

Topological Phase Transitions and Their Thermodynamic Fate in Arbitrary- S Classical Pyrochlore Spin Ice

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We develop a self-contained theoretical framework that classifies the topological phases and critical phenomena of classical pyrochlore magnets with arbitrary spin S , subject to competing exchange and single-ion anisotropies. We work first in the monopole-free (ice-rule) limit. In the small- w regime, where the single-ion term favors low spin amplitudes, dualities reveal a dichotomy: Integer spins exhibit a continuous 3D XY deconfinement transition, whereas half-integer spins remain in a U(1) Coulomb liquid without any transition. In the large- w regime, where the local spin amplitudes are maximized ($|S^z| = S$), the macroscopic flux is quantized to multiples of $2S$. By mapping the defect structure to topological loop gases, we prove that the compatibility between the physical ice rule and the modular $\mathbb{Z}_{2S}$ flux conservation holds at the vertex level if and only if $S \leq 3/2$. For $S = 3/2$, this maps the system to the three-state Potts model, whose symmetry-allowed cubic invariant drives a first-order transition. For $S \geq 2$, no mapping to a discrete clock model exists. Using a decomposition of the partition function, we show that the only processes sensitive to the discrete $\mathbb{Z}_{2S}$ structure carry exponentially small statistical weight and correspond to irrelevant operators at the 3D XY fixed point, so the deconfinement transition is of the 3D XY type. Finally, incorporating thermal monopoles, we show that they act as a symmetry-breaking effective magnetic field that severs defect strings. Consequently, the continuous transitions are rounded into crossovers, whereas the first-order $S = 3/2$ transition is predicted to survive at finite temperatures, terminating at a critical end point. Classical Monte Carlo simulations for S up to $7/2$ corroborate the predicted crossover behavior at the accessible temperatures; these temperatures lie above the estimated critical end point, so the predicted survival of the $S = 3/2$ first-order transition remains to be tested directly.

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I. INTRODUCTION

The study of geometrically frustrated magnetism on the pyrochlore lattice has been a fertile ground for discovering exotic states of matter, most notably classical and quantum spin liquids [1–4]. The quintessential example is classical spin ice, realized in rare-earth oxides such as $\text{Ho}_2\text{Ti}_2\text{O}_7$ and

$\text{Dy}_2\text{Ti}_2\text{O}_7$ [5–8]. In these materials, strong crystalline electric fields acting on the large total angular momenta ($J = 8$ for Ho^{3+} , $J = 15/2$ for Dy^{3+}) isolate a low-energy doublet, allowing the magnetic moments to be treated as effective $S = 1/2$ Ising pseudospins oriented along the local $\langle 111 \rangle$ tetrahedral axes [9]. The frustrated exchange interactions force the spins into a two-in, two-out ice rule [10], mapping the low-energy physics to a fluctuating, divergence-free effective magnetic field. This emergent electromagnetism characterizes the U(1) Coulomb liquid phase, distinguished by algebraic spin correlations and pinch-point singularities [11–15].

Recent theoretical and numerical advances have pushed beyond the rigid $S = 1/2$ paradigm by exploring $S = 1$ and higher-spin systems in which the dominant easy-axis exchange competes with a single-ion anisotropy [16–19]. Throughout this paper, S_ℓ^z denotes the spin component

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TABLE I. Phase diagram of integer-spin models in the monopole-free limit ($v = 0$). The macroscopic polarization flux $\mathbf{P}$ serves as a topological invariant distinguishing the three phases. The transition out of the trivial paramagnet belongs to the 3D XY universality class for all integer S . The deconfinement transition out of the $\mathbb{Z}_{2S}$ -confined phase is 3D Ising for $S = 1$ and 3D XY for $S \geq 2$, the latter supported by the decomposition of Sec. VC and the irrelevance of the $\mathbb{Z}_{2S}$ fusion cascade. The $S = 1$ critical fugacity is $w_{c2} = 2/(3 \tanh K_c^{\text{Ising}})$, where K_c^{Ising} is the 3D Ising critical coupling on the diamond lattice [18]. For $S \geq 2$, $w_{c2} = [2/(3\tau_1)]^{1/(2S-1)}$ with $\tau_1 := I_1(K_c^{XY})/I_0(K_c^{XY})$ (see Sec. VC). At finite temperatures ($v > 0$), thermal monopoles round all these transitions into continuous crossovers (see Sec. VI). The value $w_{c1} \approx 0.344$ is the leading-order analytic estimate of Sec. IV; the measured value for $S = 1$ is 0.3609(1) [16].

Spin S	Trivial phase	w_{c1} (transition)	U(1) Coulomb phase	w_{c2} (deconfinement)	$\mathbb{Z}_{2S}$ -confined phase
1	$\mathbf{P} = \mathbf{0}$	≈ 0.344 (3D XY)	$\mathbf{P} \in \mathbb{Z}^3$	$\frac{2}{3 \tanh K_c^{\text{Ising}}} \approx 1.88$ (3D Ising)	$\mathbf{P} \in (2\mathbb{Z})^3$
≥ 2	$\mathbf{P} = \mathbf{0}$	≈ 0.344 (3D XY)	$\mathbf{P} \in \mathbb{Z}^3$	$(\frac{2}{3\tau_1})^{1/(2S-1)} \approx (1.859)^{1/(2S-1)}$ (3D XY)	$\mathbf{P} \in (2S\mathbb{Z})^3$

along the local $\langle 111 \rangle$ axis of site ℓ (the axis joining the centers of the two tetrahedra sharing that site), the transverse components of the exchange are set to zero, and the model is treated entirely classically. For the $S = 1$ case, the competition between a dominant easy-axis exchange and a single-ion anisotropy $\mu(S^z)^2$ ($\mu > 0$) that penalizes large $|S^z|$ yields a rich phase diagram [16–18]. Unlike the $S = 1/2$ model, the $S = 1$ spins can access a nonmagnetic $S^z = 0$ state. In the monopole-free (ice-rule) limit, tuning the anisotropy drives the system through three distinct macroscopic phases: a trivial paramagnet, a U(1) Coulomb phase, and a $\mathbb{Z}_2$ -confined Coulomb phase (a Coulomb liquid whose macroscopic polarization flux is restricted to even integers, so that strings carrying a single unit of flux are confined while pairs remain free), separated by continuous transitions in the 3D XY and 3D Ising universality classes. More recently, Pandey *et al.* investigated the $S = 3/2$ case, uncovering a first-order $\mathbb{Z}_3$ flux-confinement transition separating two distinct Coulomb liquids [19]. These developments connect to the broader understanding of fractionalization and magnetic fragmentation in pyrochlore systems [20–22]. The same class of models also arises in a broader range of systems, including water ice under high pressure [23] and artificial nanomagnet arrays [24].

These discoveries raise fundamental questions. How do the macroscopic topological structures and critical phenomena generalize to an arbitrary spin S ? Why does the $S = 3/2$ model exhibit a first-order transition while $S = 1$ exhibits continuous transitions, and can the first-order character be derived from a microscopic mapping rather than inferred from symmetry considerations [19]? What is the ultimate fate of the phase transitions and universality classes for $S \geq 2$? Finally, what is the thermodynamic fate of these topological phase transitions at finite temperatures, where the strict ice rules are inevitably violated by thermally excited magnetic monopoles?

In this paper, we address these questions by developing a unified theoretical framework for the spin- S pyrochlore magnet, treating the monopole-free limit first and thermal monopoles second. In the monopole-free limit, we first

show that the phase diagram contains only the phases already identified above: Uniform backgrounds of intermediate spin amplitude are excluded by the convexity of the single-ion energy, and scenarios of “partial deconfinement,” in which strings of higher topological charge would condense before the fundamental strings, are excluded by a free-energy comparison of the competing defect strings (Sec. III).

We then determine the nature of each transition. In the small- w regime, an exact rewriting of the partition function in terms of a dual phase field shows that all integer- S models undergo a 3D XY transition at a common, S -independent coupling, whereas all half-integer- S models reduce to the ordinary $S = 1/2$ spin ice and therefore have no small- w transition at all (Sec. IV). In the large- w regime, we map the defect strings onto loop gases (Sec. V). For $S = 3/2$, the loop gas coincides with the high-temperature expansion of the three-state Potts model, which explains microscopically the first-order transition observed numerically in Ref. [19] and locates it quantitatively. For $S \geq 2$, we show that no discrete clock model reproduces the loop gas; instead, the loop gas is that of the continuous 3D XY model, up to corrections whose statistical weight is exponentially small and whose corresponding operators are irrelevant at the XY fixed point, so the transition is continuous and of the 3D XY type. The resulting classification in the monopole-free limit is summarized in Tables I and II and the schematic phase diagram in Fig. 1.

Finally, by incorporating thermal monopoles into the partition function, we show that they enter the dual descriptions as a symmetry-breaking field that allows defect strings to terminate. This rounds all the continuous transitions into crossovers at any $T > 0$ and predicts that the $S = 3/2$ first-order line is the only boundary that can survive at finite temperature, terminating at a critical end point (Sec. VI). We corroborate the crossover behavior with classical Monte Carlo simulations for S up to $7/2$ (Sec. VII); the temperatures accessible to these simulations lie above the estimated critical end point, so the survival of

TABLE II. Phase diagram of half-integer-spin models in the monopole-free limit ($v = 0$). The absence of the nonmagnetic $S^z = 0$ state forbids the trivial paramagnetic phase, reducing the diagram to two phases (except for $S = 1/2$, which has only one). For $S = 1/2$, the single-ion anisotropy is a constant and the system resides in the U(1) Coulomb phase for all w . The $S = 3/2$ deconfinement transition is first order, driven by $\mathbb{Z}_3$ defect-string fusion mapped to the three-state Potts model; the quoted $w_c \approx 1.44$ is the closed-form Bethe-Peierls estimate $w_c^2 = \sqrt{2} + 2/3 \approx 2.081$, which overestimates the Monte Carlo value $w^2 \approx 2.02$ of Ref. [19] (i.e., $w_c \approx 1.42$) by $\sim 3.0\%$. For $S \geq 5/2$, the exponential suppression of the fusion cascade restores 3D XY criticality. At finite temperatures ($v > 0$), the continuous transitions become crossovers, while the $S = 3/2$ first-order transition is predicted to persist up to a critical end point (see Sec. VI).

Spin S	U(1) Coulomb phase	w_c (deconfinement)	$\mathbb{Z}_{2S}$ -confined phase
1/2	$P \in \mathbb{Z}^3$	None [always U(1) phase]	
3/2	$P \in \mathbb{Z}^3$	≈ 1.44 (first order; 3-Potts)	$P \in (3\mathbb{Z})^3$
$\geq 5/2$	$P \in \mathbb{Z}^3$	$(\frac{2}{3\pi})^{1/(2S-1)} \approx (1.859)^{1/(2S-1)}$ (3D XY)	$P \in (2S\mathbb{Z})^3$

the $S = 3/2$ first-order line itself remains an open target for future numerics. Beyond the specific context of spin ice, our analysis illustrates in a quantitative setting how a lattice model whose microscopic conservation law is real valued—and hence U(1)—can imitate a discrete gauge structure at low energies, and when this imitation must fail.

For clarity, we state explicitly what each of the recent works on which this paper builds established, and what is new here. Reference [16] mapped out the $S = 1$ phase diagram by worm-algorithm simulations performed directly in the ice-rule manifold, locating the two transitions [$w_{c1} = 0.3609(1)$ and $w_{c2} = 1.8904(1)$] and identifying their universality classes through a mapping to an XY partition function combined with finite-size scaling; Ref. [18] (by the present authors) derived the same $S = 1$ results analytically via dual XY and loop-gas representations and quantified the effect of thermal monopoles as an explicit symmetry-breaking field in those dual representations; Ref. [17] studied a related two-dimensional model in a strong field; and Ref. [19] discovered the first-order $\mathbb{Z}_3$ transition for $S = 3/2$ by the same worm-algorithm approach and rationalized it by a symmetry-based argument.

The present paper contains all $S \geq 1$ within a single framework, and we wish to be equally explicit about where its novelty does and does not lie. The transformations themselves are not new: The dualities, loop-gas expansions, and mean-field evaluations used below are standard tools of lattice statistical mechanics, and we credit their sources where they appear. What is new is the structure these tools reveal once they are set up for arbitrary S .

