on Gutzwiller-projected fermionic wave functions representing the relevant competing orders. For each fixed S^z sector, from 0 up to $m = \frac{1}{3}$, we construct and optimize the corresponding *ansätze* (e.g., canted-stripe, umbrella, Y, and monopole states) and compare their variational energies to assess the dominant correlations. The unprojected fermionic Hamiltonian has the general form $\mathcal{H}_{\text{aux}} = \sum_{(ij),\sigma} \chi_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.} + \sum_i \vec{M}_i \cdot \vec{S}_i$, where the parameters χ_{ij} and $\vec{M}_i$ differ for each phase (details to be provided in Ref. [52]). In particular, the monopole states (corresponding to finite densities of the gapless monopole excitations of the Dirac spin liquid [53]) have $\vec{M}_i = 0$ and are generated by threading an internal gauge

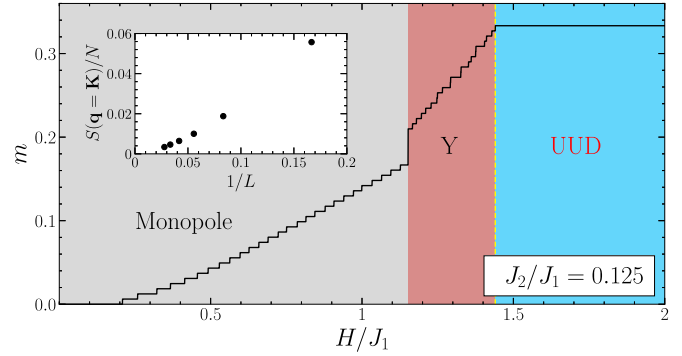


FIG. 3. Low-field magnetization curve at $J_2/J_1 = \frac{1}{8}$ obtained via VMC calculations performed on the 18×18 triangular lattice with PBC. The plateau at $m = 0$ is due to the finite-size gap of the $Q = 1$ monopole excitation. A clear first-order transition from the monopole to the Y phase is observed, and the latter continuously evolves into the UUD. Inset: Finite-size scaling of the structure factor at $\mathbf{q} = \mathbf{K} = (4\pi/3, 0)$ for the monopole states at fixed magnetization $m = 1/6$, showing lack of magnetic ordering. $N = L^2$ denotes the number of sites.

flux $2\pi Q$ uniformly through all triangles [54] and occupying the resulting $2Q$ fermionic zero modes with up spins, yielding a unique state with $S^z = Q$. The corresponding magnetization curve at $J_2/J_1 = \frac{1}{8}$ is shown in Fig. 3. The projected monopole states, despite having no tunable parameters, maintain the lowest variational energy among all competing *ansätze* up to $H/J_1 \approx 1.15$ ($m \approx \frac{1}{6}$), beyond which a sharp first-order transition occurs into the Y phase. The VMC-based estimate of the phase boundaries is provided in the bottom panel of Fig. 1. These results demonstrate that in the vicinity of the QSL, the ground state in the presence of a field is a state with a finite density of monopoles. The condensation of these monopoles is expected to yield a transverse 120° magnetic ordering [53,55,56]. To investigate this aspect, we compute the structure factor $S(\mathbf{q}) = \frac{1}{N} \sum_{ij} e^{i\mathbf{q} \cdot (\mathbf{R}_i - \mathbf{R}_j)} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$, of the monopole states at fixed magnetization $m = 1/6$ for $\mathbf{q} = \mathbf{K}$ (see the inset of Fig. 3). The presence of magnetic order would manifest in the extensive behavior of the structure factor, $S(\mathbf{K}) \propto N$. Instead, we find that $S(\mathbf{K})/N$ scales to 0 in the thermodynamic limit, indicating that the monopole phase does not have long-range order, in contrast to the expectations from field theory approaches [56]. A detailed characterization of this phase is given in a future work [52].

Discussion and conclusion. We obtained the phase diagram of the J_1 - J_2 - H triangular lattice Heisenberg antiferromagnet by integrating three complementary methods: self-consistent NLSWT (including all S^{-2} corrections), large-scale DMRG, and variational Monte Carlo. NLSWT provides global structure and identifies candidate phases; DMRG supplies an unbiased quantum benchmark along representative cuts; VMC resolves the regime where semiclassical methods fail—namely the vicinity of the classical frustration point $J_2/J_1 = \frac{1}{8}$, where the zero-field Dirac QSL emerges. Taken together, the methods yield a coherent and internally consistent phase diagram. First, nonlinear quantum fluctuations substantially enlarge both the UUD ($m = \frac{1}{3}$) and UUUD ($m = \frac{1}{2}$) plateaus in both H and J_2/J_1 . Second, these plateaus overlap in the

parameter window connected to the zero-field QSL: increasing the field produces two successive magnetization plateaux at $m = \frac{1}{3}$ and $m = \frac{1}{2}$, a distinctive experimental fingerprint of a system tuned close to the QSL regime, in particular considering the most experimentally investigated compounds, i.e., Yb-delafoffsites have J_2/J_1 at the lower end of the spin-liquid regime, if at all [24,31,32]. Third, away from phase boundaries and the QSL region, NLSWT with fully renormalized angles quantitatively reproduces the DMRG results, confirming its reliability over most of the phase diagram. Finally, VMC shows that applying a field onto a Dirac QSL leads to a finite-density monopole phase that persists up to a first-order transition into the Y state. Its detailed characterization is addressed in a future work [52].

Note added. Recently, we became aware of an independent complementary study [57], which reports a similar phase diagram. The tension close to saturation, the canted-stripe versus $\bar{V}$ state, can be attributed to geometric effects of finite-size cylinders. LSWT on an XC-8 geometry shows the canted-stripe state to be energetically favored, although this preference is not maintained in NLSWT. On large clusters, we find the $\bar{V}$ state to be energetically preferred. In addition,

we also learned of an independent study [58] investigating the monopole states, presenting results in agreement with our work.

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Data availability. Data are available upon reasonable request on Zenodo [59].

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