In the small- w regime, the arbitrary- S dual link weights expose a parity dichotomy invisible at $S = 1$: The leading XY coupling, and hence the location of the transition, is the same for every integer S , whereas for half-integer S the dual weights are antiperiodic—the dual hallmark of half-integer spin—and the model reduces to the ordinary spin ice, with no transition at all. In the large- w regime, the organizing result is the ice-rule compatibility criterion of Sec. VA, an elementary geometric statement that, to our knowledge, has

no counterpart in the literature: A discrete $\mathbb{Z}_{2S}$ description can be consistent with the physical ice rule at the vertex level only for $S \leq 3/2$, which explains with a single argument why the Ising and Potts mappings succeed at $S = 1$ and $S = 3/2$ and why every such mapping must fail for $S \geq 2$.

On the $S = 3/2$ side of this divide, the criterion upgrades the symmetry-based rationale of Ref. [19] to a microscopic derivation—the loop gas is identified with the high-temperature expansion of the three-state Potts model, so that the first-order character follows *a priori* from the symmetry-allowed cubic invariant rather than being inferred from the numerics—and a Bethe-Peierls evaluation then locates the transition in closed form, within 3% of the numerical value. On the $S \geq 2$ side, for which no previous results exist, numerical or analytic, we show that no discrete clock model reproduces the loop gas, bound the residual discrete corrections through a decomposition of the partition function, and thereby obtain both the 3D XY universality class and the closed-form critical line $w_c(S)$ for the entire family.

The completeness argument of Sec. III and the $S \geq 2$ Monte Carlo simulations of Sec. VII are likewise reported here for the first time. The same holds for the finite-temperature analysis of Sec. VI in the generality given there: Whereas thermal monopoles in spin ice are traditionally treated through the continuum electrostatic analogy [8,14,29], we represent the monopole gas exactly in the dual variables, where a charge- Q monopole is the local operator $e^{iQ\theta}$ and the gas therefore acts as an explicit U(1) symmetry-breaking field—a correspondence introduced for $S = 1$ in Ref. [18] and established here for every S , culminating in the zero-field, self-generated critical end point for $S = 3/2$, to our knowledge the first such prediction for a frustrated magnet (the known critical end point of dipolar spin ice, the field-driven monopole liquid-gas transition [8], requires a finite [111] magnetic field).

This paper is organized as follows. In Sec. II we define the model and derive the exact partition function.

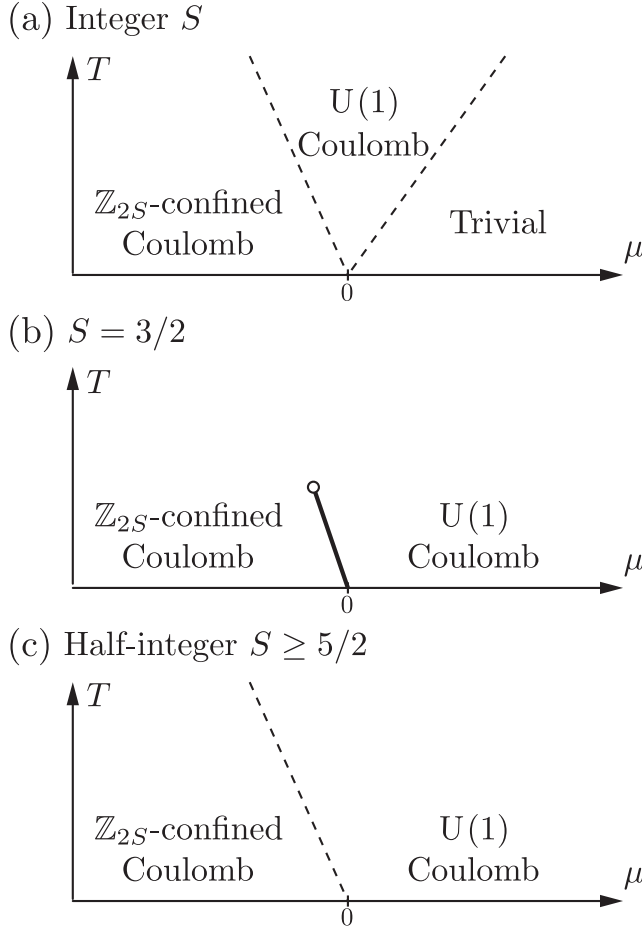


FIG. 1. Schematic phase diagram in the (μ, T) plane for (a) integer $S \geq 1$, (b) $S = 3/2$, and (c) half-integer $S \geq 5/2$; the regimes are labeled in each panel, and μ and T are quoted in units of J . Dashed lines denote crossover ridges (no thermodynamic singularity at $T > 0$); the solid line in (b) denotes the first-order coexistence line, terminating at a critical end point (open circle). The ridges and the coexistence line emanate from the origin along the rays $\mu = -T \ln w_c$ fixed by the monopole-free critical fugacities w_c of Tables I and II; on each ray μ/T is constant, and the sharp transitions are realized only in the monopole-free limit $T/J \rightarrow 0$ taken at fixed μ/T (Sec. II C). For integer S (a), the U(1) Coulomb regime is the wedge of finite opening angle bounded by the rays through w_{c1} and w_{c2} . An equivalent representation in the $(w, T/J)$ plane, in which the monopole-free transitions appear as separate points on the $T/J \rightarrow 0$ axis, is given in Sec. I of Supplemental Material [25].

Section III establishes the macroscopic flux quantization and the completeness of the phase diagram. The small- w duality mapping and the integer vs half-integer dichotomy are presented in Sec. IV, while the large- w loop-gas mappings and the classification of deconfinement transitions are developed in Sec. V. The finite-temperature effects of thermal monopoles are analyzed in Sec. VI. Section VII presents the finite-temperature Monte Carlo simulations, Sec. VIII presents an experimental outlook, and Sec. IX concludes with future directions.

II. MODEL FORMULATION AND EXACT PARTITION FUNCTION

Before embarking on the generalized theory for arbitrary spin S , we rigorously define the microscopic Hamiltonian and introduce the exact representation of the partition function that forms the foundation of all subsequent duality mappings.

A. Lattice geometry and effective Hamiltonian

The pyrochlore lattice is a network of corner-sharing tetrahedra whose sites lie at the midpoints of the links $\ell = \langle \mathbf{r}_A, \mathbf{r}_B \rangle$ of an underlying bipartite diamond lattice [7,30]. The diamond lattice comprises N vertices (equivalently, N tetrahedra of the pyrochlore lattice) and $2N$ links. We place on each site a discrete spin variable $S_\ell^z \in \{-S, -S+1, \dots, S\}$ with arbitrary positive integer or half-integer magnitude S . The local quantization axis on every link is oriented from the A -sublattice vertex $\mathbf{r}_A$ toward the B -sublattice vertex $\mathbf{r}_B$.

We study the generalized Blume-Capel Hamiltonian on this lattice [31,32], which couples an antiferromagnetic nearest-neighbor exchange $J > 0$ with a single-ion anisotropy μ :

$$H = \frac{J}{2} \sum_{\mathbf{r}} \left(\sum_{\ell \in \mathbf{r}} S_\ell^z \right)^2 + \mu \sum_{\ell} (S_\ell^z)^2, \quad (1)$$

where the outer sum runs over every diamond-lattice vertex $\mathbf{r}$ and $\ell \in \mathbf{r}$ labels its four incident links (coordination number $z = 4$). Since both terms are quadratic in S_ℓ^z , the Hamiltonian is invariant under a simultaneous sign flip $S_\ell^z \rightarrow -S_\ell^z$ on *all* links (global time-reversal symmetry). Moreover, because the exchange energy at each vertex is the squared divergence $(\sum_{\ell \in \mathbf{r}} S_\ell^z)^2 = (-\sum_{\ell \in \mathbf{r}} S_\ell^z)^2$, its value is independent of the sublattice sign convention adopted for the link orientations. Accounting for the sublattice orientation of each link, the discrete lattice divergence is defined as $\nabla \cdot \mathbf{S}_{\mathbf{r}_A} := +\sum_{\ell \in \mathbf{r}_A} S_\ell^z$ and $\nabla \cdot \mathbf{S}_{\mathbf{r}_B} := -\sum_{\ell \in \mathbf{r}_B} S_\ell^z$ (the sign flip on the B sublattice arises because the local quantization axis on each link is oriented from A to B), which can be interpreted as a magnetic monopole charge [33].

B. Exact partition function

At temperature T the canonical partition function is

$$Z := \sum_{\{S_\ell^z\}} e^{-H/T}. \quad (2)$$

We parametrize the Boltzmann weights by two dimensionless fugacities: $w := e^{-\mu/T}$, governing the single-ion cost, and $v := e^{-J/(2T)}$, governing the monopole cost. Physically, $\mu > 0$ ($w < 1$) penalizes large spin amplitudes (easy-plane tendency), whereas $\mu < 0$ ($w > 1$) favors the maximal amplitude $|S^z| = S$ (easy-axis tendency). Introducing an independent monopole charge variable $Q_r \in \mathbb{Z}$ at each

vertex and enforcing $Q_r = \nabla \cdot \mathbf{S}_r$ via a Kronecker delta, we rewrite the partition function as

$$Z = \sum_{\{Q_r\}} \sum_{\{S_\ell^z\}} \left(\prod_r \delta_{\nabla \cdot \mathbf{S}_r, Q_r} \right) v \sum_r Q_r^2 w \sum_\ell (S_\ell^z)^2, \quad (3)$$

which cleanly separates the topological weight v^{Q^2} from the local anisotropy weight $w^{(S^z)^2}$ and holds for arbitrary S and T . This representation is the starting point for all analytical results derived below.

C. Monopole-free limit and macroscopic polarization flux

When $T \ll J$ the monopole fugacity v is exponentially small, so configurations with any $Q_r \neq 0$ carry a prohibitive Boltzmann penalty. Retaining only the $Q_r = 0$ sector in Eq. (3) imposes the ice rule $\nabla \cdot \mathbf{S}_r = 0$ at every vertex. This monopole-free limit ($v = 0$) is the setting of a large fraction of this paper: Sections III–V work exclusively at $v = 0$, and the effects of $v > 0$ are analyzed in Sec. VI and probed numerically in Sec. VII. We stress that $v \rightarrow 0$ at fixed w is a joint limit on both couplings rather than a zero-temperature limit at fixed couplings: Since $w = e^{-\mu/T}$, holding w fixed as $T/J \rightarrow 0$ means holding $\mu/T = -\ln w$ fixed, so that $|\mu|/J$ vanishes together with T/J . The variable w therefore describes the physically natural hierarchy $|\mu| \ll J$ with T of order $|\mu|$, in which the residual thermal fluctuations within the ice-rule manifold are controlled by w rather than by T itself. Equivalently, for a material with fixed μ and J , cooling sweeps $w = e^{-\mu/T}$ monotonically away from unity, so that the regimes organized by w are traversed on cooling to T of order $|\mu|$ —still far below J , where v is exponentially small. This is the limit in which the phase diagrams of Refs. [16,19] were obtained. We emphasize that the sharp transitions analyzed in Secs. III–V exist strictly on the $v = 0$ manifold: At any $T > 0$ the monopole fugacity is nonzero, and, as shown in Sec. VI, the continuous transitions are then rounded into crossovers, with the sole exception of the first-order line at $S = 3/2$.

The ice-rule manifold further decomposes into topologically distinct sectors labeled by a macroscopic polarization flux $\mathbf{P}$. Under periodic boundary conditions the component along a cubic axis z reads

$$P_z = \sum_{\ell \in C_k} \text{sgn}(z_B - z_A) S_\ell^z, \quad (4)$$

where C_k denotes the set of links intersected by any plane of constant z cutting through the lattice. The sign factor projects each local spin onto the global z direction. Because the divergence-free condition forces all flux entering a slab to exit, P_z is independent of the choice of C_k and therefore constitutes a conserved topological quantum number [20,34].

D. Review of the foundational cases ($S = 1/2$ and $S = 1$)

For the foundational $S = 1/2$ case, individual spins can only take values $\pm 1/2$. The single-ion anisotropy term

evaluates to a constant: $\mu(S_\ell^z)^2 = \mu/4$. Because this uniformly shifts the global energy, the parameter w is rendered physically irrelevant. The thermodynamics is dictated solely by the topological ice rule. The macroscopic flux can freely take any integer value, $\mathbf{P} \in \mathbb{Z}^3$ (since any macroscopic plane intersects an even number of links, and summing an even number of half-integer spins yields an integer). The macroscopic state is the canonical U(1) Coulomb liquid phase [11,14,35].

The $S = 1$ limit introduces the nonmagnetic state $S_\ell^z = 0$. For $w \ll 1$ ($\mu > 0$), the nonmagnetic state is energetically favored, collapsing the system into a trivial paramagnet with $\mathbf{P} = \mathbf{0}$. As w increases, defect strings of $S_\ell^z = \pm 1$ condense through a 3D XY continuous phase transition, yielding a U(1) Coulomb phase.

For $w \gg 1$ ($\mu < 0$), the energetic penalty forces the spins to maximize their amplitude, settling into $S_\ell^z = \pm 1$ on all links. Because any macroscopic plane on the bipartite diamond lattice is intersected by an even number of links, summing an even number of ± 1 states strictly quantizes the macroscopic flux to even integers, $\mathbf{P} \in (2\mathbb{Z})^3$, stabilizing a $\mathbb{Z}_2$ -confined Coulomb phase. In the monopole-free limit, the ice rule forbids isolated defect links, so the elementary excitations are *closed loops* of $S_\ell^z = 0$ links. Because $0 = -0$, these loops lack internal orientation. The resulting undirected loop gas maps onto the high-temperature expansion of the 3D Ising model, placing the deconfinement transition in the 3D Ising universality class [18], in agreement with the independent symmetry-based argument and the finite-size-scaling analysis of Ref. [16]; the loop-gas estimate $w_{c2} \approx 1.884$ [18] agrees with the numerical transition point $w_{c2} = 1.8904(1)$ of Ref. [16] to 0.3%.

III. MACROSCOPIC FLUX QUANTIZATION AND THE COMPLETENESS OF THE PHASE DIAGRAM

When generalizing to arbitrary $S \geq 3/2$, the enlarged local state space raises the question of whether more complex phase structures—such as intermediate uniform backgrounds or partial deconfinement cascades—can arise. Throughout this section, we work in the monopole-free limit $v = 0$. We first characterize the macroscopic topology in both limiting regimes of w , and then argue that intermediate phases are excluded.

A. Macroscopic flux quantization in the large- w limit

In the large- w limit, the vacuum resides exclusively at $S_\ell^z = S\sigma_\ell$ with polarities $\sigma_\ell \in \{-1, 1\}$. To characterize the macroscopic topology, we compute the global polarization flux P_z across a macroscopic cross-sectional plane C_k :

$$P_z = S \sum_{\ell \in C_k} \text{sgn}(z_B - z_A) \sigma_\ell = S \sum_{\ell \in C_k} \tilde{\sigma}_\ell, \quad (5)$$

where $\tilde{\sigma}_\ell := \text{sgn}(z_B - z_A) \sigma_\ell \in \{-1, 1\}$.

A macroscopic plane completely traverses the bipartite diamond lattice. The total number of links $N_\perp$ intersecting this plane is strictly an even integer (e.g., $N_\perp = 4L^2$ for a plane orthogonal to a cubic axis in a periodic lattice of L^3 unit cells). Let N_+ be the number of links crossing the plane with positive projected polarity ($\tilde{\sigma}_\ell = +1$), and N_- be the number with negative projected polarity ($\tilde{\sigma}_\ell = -1$). We have the geometric identity $N_+ + N_- = N_\perp$. The algebraic sum of the projected polarities evaluates to

$$\begin{aligned} \sum_{\ell \in C_k} \tilde{\sigma}_\ell &= N_+(1) + N_-(-1) \\ &= (N_\perp - N_-) - N_- = N_\perp - 2N_-. \end{aligned} \quad (6)$$

Because $N_\perp$ is an even integer, the quantity $N_\perp - 2N_-$ is manifestly an even integer, denoted as $2k$ ($k \in \mathbb{Z}$). Substituting this topological constraint back into the macroscopic flux equation yields:

$$P_z = S(2k) = 2Sk, \quad \text{and hence} \quad \mathbf{P} \in (2S\mathbb{Z})^3. \quad (7)$$

This elementary parity argument shows that the macroscopic flux in the large- w limit is quantized to multiples of $2S$, defining a $\mathbb{Z}_{2S}$ -confined Coulomb phase for any S . The same fact was noted for $S = 1$ in Refs. [16,18] and for $S = 3/2$ in Ref. [19]; we have recorded here its form for general S .

B. Macroscopic flux quantization in the small- w limit

In the opposite limit $w \ll 1$ ($\mu > 0$), the single-ion anisotropy favors the smallest accessible spin amplitude on every link. The nature of the resulting ground-state manifold depends qualitatively on whether S is an integer or a half-integer.

For integer S , the unique minimum of the single-ion energy μm^2 is $m = 0$. In this regime every link is occupied by the nonmagnetic state $S_\ell^z = 0$, giving $P_z = 0$ identically. Thermal excitations with $|m| \geq 1$ are dilute (fugacity $w \ll 1$) and form small, closed loops under the ice rule, so the macroscopic flux remains locked at $\mathbf{P} = \mathbf{0}$. The system is a trivial paramagnet, with a unique ground state and local (closed-loop) excitations.

For half-integer S , the minimum amplitude is $|m| = 1/2$, and the ground-state manifold consists of all ice-rule-satisfying configurations of $S_\ell^z = \pm 1/2$. This is precisely the $S = 1/2$ spin ice, irrespective of the original value of S . Substituting $S \rightarrow 1/2$ into the large- w result $\mathbf{P} \in (2S\mathbb{Z})^3$ immediately yields $\mathbf{P} \in \mathbb{Z}^3$. The small- w phase of any half-integer spin is therefore a fully deconfined U(1) Coulomb liquid, topologically equivalent to the canonical $S = 1/2$ spin ice [11,14,35].

To summarize, the two limiting regimes exhibit the following macroscopic flux sectors: For integer S , the accessible sectors change from $\mathbf{P} = \mathbf{0}$ (small w) to $\mathbf{P} \in (2S\mathbb{Z})^3$ (large w); for half-integer S , they change from $\mathbf{P} \in \mathbb{Z}^3$ (small w) to $\mathbf{P} \in (2S\mathbb{Z})^3$ (large w). In both cases, the

set of thermodynamically accessible flux sectors differs between the two limits, guaranteeing the existence of at least one phase boundary as w is varied: For integer S , the nonzero sectors in $(2S\mathbb{Z})^3$ must be activated (deconfinement), while for half-integer S , the sectors in $\mathbb{Z}^3 \setminus (2S\mathbb{Z})^3$ must be suppressed (confinement). The remaining question is whether intermediate phases can intervene between these two extremes.

C. Prohibition of intermediate background phases

Let us evaluate whether a macroscopic uniform background comprised predominantly of intermediate spin amplitudes ($|S_\ell^z| = m$, where $0 < m < S$) can emerge as a thermodynamically stable phase.

In the strict monopole-free limit ($v \rightarrow 0$), the thermodynamic competition between different uniform backgrounds is dictated by the local single-ion anisotropy energy function, $\mathcal{E}(m) \propto \mu m^2$. For the small- w regime ($\mu > 0$), this is a strictly convex parabola, minimizing uniquely at the smallest possible amplitude (0 for integer S , $\pm 1/2$ for half-integer S). For the large- w regime ($\mu < 0$), the concave nature of $\mathcal{E}(m)$ places the minimum at the boundaries $m = \pm S$.

Because any intermediate spin state ($0 < m < S$) carries an extensive energy penalty compared to either the minimal- or maximal-amplitude states, both intermediate uniform and mixed backgrounds are thermodynamically forbidden. The system must transit directly between the minimal- and maximal-amplitude backgrounds.

D. Hierarchy of string free energies and the absence of partial deconfinement

Even after excluding intermediate backgrounds, one might envision a cascade of partial deconfinement transitions within the large- w regime, in which defect strings of successively higher topological charge ϕ condense at different fugacities. Here, a charge- ϕ defect string denotes a connected string of links on which S_ℓ^z deviates from its vacuum value by ϕ units, $S_\ell^z = \pm(S - \phi)$ with $1 \leq \phi \leq 2S - 1$; the equivalent flux formulation of this charge is given in Sec. VA. We now show that this scenario is also excluded.

In the $\mathbb{Z}_{2S}$ -confined phase ($\mu < 0$), the deconfinement transition out of the vacuum ($S_\ell^z = \pm S$) is driven by the thermal proliferation of topological defect strings. A defect string carrying a relative integer topological charge ϕ incurs a string tension ΔE_ϕ :

$$\begin{aligned} \Delta E_\phi &= -|\mu|(S - \phi)^2 - (-|\mu|S^2) \\ &= |\mu|(2S\phi - \phi^2), \quad (1 \leq \phi \leq 2S - 1). \end{aligned} \quad (8)$$

This tension forms an inverted parabola over $\phi \in [1, 2S - 1]$. The absolute minimum tension is strictly achieved at the boundaries: the fundamental unit charge ($\phi = 1$) and its dual ($\phi = 2S - 1$).

$$\Delta E_1 = \Delta E_{2S-1} = |\mu|(2S-1). \quad (9)$$

For $S \geq 2$, any intermediate-charge defect ($1 < \phi < 2S-1$) incurs a strictly larger string tension ($\Delta E_\phi > \Delta E_1$). (For $S = 3/2$, the only available charges are the fundamental string $\phi = 1$ and its dual $\phi = 2$, which share the identical minimum tension and thus cocondense; no intermediate defect exists.)

The tension comparison above is purely energetic, and the quantity that actually controls which strings proliferate is the free energy per unit length, which also contains the configurational entropy of the string. We therefore formulate the argument in terms of free energies. A charge- ϕ string of length $|C|$ contributes a statistical weight $[e^{s_\phi w^{-\phi(2S-\phi)}}]^{|C|}$, where e^{s_ϕ} collects the entropic factors per unit length: the number of lattice embeddings, governed by the connective constant $\mu_{\text{SAW}} \approx 2.88$ of self-avoiding walks on the diamond lattice, and local vertex-weight and internal-degeneracy factors, which are bounded above and below by S -independent constants of order unity. Within Pauling's independent-vertex approximation, each such factor is a ratio of ice-rule state counts at a four-coordinated diamond-lattice vertex times a link degeneracy of at most 2, and is therefore bounded independently of both S and ϕ (Sec. VA 2 carries out the explicit evaluation for the fundamental strings).

Crucially, all string species live on the same lattice, so the embedding entropy is common to every ϕ , and the species-dependent part of s_ϕ is bounded. A charge- ϕ string can proliferate—its free energy per unit length can turn non-positive—only when $\phi(2S-\phi) \ln w \leq s_\phi$. Because the tension exponent $\phi(2S-\phi)$ is strictly minimized at the boundaries $\phi = 1$ and $\phi = 2S-1$, while s_ϕ varies only within bounded $\mathcal{O}(1)$ limits, the proliferation threshold is reached first—i.e., at the largest value of w as w is lowered from deep inside the confined phase—by the fundamental strings. For an intermediate-charge string to condense first, its entropy per unit length would have to exceed that of the fundamental string by an amount that grows with the tension gap $[\phi(2S-\phi) - (2S-1)] \ln w > 0$, which the bounded local factors cannot supply.

We emphasize the logical status of this argument: The tension hierarchy is exact, while the entropic bounds invoke the same independent-vertex (Pauling) treatment that is used—and validated at the few-percent level against the Monte Carlo data of Refs. [16,19]—throughout Sec. V. Within this controlled treatment, partial deconfinement is excluded; the simulations of Sec. VII, which show no intermediate *cooperative* anomaly between the two cross-over scales, corroborate this conclusion (the broad secondary shoulder present for $S \geq 2$ is a size-independent single-ion Schottky feature, as established in Sec. VII). We also note that the entropic process by which a charge-2 string splits into two charge-1 strings works in favor of this

conclusion, since it converts higher-charge strings into fundamental strings.

Once the fundamental strings proliferate as winding strings around the torus, each such string shifts the macroscopic flux across a cross-sectional plane by ± 1 , so $\mathbf{P} \in \mathbb{Z}^3$ —full deconfinement into the U(1) Coulomb liquid in a single step. More generally, condensation of charge- n defect strings would change the accessible flux sectors from $(2S\mathbb{Z})^3$ to $[\gcd(n, 2S)\mathbb{Z}]^3$, since each winding string shifts the flux by $\pm n$. For $n = 1$, $\gcd(1, 2S) = 1$ recovers $\mathbb{Z}^3$. Since the fundamental strings reach their proliferation threshold first and already achieve complete deconfinement, intermediate fractionalized phases with partial flux quantization [e.g., $\mathbf{P} \in (S\mathbb{Z})^3$, which would require $n \geq 2$ strings to condense before $n = 1$] do not occur. Combining this result with the macroscopic flux quantization in both limits (Secs. III A and III B) and the prohibition of intermediate backgrounds (Sec. III C), we conclude that the global phase diagram is limited to exactly three phases for integer S [trivial paramagnet, U(1) Coulomb liquid, $\mathbb{Z}_{2S}$ -confined phase] and two phases for half-integer S [U(1) Coulomb liquid, $\mathbb{Z}_{2S}$ -confined phase].

IV. SMALL- w REGIME: EXACT DUALITY MAPPING AND THE SPIN PARITY DICHOTOMY

When $w \ll 1$ ($\mu > 0$), large spin amplitudes are energetically penalized and the thermodynamics depends qualitatively on the parity of $2S$. We expose this integer vs half-integer dichotomy through an exact duality transformation of the monopole-free partition function [36,37]. We continue to work at $v = 0$ throughout this section. The transformation below is the standard duality between integer-valued, divergence-free link currents and a compact phase field, familiar from the analyses of the XY model by José *et al.* [38] and by Dasgupta and Halperin [39] (see also the textbook treatment in Ref. [40]), here run in reverse: We start from the physical currents S_ℓ^z and reconstruct the phase field. The same mapping onto an XY model was used for $S = 1$ in Refs. [16,18] and for $S = 3/2$ in Ref. [19]; the derivation below generalizes this mapping to arbitrary S while keeping track of the exact link weights.

A. Exact dual representation

From Eq. (3), taking the exact limit $v \rightarrow 0$, the partition function is restricted to the minimally frustrated manifold where $Q_r = 0$ identically:

$$Z_{v=0} = \sum_{\{S_\ell^z\}} \left(\prod_r \delta_{Q_r,0} \right) \prod_\ell w^{(S_\ell^z)^2}. \quad (10)$$

Each Kronecker delta is resolved by a Lagrange-multiplier phase $\theta_r \in [0, 2\pi)$:

$$\delta_{Q_r,0} = \int_0^{2\pi} \frac{d\theta_r}{2\pi} e^{-i\theta_r Q_r}. \quad (11)$$

Substituting into $Z_{v=0}$ and exchanging the order of summation and integration gives

$$Z_{v=0} = \sum_{\{S_\ell^z\}} \int \mathcal{D}\theta \exp \left(-i \sum_r \theta_r Q_r \right) w^{\sum_\ell (S_\ell^z)^2}, \quad (12)$$

with $\mathcal{D}\theta := \prod_r [(d\theta_r)/(2\pi)]$.

A discrete summation by parts converts the vertex sum in the exponent into a sum over oriented links $\ell = \langle \mathbf{r}_A, \mathbf{r}_B \rangle$:

$$\begin{aligned} \sum_r \theta_r Q_r &= \sum_{\mathbf{r}_A} \theta_{\mathbf{r}_A} \left(\sum_{\ell \in \mathbf{r}_A} S_\ell^z \right) - \sum_{\mathbf{r}_B} \theta_{\mathbf{r}_B} \left(\sum_{\ell \in \mathbf{r}_B} S_\ell^z \right) \\ &= - \sum_{\ell = \langle \mathbf{r}_A, \mathbf{r}_B \rangle} (\theta_{\mathbf{r}_B} - \theta_{\mathbf{r}_A}) S_\ell^z \\ &= - \sum_\ell (\nabla \theta)_\ell S_\ell^z, \end{aligned} \quad (13)$$

where we have defined the phase difference along the link as $\nabla \theta_\ell := \theta_{\mathbf{r}_B} - \theta_{\mathbf{r}_A}$.

This transformation decouples the global constraint, allowing the summation over $S_\ell^z \in \{-S, -S+1, \dots, S\}$ to factorize into a product of independent local sums:

$$Z_{v=0} = \int \mathcal{D}\theta \prod_\ell W_S(\nabla \theta_\ell), \quad (14)$$

where we define the exact local link weight function:

$$W_S(\nabla \theta_\ell) := \sum_{m=-S}^S w^{m^2} e^{im\nabla \theta_\ell}. \quad (15)$$

The macroscopic statistical mechanics of this exact dual continuous representation is thus governed by the effective action $S_{\text{eff}}[\theta] := - \sum_\ell \ln W_S(\nabla \theta_\ell)$.

B. Integer spins: Protection of 3D XY universality

For integer spins ($S \in \mathbb{Z}$), the absolute minimum of the energy uniquely defines the trivial nonmagnetic vacuum state $m = 0$, which carries a weight of $w^0 = 1$. The elementary thermal excitations are the fundamental defects with $m = \pm 1$, carrying a suppressed weight $w \ll 1$. Higher-spin states, such as $m = \pm 2$, carry penalized weights $\mathcal{O}(w^4)$.

For integer $S \geq 2$, the exact link weight $W_S(\nabla \theta_\ell)$ expands as

$$W_S(\nabla \theta_\ell) = 1 + 2w \cos(\nabla \theta_\ell) + 2w^4 \cos(2\nabla \theta_\ell) + \dots \quad (16)$$

Expanding $\ln W_S = \ln(1+x)$ with $x = W_S - 1$, we obtain the effective action:

$$\begin{aligned} S_{\text{eff}}[\theta] &= \sum_\ell \left[-(2w + 2w^3) \cos(\nabla \theta_\ell) + w^2 \cos(2\nabla \theta_\ell) \right. \\ &\quad \left. - \frac{2}{3} w^3 \cos(3\nabla \theta_\ell) + \frac{1}{2} w^4 \cos(4\nabla \theta_\ell) \right] \\ &\quad + \mathcal{O}(w^5). \end{aligned} \quad (17)$$

The dominant term, $-(2w + 2w^3) \sum_\ell \cos(\nabla \theta_\ell)$, is independent of S (it holds for all integer $S \geq 1$; see below) and maps the small- w regime to the classical 3D XY model [38] with an effective coupling $K_{\text{eff}} = 2w + 2w^3 + \mathcal{O}(w^5)$. The critical point w_{c1} is determined by $K_{\text{eff}}(w_{c1}) = K_c^{XY}$, where K_c^{XY} is the 3D XY critical coupling on the diamond lattice. Our Monte Carlo simulations of the classical XY model on the diamond lattice (the ferromagnetic and antiferromagnetic models share the same T_c on this bipartite lattice) yield $T_c^{XY} = 1.30036(1)$ [41], corresponding to $K_c^{XY} = 1/T_c^{XY} \approx 0.769$. Solving $2w + 2w^3 = K_c^{XY}$ to $\mathcal{O}(w^3)$ gives $w_{c1} \approx 0.344$, in good agreement with the numerical result $w_{c1} = 0.3609(1)$ obtained for $S = 1$ by Pandey and Damle [16].

All non-XY harmonics $\cos(p\nabla \theta_\ell)$ ($p \geq 2$) are strongly irrelevant operators at the 3D XY fixed point [38,42], so the small- w regime belongs to the 3D XY universality class for all integer S . Two remarks clarify the logic here. First, the 3D XY universality is ultimately a consequence of the exact U(1) invariance of the dual action, which encodes the real-valued divergence-free constraint; the harmonic expansion serves to identify the two phases that the transition connects (an XY paramagnet, corresponding to the trivial phase, and an XY “ferromagnet,” corresponding to the Coulomb liquid) and to locate the transition quantitatively. Second, by 3D XY universality we refer to the critical fixed point governing the transition at w_{c1} . The ordered phase of the dual XY model is not merely an auxiliary construct: Its spin stiffness maps onto the stiffness of the emergent gauge field of the Coulomb liquid, so the dual description remains physically informative on both sides of w_{c1} , although the truncation to the leading harmonic is quantitatively controlled only for small w .

The leading XY coupling $-(2w + 2w^3) \cos(\nabla \theta_\ell)$ is completely independent of S for all integer $S \geq 1$; only the irrelevant higher harmonics ($p \geq 2$) are sensitive to the available spin states. The critical point w_{c1} is therefore universal across all integer spins. For $S = 1$, the absence of $m = \pm 2$ states renders $W_1(\nabla \theta_\ell) = 1 + 2w \cos(\nabla \theta_\ell)$ exact, so the higher-harmonic coefficients differ from Eq. (17) at subleading orders [e.g., $\cos(2\nabla \theta_\ell)$ acquires an additional $+2w^4$ correction]. These differences are confined to the irrelevant sector and do not affect the universal XY critical behavior.

C. Half-integer spins: Absence of phase transitions

The physical conclusion of this subsection can be stated simply: As $w \rightarrow 0$, a half-integer- S model reduces to the

ordinary $S = 1/2$ spin ice, because the minimal doublet $S^z = \pm 1/2$ is the only surviving degree of freedom. The small- w phase is therefore the U(1) Coulomb liquid, and no thermodynamic phase transition can occur at small w . The purpose of the analysis below is to make this statement quantitative—in particular, to show that the leading corrections in w do not generate any relevant (confining) perturbation but merely renormalize the stiffness of the Coulomb liquid.

For half-integer spins ($S = 1/2, 3/2, 5/2, \dots$), the non-magnetic integer state $m = 0$ is strictly forbidden. The lowest-energy states available to each link are the physical doublets $m = \pm 1/2$, both carrying an identical Boltzmann weight $w^{1/4}$. The higher-spin thermal states (e.g., $m = \pm 3/2$) carry weights $w^{9/4}$, which are heavily suppressed by a factor of $w^2 \ll 1$.

For $S \geq 3/2$, evaluating the exact link weight function yields the analytical expansion:

$$W_S(\nabla\theta_\ell) = 2w^{1/4} \cos\left(\frac{\nabla\theta_\ell}{2}\right) + 2w^{9/4} \cos\left(\frac{3\nabla\theta_\ell}{2}\right) + \mathcal{O}(w^{25/4}). \quad (18)$$

Factoring out $2w^{1/4} \cos(\nabla\theta_\ell/2)$, expanding the logarithm, and applying the identity $\cos(3x)/\cos x = 2\cos(2x) - 1$ with $x = \nabla\theta_\ell/2$, we obtain the effective action (up to constants):

$$S_{\text{eff}}[\theta] = -\sum_\ell \ln \cos\left(\frac{\nabla\theta_\ell}{2}\right) - 2w^2 \sum_\ell \cos(\nabla\theta_\ell) + \mathcal{O}(w^4). \quad (19)$$

The physical tuning parameter w factors out of the leading action term as an overall global normalization constant. While this shifts the global energy scale, it does not lift the topological degeneracy of the system. The leading, w -independent effective action, $-\sum_\ell \ln \cos[(\nabla\theta_\ell)/2]$, is identical to the gauge theory formulation of the classical $S = 1/2$ spin ice [11,13]. This action describes the degenerate manifold of two-in, two-out configurations, which hosts the U(1) Coulomb liquid phase characterized by algebraic dipolar correlations and unconfined integer fluxes ($\mathbf{P} \in \mathbb{Z}^3$).

The subleading $\mathcal{O}(w^2)$ correction is a global U(1)-symmetric XY rotor coupling $-2w^2 \cos(\nabla\theta_\ell)$ —the same functional form as the standard 3D XY model action. In the dual framework, this term strictly preserves the continuous U(1) symmetry and merely renormalizes the phase stiffness [corresponding to the photon stiffness of the emergent U(1) gauge field] without introducing any symmetry-breaking relevant operator (such as a monopole potential $\cos \theta_r$) that could generate a confining gap. More broadly, the 3D U(1) Coulomb phase is intrinsically robust against arbitrary

small local perturbations [11,14], and the $\mathcal{O}(w^2)$ perturbation does not generate any relevant operator that could confine the gauge field. Notably, this $\mathcal{O}(w^2)$ photon stiffness vanishes identically in the pure $S = 1/2$ limit, where $W_{1/2} = 2w^{1/4} \cos(\nabla\theta_\ell/2)$ contains no higher harmonics. It is the admixture of higher spin states ($|m| \geq 3/2$), available only for $S \geq 3/2$, that generates the phase stiffness through virtual fluctuations. Consequently, the duality mapping confirms and quantifies the simple picture stated at the beginning of this subsection: For any half-integer S , the small- w regime is the $S = 1/2$ Coulomb liquid with a weakly renormalized stiffness, and no thermodynamic phase transition occurs.

A technical remark: The link weight $W_S(\alpha)$ of any half-integer S is antiperiodic, $W_S(\alpha + 2\pi) = -W_S(\alpha)$ —the dual manifestation of the half-integer spin, reminiscent of the (-1) phase acquired by a spin-1/2 wave function under a 2π rotation. The dual integrand nonetheless remains single valued under $\theta_r \rightarrow \theta_r + 2\pi$, because each such shift flips the sign of exactly $z = 4$ incident link weights and $(-1)^4 = +1$; the even coordination number of the diamond lattice is what makes the half-angle representation consistent, and the partition function is strictly real and positive. Alternatively, all half-angles can be avoided from the outset by treating $2S_\ell^z \in \{\pm 1, \pm 3, \dots\}$ as the integer-valued conserved current and coupling the dual phase field to it; the resulting link weights involve only integer harmonics $\cos(p\nabla\theta_\ell)$ and lead to identical conclusions. We have kept the half-angle convention to maintain an explicit connection to the physical spin variables.

V. LARGE- w REGIME: GRAPHICAL MAPPINGS AND THE NATURE OF THE DECONFINEMENT TRANSITIONS

In the large- w limit ($\mu \rightarrow -\infty$), the system uniquely resides in the highly confined vacuum state where all spins take their maximum absolute values, $S_\ell^z = S\sigma_\ell$, with background polarities $\sigma_\ell \in \{-1, 1\}$. Defect strings, characterized by a reduced spin amplitude $|S^z| < S$, form graphs constrained by the local ice rule. In this section, working again at $v = 0$, we derive graphical (loop-gas) representations of the partition function and use them to determine the nature of the deconfinement transition. The outcome is a sharp dichotomy: For $S \leq 3/2$ the loop gas coincides with the high-temperature expansion of a *discrete* spin model (Ising for $S = 1$, three-state Potts for $S = 3/2$), whereas for $S \geq 2$ it coincides with that of the *continuous* 3D XY model.

A. Defect graphs, ice-rule compatibility, and configurational entropy

1. Ice-rule compatibility criterion

To analyze the macroscopic defect statistics, we map the physical spin variables into a discrete effective flux.

For each link ℓ , we define the shifted nonnegative variable, $\phi_\ell := S_\ell^z + S \in \{0, 1, \dots, 2S\}$. In this representation, the maximal-amplitude vacuum states correspond to $\phi_\ell \in \{0, 2S\} \equiv 0 \pmod{2S}$. Consequently, any link hosting an elementary defect ($|S_\ell^z| < S$) carries a nonzero $\mathbb{Z}_{2S}$ flux $\phi_\ell \in \{1, 2, \dots, 2S-1\}$.

At each vertex, $\sum_{\ell \in r} \phi_\ell = \sum_{\ell \in r} S_\ell^z + 4S$. The ice rule ($\nabla \cdot \mathbf{S}_r = 0$) strictly fixes the first sum to zero on both sublattices, giving the *exact* constraint $\sum_{\ell \in r} \phi_\ell = 4S$. Taking this equation modulo $2S$ yields a weaker, purely local conservation law:

$$\sum_{\ell \in r} \phi_\ell \equiv 0 \pmod{2S}. \quad (20)$$

Because $4S \equiv 0 \pmod{2S}$, the ice rule implies Eq. (20), but the converse need not hold: The modular condition admits solutions with $\sum_{\ell \in r} \phi_\ell = 2S, 6S, \dots$ that violate $Q_r = 0$.

Given a configuration of defect links (those with $\phi_\ell \in \{1, \dots, 2S-1\}$) satisfying Eq. (20) at every vertex, a natural question arises: Can one always choose the values of the remaining vacuum links ($\phi_\ell \in \{0, 2S\}$) so that the strict ice-rule constraint $\sum_{\ell \in r} \phi_\ell = 4S$ holds at every vertex? Such a choice is called an *ice-rule-compatible vacuum assignment*.

The answer reveals a topological dichotomy.

Ice-rule compatibility criterion. Consider any $\mathbb{Z}_{2S}$ -conserving defect configuration on the diamond lattice and any single vertex r of it. The modular conservation law alone guarantees—for every such configuration and every such vertex—that the nondefect links of r can be assigned vacuum values $\phi_\ell \in \{0, 2S\}$ such that the ice rule $\sum_{\ell \in r} \phi_\ell = 4S$ holds at r if and only if $S \leq 3/2$. For $S \geq 2$ the assignment still exists whenever fewer than four links of r carry defects, and can fail only at fully excited vertices.

Proof. Let k denote the number of defect bonds ($\phi_\ell \in \{1, \dots, 2S-1\}$) at a vertex, and write Σ_{def} for their partial sum. The remaining $4-k$ vacuum bonds each carry $\phi_\ell \in \{0, 2S\}$; if n_+ of them take the value $2S$, the ice rule $\sum_{\ell \in r} \phi_\ell = 4S$ becomes

$$n_+ = \frac{4S - \Sigma_{\text{def}}}{2S} = 2 - \frac{\Sigma_{\text{def}}}{2S}, \quad (21)$$

which must be solved with $n_+ \in \{0, 1, \dots, 4-k\}$.

- (i) $k < 4$ (at least one vacuum bond exists, so n_+ is adjustable). Case by case: $k = 0$: Trivially $\Sigma_{\text{def}} = 0$ and $n_+ = 2$. $k = 1$: $\Sigma_{\text{def}} \in [1, 2S-1]$ is never a multiple of $2S$, so $k = 1$ is forbidden by $\mathbb{Z}_{2S}$ conservation itself. $k = 2$: $\Sigma_{\text{def}} \in [2, 4S-2]$; the unique multiple of $2S$ is $2S$ itself, giving $n_+ = 1 \leq 2$, which is satisfiable. $k = 3$: $\Sigma_{\text{def}}/(2S) \in \{1, 2\}$ with $n_+ \in \{1, 0\}$, both in $[0, 1]$, again satisfiable. Thus every vertex with $k < 4$ admits an ice-rule-compatible vacuum assignment for all S .

TABLE III. Ice-rule compatibility for a fully excited vertex ($k = 4$). The interval $[4, 4(2S-1)]$ lists the allowed range of $\sum_{\ell \in r} \phi_\ell$. The ice rule requires $\sum_{\ell \in r} \phi_\ell = 4S$; for $S \geq 2$, additional multiples of $2S$ appear in the interval, so the modular condition no longer guarantees the ice rule (ice-rule incompatibility).

Spin S	Interval	Multiples of $2S$ in the interval	Compatible?
1	$[4, 4]$	4	✓
3/2	$[4, 8]$	6	✓
2	$[4, 12]$	4, 8, 12	✗
$\geq 5/2$	$[4, 4(2S-1)]$	$2S, 4S, \dots$	✗

- (ii) $k = 4$ (all bonds excited; no adjustable vacuum bonds). Since $\phi_\ell \in [1, 2S-1]$, we have $\Sigma_{\text{def}} \in [4, 4(2S-1)]$. With no vacuum bonds available, Eq. (21) has no free variable, and the strict ice rule demands $\Sigma_{\text{def}} = 4S$. The modular conservation law $\Sigma_{\text{def}} \equiv 0 \pmod{2S}$ guarantees this if and only if $4S$ is the unique multiple of $2S$ within the kinematically allowed interval $[4, 4(2S-1)]$ (Table III). For $S \leq 3/2$, $4S$ is the unique multiple, so $\mathbb{Z}_{2S}$ conservation guarantees $Q_r = 0$. For $S \geq 2$, extra multiples of $2S$ appear in the interval, satisfying $\mathbb{Z}_{2S}$ conservation but giving $Q_r \neq 0$ —a situation we refer to as *ice-rule incompatibility*. (We deliberately avoid the term “monopole” here: The physical, thermally excited monopoles of Sec. VI are absent in the present $v = 0$ setting, and the incompatibility is a purely arithmetic property of the modular conservation law.)

Combining (i) and (ii) completes the proof. ■

This criterion establishes a sharp dichotomy at the vertex level. For $S \leq 3/2$, the modular conservation law guarantees vertex-by-vertex compatibility with the ice rule. One caveat must be recorded: Vertex-level compatibility does not by itself guarantee a *globally* consistent vacuum assignment, because vacuum links are shared between vertices. For $S = 1$, this mechanism does not arise (junctions are absent, and no vacuum value is ever forced). For $S = 3/2$, however, a cubic junction fixes the value of its unique vacuum link ($\phi = 2S$ when all three defect currents point in, $\phi = 0$ when they point out), so rare arrangements in which the forced vacuum links of two like-oriented junctions meet at a common pass-through vertex admit no consistent assignment and are excluded from the physical ensemble. This exclusion acts as a short-range, $\mathbb{Z}_3$ -symmetric hard-core constraint between nearby junctions; it first arises at second order in the junction density, and its role is accounted for in Sec. V B. The minimal excluded configuration, together with an exact finite-lattice verification, is recorded in Sec. V of Supplemental Material [25]. For $S \geq 2$, compatibility fails already at the single-vertex level. As a concrete illustration, consider $S = 2$

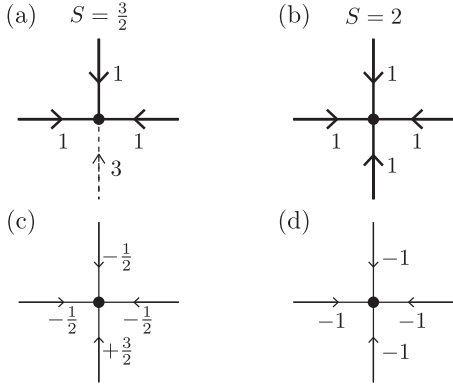


FIG. 2. Ice-rule compatibility at a single $z = 4$ diamond-lattice vertex; arrows indicate the bipartite $A \rightarrow B$ link orientation along which ϕ_ℓ is defined. (a) $S = 3/2$: three fundamental defects ($\phi = 1$) annihilate at a single vertex, and the remaining vacuum link at $\phi = 2S$ completes the ice rule $\sum_{\ell \in r} \phi_\ell = 4S$. (b) $S = 2$: four fundamental defects give $\sum_{\ell \in r} \phi_\ell = 4 = 2S \neq 4S$ —the modular condition is satisfied but the ice rule is violated. (c), (d) The spin configurations S_ℓ^z corresponding to (a) and (b), with $\sum_{\ell \in r} S_\ell^z = 0$ and -4 , respectively. The four bonds are drawn as a planar cross for clarity; on the diamond lattice they point toward the corners of a tetrahedron.

[Figs. 2(b) and 2(d)]: A vertex with $(\phi_1, \phi_2, \phi_3, \phi_4) = (1, 1, 1, 1)$ gives $\Sigma_{\text{def}} = 4 = 2S$, while $(3, 3, 3, 3)$ gives $\Sigma_{\text{def}} = 12 = 6S$. Both satisfy $\mathbb{Z}_4$ conservation but violate the ice rule $\Sigma_{\text{def}} = 4S = 8$, producing charges $Q_r = \pm 4$. Consequently, for $S \geq 2$, any loop model built on $\mathbb{Z}_{2S}$ conservation alone would include configurations that the spin-ice model forbids. Together with the mismatch of defect fugacities quantified in Sec. V C, this obstructs a mapping to a discrete $\mathbb{Z}_{2S}$ spin or gauge model [37,43,44].

2. Configurational entropy

The Boltzmann weight of a single defect link relative to the vacuum background changes by a factor of $w^{(S-1)^2 - S^2} = w^{1-2S}$. To evaluate the full loop-gas partition function, we must additionally account for the macroscopic configurational entropy of the background spins.

We employ Pauling’s independent-vertex approximation [10]. In the vacuum, each vertex has $\binom{4}{2} = 6$ valid ice-rule configurations out of $2^4 = 16$ unconstrained binary assignments, yielding a Pauling fraction $p_0 = 3/8$. We now compute, following Ref. [18], the ratio $W(C)/W(\emptyset)$, where $W(C)$ denotes the number of ice-rule-satisfying background spin configurations in the presence of a defect loop C of length $|C|$, and $W(\emptyset)$ is the corresponding count in the defect-free vacuum.

For $S \geq 3/2$, the defect retains a nonzero amplitude $[S_\ell^z = \pm(S-1) \neq 0]$, so each defect link carries an internal arrow (the sign of S^z), making the loops directed. For such a directed loop with a fixed orientation, the two defect links at each loop vertex are completely determined—their ϕ

values are fixed by the loop’s flux charge—leaving only the two background links as free variables. Each background link carries $\phi \in \{0, 2S\}$, and the ice rule $\sum_{\ell \in r} \phi_\ell = 4S$ constrains the pair: If the defect links contribute Σ_{def} to the vertex sum, the two background links must sum to $4S - \Sigma_{\text{def}} = 2S$, which is uniquely satisfied by one link carrying 0 and the other $2S$. There are exactly two such assignments (either ordering), so out of $2^2 = 4$ background configurations, exactly two satisfy the ice rule, giving a vertex fraction $p_{\text{loop}} = 1/2$. This holds uniformly for all S . In addition, each defect link replaces a two-state vacuum link ($S_\ell^z = \pm S$) with a single fixed state, contributing a link-degeneracy factor of $1/2$ per defect link. Combining both factors, the Pauling entropy reduction per loop link is

$$\frac{W(C)}{W(\emptyset)} \approx \left(\frac{1}{2} \times \frac{p_{\text{loop}}}{p_0} \right)^{|C|} = \left(\frac{1}{2} \times \frac{4}{3} \right)^{|C|} = \left(\frac{2}{3} \right)^{|C|}. \quad (22)$$

Together with the bare Boltzmann weight w^{1-2S} per defect link, the effective fundamental string fugacity evaluates to (see Secs. II and III of Supplemental Material [25] for detailed derivations)

$$\tilde{x}_1 = \frac{2}{3} w^{-(2S-1)}. \quad (23)$$

The internal degrees of freedom n hosted by each continuous loop depend on S . For $S = 1$, the defect is $S_\ell^z = 0$, yielding undirected loops ($n = 1$). For $S \geq 3/2$, as noted above, the nonzero defect amplitude preserves the sign of the displacement, yielding chiral, directed loops that host $n = 2$ distinct physical states.

B. Mapping to the three-state Potts model for $S = 3/2$

For the specific case of $S = 3/2$, our ice-rule compatibility criterion guarantees that the geometric $z = 4$ lattice constraints and the $\mathbb{Z}_3$ flux conservation are matched. Up to the short-range junction-junction exclusion recorded in Sec. V A, every $\mathbb{Z}_3$ -conserving defect graph is realizable within the physical ice-rule manifold, and the loop expansion below is that of a discrete three-state spin model.

The fundamental defects $S_\ell^z = \pm 1/2$ naturally act as conjugate strings carrying fluxes $\phi = 1$ and $\phi = 2 \equiv -1 \pmod{3}$. The strict $\mathbb{Z}_3$ conservation geometrically permits degree-2 pass-throughs, degree-4 crossings, and uniquely, degree-3 junctions where three fundamental strings converge [$\sum_{\ell \in r} \phi_\ell = 1 + 1 + 1 = 3 \equiv 0 \pmod{3}$]. This geometry accommodates the simultaneous local annihilation of exactly three topological strings at a single vertex [Figs. 2(a) and 2(c)].

The vertex weights are determined by the ice-rule state counts at each vertex degree. In the defect-free vacuum (degree $d_0 = 0$), each vertex has $\binom{4}{2} = 6$ valid configurations out of $2^4 = 16$ possibilities, giving a local state sum $z(0) = 6$. At a degree-2 (pass-through) vertex, the two

defect links are fixed by the loop direction, and the two remaining vacuum links must satisfy the ice rule, giving $z_{\text{dir}}(2)/z(0) = 2/6 = 1/3$. At a degree-3 (cubic junction) vertex, the $\mathbb{Z}_3$ conservation law already forces all three defect currents to share one orientation ($|\Sigma_{\text{def}}| = 3$; i.e., all ingoing or all outgoing); the ice rule additionally fixes the value of the single remaining vacuum link, which halves the allowed configurations relative to the degree-2 baseline, giving $z_{\text{dir}}(3)/z(0) = 1/6$. At a degree-4 (crossing) vertex, all four bonds are occupied by defects (no vacuum links remain); the directed ice rule then uniquely fixes the defect configuration, giving $z_{\text{dir}}(4)/z(0) = 1/6$. The vertex fugacities, normalized relative to the degree-2 weight, are thus $\lambda_3 = (1/6)/(1/3)^{3/2} = \sqrt{3}/2 \approx 0.866$ (penalty at cubic junctions) and $\lambda_4 = (1/6)/(1/3)^2 = 3/2$ [enhancement at crossings; the denominator is $(1/3)^2$ because a crossing replaces two independent degree-2 vertices]. Utilizing the standard topological graph identity $\sum d V_d = 2|G|$, the complete monopole-free partition function takes the form

$$Z_{v=0} = Z_{\text{vac}} \sum_G 2^{N_{\text{comp}}(G)} \tilde{x}_1^{|G|} \lambda_3^{V_3(G)} \lambda_4^{V_4(G)}, \quad (24)$$

where Z_{vac} is the partition function of the vacuum sector, in which every link carries maximum amplitude $|S_\ell^z| = S$ subject to the ice rule. Each vacuum configuration contributes a Boltzmann weight w^{2NS^2} , and the Pauling approximation (Sec. V A 2) yields an ice-rule degeneracy $(3/2)^N$, so that $Z_{\text{vac}} \approx w^{2NS^2} (3/2)^N$. The sum runs over all graphs G on the diamond lattice whose edges carry directed $\mathbb{Z}_3$ fluxes satisfying the conservation law $\sum_{\ell \in r} \phi_\ell \equiv 0 \pmod{3}$ at every vertex r [Eq. (20)], excluding the short-range junction-junction configurations identified in Sec. V A; $|G|$ is the total number of edges, $V_3(G)$ and $V_4(G)$ are the numbers of degree-3 and degree-4 vertices, respectively, and $N_{\text{comp}}(G)$ is the number of closed defect strands, each carrying two chiral orientations (at a degree-4 crossing, the four incident defect links pair into two through-going strands, so two loops crossing at a vertex count as two strands).

This graph ensemble is isomorphic to the high-temperature graphical expansion of the classical three-state Potts model on the diamond lattice [36,45] (see Secs. III and V of Supplemental Material [25] for detailed derivations),

$$Z_{3\text{-Potts}} = \sum_{\{\sigma_r \in \mathbb{Z}_3\}} \exp\left(K \sum_{\langle rr' \rangle} \delta_{\sigma_r, \sigma_{r'}}\right). \quad (25)$$

The standard Fourier decomposition on $\mathbb{Z}_3$ expands each bond weight as $e^{K\delta_{\sigma,\sigma'}} = a_0[1 + t(\omega^{\sigma-\sigma'} + \omega^{-(\sigma-\sigma')})]$ with $\omega = e^{2\pi i/3}$, $a_0 = (e^K + 2)/3$, and $t = (e^K - 1)/(e^K + 2)$. Summing over the spin variables, the $\mathbb{Z}_3$ flux conservation at every vertex generates exactly the same graph ensemble as above, yielding

$$Z_{3\text{-Potts}} = a_0^{2N} 3^N \sum_G 2^{N_{\text{comp}}(G)} t^{|G|}. \quad (26)$$

The identification with the spin-ice expansion is established by the correspondence $t = \tilde{x}_1$; the local geometric weights λ_3 and λ_4 act merely as short-distance renormalizations of the bare coupling and do not alter the universality class.

We spell out the status of this mapping. The correspondence between the two graph ensembles is fixed by the $\mathbb{Z}_3$ conservation law and the vertex-level compatibility criterion, up to the explicit short-range exclusion recorded in Sec. V A: Configurations in which the forced vacuum links of two like-oriented junctions collide occur in the Potts ensemble but not in the spin-ice ensemble. The vertex weights, by contrast, are computed within Pauling's independent-vertex approximation: Correlations of the background ice manifold induce additional interactions between defect strings beyond the independent-vertex level. In particular, a cubic junction, which forces its single background link to $\phi = 2S$, acts as a localized perturbation (an effective charge) for the background height field, so junctions experience entropic, dipolar-type interactions mediated by the background Coulomb phase.

These interactions are short ranged or screened at finite defect density—including, at shortest distance, the strict junction-junction exclusion above, which acts as a hard core—and, crucially, they respect the $\mathbb{Z}_3$ symmetry of the loop gas; they therefore renormalize the couplings of the effective Potts description but do not affect the symmetry classification on which the Landau argument below rests. Their quantitative smallness is supported *a posteriori* by the accuracy of the same approximation elsewhere: It reproduces the $S = 1$ transition point $w_{c2} = 1.8904(1)$ of Ref. [16] to within 0.3% [18] and the $S = 3/2$ transition point of Ref. [19] to within $\sim 3.0\%$ (below).

Finally, for $q = 3$ the Potts and clock descriptions are equivalent. Since the Kronecker delta on $\mathbb{Z}_3$ satisfies $\delta_{\sigma,\sigma'} = \frac{1}{3}\{1 + 2\cos[2\pi(\sigma - \sigma')/3]\}$, the three-state Potts model is equivalent to the three-state clock model—the identity $\cos(2\pi/3) = \cos(4\pi/3)$ ensures that all nonidentical spin pairs receive equal weight, making the clock interaction identical to the Potts Kronecker delta. This equivalence holds for $q \leq 3$ but fails for $q \geq 4$, where different angular separations yield distinct weights (cf. Sec. V C).

In the continuum Landau-Ginzburg-Wilson effective action, the $\mathbb{Z}_3$ defect-string fusion generates a symmetry-allowed cubic invariant ($\sim \Phi^3$). Within Landau mean-field theory, a cubic invariant drives the transition first order, and in three dimensions this expectation is borne out: Indeed, extensive Monte Carlo studies have established that the three-state Potts model in three dimensions undergoes a first-order transition [45,46]. The graphical mapping derived above thus provides a theoretical explanation for

the *first-order phase transition* observed numerically by Pandey *et al.* for $S = 3/2$ [19].

We note that Ref. [19] itself provided a rationale for the first-order character by a different, symmetry-based route: Through the mapping to an XY partition function and the observation that the large- w phase exhibits long-range order of $e^{3i\theta}$ but not of $e^{i\theta}$, the transition was identified there with that of a three-state spin system. The graphical derivation given here reaches the same conclusion from a complementary, microscopic starting point, and in addition yields a quantitative estimate of the transition point, as follows.

The location of the first-order transition can be estimated analytically via the Bethe-Peierls (cavity) approximation [47]. The idea is to replace the diamond lattice ($z = 4$) by the Bethe lattice (Cayley tree) with the same coordination number, on which the partition function of the $q = 3$ Potts model can be evaluated exactly via a single-variable cavity recursion. On this tree, each site has $b = z - 1 = 3$ “children”; the cavity message—the ratio $r := P(\sigma = \sigma_0)/P(\sigma = \sigma_1)$ ($\sigma_1 \neq \sigma_0$) of the probability that a boundary spin matches a reference state σ_0 to that of any single nonreference state σ_1 (the $q - 1$ nonreference states are equivalent by the S_q symmetry of the Potts model)—satisfies the self-consistency equation,

$$r = \left[\frac{e^K r + 2}{r + e^K + 1} \right]^b, \quad (27)$$

where K is the Potts coupling and $b = 3$.

The disordered solution $r = 1$ is always present; for the $q = 3$ Potts model, a second solution $r^* > 1$ (the ordered phase) appears discontinuously—a hallmark of a first-order transition driven by the cubic Φ^3 invariant. Equating the Bethe free energies of the two solutions (see Sec. VIII of Supplemental Material [25]) determines the coexistence point *in closed form*: $e^{K_c} = 1 + \sqrt{2}$, i.e., $t_c = (3\sqrt{2} - 2)/7 \approx 0.3204$, where $t = (e^K - 1)/(e^K + 2)$ is the Potts high-temperature parameter identified with the spin-ice fugacity via $t = \tilde{x}_1 = \frac{2}{3}w^{-2}$. Converting back to the spin-ice fugacity gives the closed-form estimate

$$w_c^2 = \sqrt{2} + \frac{2}{3} \approx 2.081, \quad w_c \approx 1.443 \quad (28)$$

(note that Ref. [19] uses w to denote what corresponds to w^2 in our convention). This overestimates the Monte Carlo value $w^2 \approx 2.02$ [19] by only $\sim 3.0\%$, a level of accuracy expected for the Bethe approximation on a $z = 4$ lattice: At a first-order transition the correlation length remains finite, so the absence of loops on the Bethe lattice—its only structural deficiency—has a minor quantitative effect (see Sec. VIII of Supplemental Material [25] for the full derivation including free-energy evaluation).

C. $S \geq 2$: 3D XY universality

1. Breakdown of the clock mapping and continuous $U(1)$ baseline

We begin by recalling a fact already used in Sec. IV: The ice rule is a *real-valued* constraint—the lattice divergence of S^z vanishes exactly, not merely modulo an integer—so the microscopic model possesses an exact $U(1)$ structure for every S . This is precisely what underlies the dual XY representations here and in Refs. [16,18,19]. The question addressed in this subsection is therefore *not* how a $U(1)$ symmetry emerges, but the converse: whether the large- w defect ensemble reduces this microscopic $U(1)$ structure to a discrete one, as it does for $S = 1$ (Ising) and $S = 3/2$ (Potts). We show that for $S \geq 2$ it does not: No discrete clock model reproduces the loop gas, and the transition is governed by the microscopic $U(1)$ structure; i.e., it is of the 3D XY type.

For $S \geq 2$, the situation changes qualitatively relative to $S \leq 3/2$. As shown by the ice-rule compatibility criterion (Sec. VA), the $\mathbb{Z}_{2S}$ Gauss law no longer coincides with the physical ice rule (ice-rule incompatibility). Furthermore, the hierarchy of defect tensions creates a bond-fugacity mismatch. The natural comparison model is the $\mathbb{Z}_{2S}$ clock model [38] (rather than the Potts model), because the defect charges $\phi = 1, 2, \dots, 2S - 1$ naturally correspond to the clock-model current harmonics, which distinguish different angular separations—a structure absent in the Potts model that treats all nonidentical states equally. In a standard $\mathbb{Z}_{2S}$ clock model, higher-current harmonics yield polynomial fugacity decay ($t_m \sim K^m/m!$ at high temperature), whereas in the spin-ice model, each defect level carries an independent chemical potential with fugacities $x_\phi := w^{-\phi(2S-\phi)}$ ($\phi = 1, \dots, 2S - 1$) that decay exponentially.

A key consequence is the arithmetic prohibition of the cubic junction. For $S = 3/2$ ($2S = 3$), three fundamental strings satisfy $1 + 1 + 1 = 3 \equiv 0 \pmod{3}$, permitting a cubic vertex that maps to the symmetry-breaking Φ^3 invariant driving the first-order Potts transition (Sec. VB). For $S \geq 2$ ($2S \geq 4$), however, $1 + 1 + 1 = 3 \not\equiv 0 \pmod{2S}$, so a cubic junction composed solely of fundamental strings is strictly forbidden by the $\mathbb{Z}_{2S}$ conservation law itself. This arithmetic obstruction inherently suppresses the Φ^3 invariant that would otherwise drive a first-order transition.

A second, purely geometric, obstruction emerges in the annihilation of fundamental strings. In a $\mathbb{Z}_{2S}$ clock model, the modular conservation law $\sum_{\ell \in r} n_\ell \equiv 0 \pmod{2S}$ allows up to $z = 4$ fundamental currents to merge at a single vertex whenever $2S \leq z$; in particular, for $S = 2$ ($q = 4$), all four fundamentals annihilate locally with no intermediate bonds and unit penalty (Table IV). Even for $S > 2$, a short cascade of only $\lceil S - 2 \rceil$ intermediate bonds carrying odd currents $n = 3, 5, \dots$ suffices (see Sec. VI of Supplemental Material [25]).

TABLE IV. Number of intermediate bonds and total cascade penalty for annihilating $2S$ fundamental strings on the diamond lattice ($z = 4$). Each row shows the number of intermediate bonds connecting the fusion vertices and the product of their fugacities (the “penalty”); a penalty of 1 means no intermediate bond is needed. For $S \leq 3/2$ the two models agree and no cascade is needed. For $S \geq 2$ they diverge: the clock model requires at most $\lceil S - 2 \rceil$ bonds with polynomially suppressed fugacities t_n (Sec. IV of Supplemental Material [25]), while the spin-ice model requires $2S - 3$ bonds with exponentially suppressed fugacities $x_\phi = w^{-\phi(2S-\phi)}$; see the text for details.

Spin S	$\mathbb{Z}_{2S}$ clock		Spin ice	
	Bonds	Penalty	Bonds	Penalty
1	0	1	0	1
3/2	0	1	0	1
2	0	1	1	w^{-4}
5/2	1	t_3	2	w^{-12}
3	1	t_3	3	w^{-24}
7/2	2	$t_3 t_5$	4	w^{-42}

In the spin-ice model, by contrast, the exact ice rule $\sum_{\ell \in r} \phi_\ell = 4S$ is more restrictive than the modular condition: It forbids simultaneous merging even for $2S = 4$ [Figs. 2(b) and 2(d)] and, more generally, forbids any vertex from absorbing more than two *fundamental* strings (with three or four fundamentals at a vertex, $\sum_{\ell \in r} \phi_\ell \leq 3 + 2S < 4S$ for $S \geq 2$). The $2S$ fundamentals therefore fuse pairwise into composite strands, which fuse further through a fusion tree containing at least $2S - 3$ intermediate bonds with charges $2 \leq \phi \leq 2S - 2$; the linear chain, in which one fundamental is absorbed at a time ($\phi = 2, 3, \dots, 2S - 2$; Fig. 3), is the simplest such tree.

These combined obstructions—the ice-rule incompatibility, the exponential bond-fugacity mismatch, and the extended cascade geometry—mean that, unlike for $S \leq 3/2$, the large- w loop gas is *not* the high-temperature expansion of any discrete $\mathbb{Z}_{2S}$ clock model. The only processes that could distinguish the discrete $\mathbb{Z}_{2S}$ conservation law from the

full U(1) conservation law are the fusion cascades themselves, whose statistical weight we now quantify.

Quantitatively, each intermediate bond incurs a fugacity $x_\phi = w^{-\phi(2S-\phi)}$, so the total statistical cost of a fusion channel—the *bridge penalty*—is the product of its intermediate fugacities (see Supplemental Material [25], Sec. II, for a self-contained derivation). For the linear chain,

$$\begin{aligned} \mathcal{P}_{\text{bridge}} &= \prod_{\phi=2}^{2S-2} x_\phi = w^{-\sum_{\phi=2}^{2S-2} \phi(2S-\phi)} \\ &= w^{-(2S-3)(2S-1)(2S+4)/6}. \end{aligned} \quad (29)$$

Other fusion trees carry slightly different exponents [for $S = 3$, the cheapest channel fuses the fundamentals pairwise into three charge-2 bonds of fugacity $x_2 = w^{-8}$ each, costing w^{-24} instead of the chain’s w^{-25} —a minimum shared by the pairwise-doubling channel $2 + 2 \rightarrow 4$ terminated by $(4, 1, 1)$; see Fig. 4], but the following bound is channel independent. Each pairwise fusion produces exactly one intermediate bond, so a channel that starts from the $2S$ fundamentals and terminates at a vertex absorbing $k \in \{2, 3\}$ strands contains $2S - k$ fusion outputs; of these, at most one—a conjugate fundamental with $\phi = 2S - 1$, which can only be consumed in the pair termination $(2S - 1, 1)$ —falls outside the counted range $2 \leq \phi \leq 2S - 2$. Every channel therefore contains at least $2S - 3$ counted intermediate bonds and, since the tension exponent $\phi(2S - \phi)$ is minimized at the edges of this range, each of them costs at least $w^{-2(2S-2)}$. Hence the penalty of *any* channel is bounded by

$$\mathcal{P}_{\text{bridge}} \leq w^{-4(S-1)(2S-3)}. \quad (30)$$

For $S = 2$, $\mathcal{P}_{\text{bridge}} = w^{-4}$; for $S = 5/2$, $\mathcal{P}_{\text{bridge}} = w^{-12}$; and the suppression strengthens rapidly with S , the penalty decaying at least as fast as e^{-cS^2} at fixed $w > 1$. We also note that the exponent $4(S - 1)(2S - 3)$ vanishes precisely

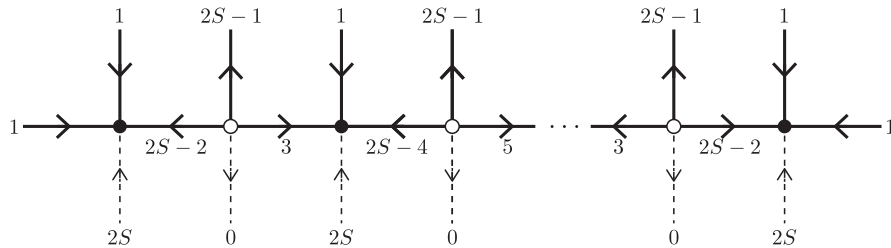


FIG. 3. The simplest (linear-chain) fusion channel for $S \geq 2$: at each of the $2S - 2$ fusion vertices, an incoming fundamental defect ($\phi = 1$) merges with the accumulated intermediate defect, incrementing the effective charge by one. Arrows indicate the bipartite $A \rightarrow B$ link orientation along which ϕ_ℓ is defined; open and filled circles denote A- and B-sublattice vertices. The displayed link labels alternate between ϕ and $2S - \phi$ along the chain because the vertices alternate between the two sublattices. The half-odd-integer case is shown; for integer S the same structure applies with uniform link orientations. The chain is drawn as a straight line for clarity; on the diamond lattice the backbone follows a zigzag path.

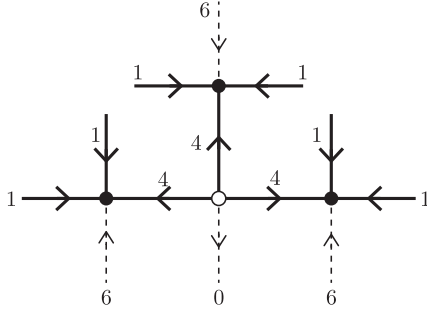


FIG. 4. The cheapest annihilation channel for $S = 3$ ($2S = 6$): six fundamental strings ($\phi_\ell = 1$) fuse pairwise at three vertices with link values (1, 1, 4, 6), and the three resulting charge-2 intermediate bonds (displayed link value $\phi_\ell = 4 = 2S - 2$) annihilate at a common vertex with link values (4, 4, 4, 0), whose vacuum link absorbs the total charge $2S$. Arrows indicate the bipartite $A \rightarrow B$ link orientation along which ϕ_ℓ is defined; solid and dashed lines denote defect and vacuum links; open and filled circles denote A- and B-sublattice vertices. An equivalent configuration is obtained by the global flip $\phi_\ell \rightarrow 2S - \phi_\ell$.

for $S \leq 3/2$ —the minimal number of intermediate bonds in any annihilation channel is $\max(0, 2S - 3)$ —recovering the *unsuppressed* pair annihilation of the $S = 1$ loops and the unsuppressed cubic junction at $S = 3/2$. The exponential protection of the U(1) structure thus sets in exactly at $S = 2$, encoding the $S \leq 3/2$ vs $S \geq 2$ dichotomy of Sec. VA in a single formula.

In the $\mathbb{Z}_{2S}$ clock model, by contrast, the weaker modular conservation $\sum_{\ell \in r} n_\ell \equiv 0 \pmod{2S}$ (rather than the exact ice rule) permits a qualitatively shorter cascade. For $2S \leq z = 4$ (i.e., $S \leq 2$), all $2S$ fundamental currents annihilate at a single vertex ($\underbrace{1 + \dots + 1}_{2S} = 2S \equiv 0$), so no intermediate

bond is needed and the penalty is unity. For $S > 2$, a cascade is required but is shorter than in the spin-ice model. For example, at $S = 3$ ($q = 6$), three fundamental currents ($n = 1$ each) merge at the first vertex to produce an intermediate bond with current $n = 3$ (using three of the four links); at the second vertex, this intermediate bond meets three more fundamentals, and $3 + 1 + 1 + 1 = 6 \equiv 0 \pmod{6}$ terminates the cascade with just one intermediate bond (carrying $n = 3$, with fugacity t_3), compared to $2S - 3 = 3$ intermediate bonds in the spin-ice model. In general, the clock-model cascade requires only $\lceil S - 2 \rceil$ intermediate bonds with polynomially suppressed fugacities (Sec. IV of Supplemental Material [25]). A comparison of the two cascade costs is given in Table IV.

Because the cascade is exponentially suppressed by the spin stiffness, at leading order the active macroscopic graph ensemble is stripped of degree-3 branching junctions and collapses to fundamental strings forming closed directed loops and degree-4 loop crossings. This restricted ensemble is topologically isomorphic to the high-temperature graphical expansion of the continuous classical 3D XY model [42], differing only in short-distance vertex weights.

2. Decomposition of the partition function and 3D XY universality

To turn this continuous U(1) baseline into a controlled analytical argument for the 3D XY universality class for $S \geq 2$, we construct a decomposition of the vacuum-normalized partition function $\tilde{Z}_{\text{ice}} := Z_{v=0}/Z_{\text{vac}}$, where Z_{vac} is the partition function restricted to the vacuum sector in which every link carries the maximal amplitude $|S_\ell^z| = S$ subject to the ice rule (i.e., the $\mathbb{Z}_{2S}$ -confined phase with no defects). The ratio $\tilde{Z}_{\text{ice}}$ thus measures the total statistical weight of all defect configurations relative to the defect-free background. We decompose $\tilde{Z}_{\text{ice}}$ into a continuous U(1) sector and an exponentially suppressed discrete $\mathbb{Z}_{2S}$ correction.

To separate the U(1)-conserving sector from the cascade corrections, we note that at crossing vertices (degree 4), the $S \geq 2$ spin ice carries a constant Pauling weight $\lambda_4 = (1/6)/(1/3)^2 = 3/2$ relative to two independent passing strings. We therefore define a *decorated XY model*, denoted $\tilde{Z}_{XY}^{(3/2)}$, which employs the ice-model bond fugacities $\tilde{x}_{|n|}$ for currents $|n| \leq 2S - 1$ and exact U(1) current conservation at every vertex (the same Gauss law as the ice rule), while additionally enhancing every crossing vertex by a factor $\beta = 3/2$.

Since $\lambda_4 = 3/2$ is a constant independent of S and w , the crossing decoration acts as a short-range quartic composite operator that flows to zero under the renormalization group (RG). Because $\tilde{Z}_{XY}^{(3/2)}$ employs the same bond fugacities $\tilde{x}_{|n|}$ as the ice model, every noncascade graph of the spin-ice loop gas appears in both partition functions with the same weight, the weights being evaluated—here as throughout this section—within the independent-vertex approximation.

There are two remaining differences to keep track of. First, the spin-ice configurations not captured by the decorated XY model are the fusion cascades analyzed above, whose total contribution $\delta Z_{\text{cascade}}$ is controlled by the bridge penalty $\mathcal{P}_{\text{bridge}}$ [Eq. (29)] and is exponentially small in $1/T$. Second, the decorated XY ensemble contains some local current configurations with no spin-ice counterpart [e.g., a vertex with currents $(+1, +1, +1, -3)$, which conserves the U(1) charge but is incompatible with the ice rule, which permits at most two positive-deviation links at any vertex]; excluding them is a U(1)-symmetric, short-range modification of vertex weights, on the same footing as the crossing decoration, and is treated as such in the RG argument below. With this bookkeeping (see Supplemental Material [25], Sec. VII), the partition function decomposes as

$$\tilde{Z}_{\text{ice}} = \tilde{Z}_{XY}^{(3/2)} + \delta Z_{\text{cascade}}. \quad (31)$$

The physical content of this decomposition is as follows. The decorated XY model $\tilde{Z}_{XY}^{(3/2)}$ captures the

U(1)-conserving sector of the spin-ice loop gas, and shares the 3D XY universality class (as shown below). The cascade contribution $\delta Z_{\text{cascade}}$ is the only term sensitive to the discreteness of the $\mathbb{Z}_{2S}$ conservation law, and its bare weight is exponentially suppressed by the lattice geometry. Combined with RG arguments, this decomposition places $\tilde{Z}_{\text{ice}}$ in the 3D XY universality class, as follows.

First, the crossing decoration operator β^{V_4} introduced in the decorated XY model preserves the continuous U(1) current conservation at every vertex and therefore corresponds to a U(1)-symmetric irrelevant perturbation. At the 3D XY critical fixed point, the leading correction-to-scaling exponent is $\omega \approx 0.79$ [48], so the scaling dimension of this operator is $\Delta = 3 + \omega \approx 3.79 > 3$. Likewise, the differences between the ice-model bond fugacities $\tilde{x}_{|n|}$ and the Bessel ratios $\tau_{|n|}$ are U(1)-symmetric short-range perturbations involving higher-current operators ($|n| \geq 2$), which are even more strongly irrelevant at the XY fixed point. Being irrelevant, the RG flow guarantees that the decorated XY model flows to the 3D XY universality class.

Second, the cascade correction $\delta Z_{\text{cascade}}$ is the only mechanism that distinguishes the discrete $\mathbb{Z}_{2S}$ conservation law from the continuous U(1) conservation law; in the coarse-grained XY description it is represented by the leading discrete anisotropy $\cos(2S\theta)$. Two logically independent facts now combine. (i) *RG irrelevance*: At the 3D XY fixed point, the anisotropy $\cos(p\theta)$ has scaling dimension $\Delta_p > 3$ for all $p \geq 4$ ($\Delta_4 \approx 3.11$ from Monte Carlo RG studies [49,50], and Δ_p increases monotonically with p ; here $p = 2S \geq 4$). It is therefore a (dangerously) irrelevant operator [38,49]: It cannot alter the critical universality class for any bare coupling within the basin of attraction of the XY fixed point—in particular, for any sufficiently weak bare coupling. (A sufficiently strong bare anisotropy can escape this basin: The hard $\mathbb{Z}_4$ clock model, the infinite-anisotropy limit at $p = 4$, decomposes into two decoupled Ising models and orders with Ising rather than XY exponents; this is precisely why the following point matters). (ii) *Bare smallness*: The decomposition shows that the bare weight of this operator is not merely small but exponentially small [$\mathcal{O}(e^{-c/T})$, Eqs. (29) and (30)], placing the system deep inside the basin of attraction. It also controls the crossover scale: The length scale beyond which the asymptotic XY behavior becomes visible is short, so no remnant of the discreteness should be observable even in moderate-size simulations. Together, (i) and (ii) place the deconfinement transitions of the $S \geq 2$ pyrochlore spin ice in the 3D XY universality class, with an early onset of the asymptotic critical behavior.

3. Quantitative estimate of w_c via $O(2)$ loop-gas mapping

Because the discrete anisotropy is highly suppressed and irrelevant for $S \geq 2$, the system asymptotes to a continuous $O(2)$ symmetry near criticality. We can thus quantitatively

estimate the deconfinement transition point by mapping the dilute directed-loop gas to the high-temperature graphical expansion of the classical 3D XY model on the diamond lattice [42]. The transition occurs when the fundamental string fugacity $\tilde{x}_1 = \frac{2}{3}w^{-(2S-1)}$ reaches the critical fugacity $\tau_1 := I_1(K_c^{XY})/I_0(K_c^{XY})$, where K_c^{XY} is the 3D XY critical coupling on the diamond lattice. Equating $\tilde{x}_1 = \tau_1$, we obtain the general scaling formula:

$$w_c(S) = \left(\frac{2}{3\tau_1}\right)^{1/(2S-1)}, \quad S \geq 2. \quad (32)$$

From our Monte Carlo determination [41] $K_c^{XY} \approx 0.769$ [i.e., $T_c^{XY} = 1.30036(1)$], we obtain $\tau_1 \approx 0.359$ and $2/(3\tau_1) \approx 1.859$, giving $w_c(S) \approx (1.859)^{1/(2S-1)}$. As $S \rightarrow \infty$, the critical fugacity asymptotes to $w_c \rightarrow 1$ (i.e., $\mu \rightarrow 0$), consistent with the classical continuous-spin limit: as $S \rightarrow \infty$ the discrete spin variable $S_\ell^z \in \{-S, \dots, S\}$ approaches a continuous variable, the $\mathbb{Z}_{2S}$ flux quantization becomes infinitely fine, and the discrete $\mathbb{Z}_{2S}$ -confined phase vanishes; any weak easy-axis anisotropy, i.e., w slightly below $w_c(S)$, within the present model then suffices to stabilize the continuous U(1) Coulomb liquid. The geometric suppression of the $\mathbb{Z}_{2S}$ fusion cascade, established by the decomposition above, ensures that the continuous $O(2)$ approximation underlying this formula remains accurate for all $S \geq 2$. The complete classification of phases, flux quantization, and critical phenomena obtained in the monopole-free limit is collected in Tables I and II and illustrated schematically in Fig. 1.

VI. FINITE-TEMPERATURE EFFECTS: MAGNETIC MONOPOLES, STRING SEVERING, AND CROSSOVERS

The analysis in the previous sections relied on the strict enforcement of the local ice rule, $Q_r = 0$. This monopole-free limit is realized in the limit $T/J \rightarrow 0$ taken at fixed w , i.e., at fixed μ/T (Sec. II C). At any realistic finite temperature $T > 0$, the finite exchange J permits the thermal excitation of magnetic monopoles [8,29], characterized by a small but strictly nonzero fugacity $v := \exp(-J/2T) \ll 1$.

In this section, we return to the exact partition function generated in Eq. (3). It is well established on general grounds that three-dimensional topological order is fragile against thermal fluctuations [33,51,52]. Building on this principle, we show concretely that the thermal excitation of monopoles explicitly breaks the microscopic U(1) invariance encoded in the divergence-free constraint—entering the dual description of the small- w regime as a symmetry-breaking field—and acts as a topological severing of defect strings in the large- w regime [18,23], destroying the macroscopic topological invariants and rounding the phase

transitions into crossovers for all S (with the exception of $S = 3/2$).

A. Small- w regime: Emergence of a symmetry-breaking sine-Gordon field

The construction in this subsection is standard [36,38], and we keep the derivation brief for self-containedness; the conclusion that thermal monopoles act as an effective external field in the dual XY language was reached for $S = 1$ in Ref. [18]. We note, however, that this dual viewpoint is itself recent: Thermal monopoles in spin ice have traditionally been treated through the continuum electrostatic analogy, with screening inserted at the Debye level [8,14,29]. In the exact dual representation below, by contrast, a monopole of charge Q_r appears as the local vertex operator $e^{iQ_r\theta_r}$, so the full monopole gas enters the partition function—for every S at once—as an explicit U(1) symmetry-breaking site weight, from which the screening physics follows rather than being assumed. To properly capture the effect of thermal monopoles in the small- w limit (Sec. IV), we relax the constraint in the partition function by reinstating the sum over local divergences. The partition function in the dual phase field representation becomes

$$Z = \sum_{\{Q_r\}} \sum_{\{S_\ell^z\}} \int \mathcal{D}\theta \times \exp \left(-i \sum_r \theta_r (\nabla \cdot \mathbf{S}_r - Q_r) \right) v \sum_r Q_r^2 w \sum_\ell (S_\ell^z)^2. \quad (33)$$

Following the exact discrete integration by parts introduced previously, the exact spin sector decouples and maps to the local link weights $W_S(\nabla\theta_\ell)$ as before. The new addition is the unconstrained independent summation over the local discrete monopole charges Q_r at every single site, which we define as the local site action $M(\theta_r)$:

$$M(\theta_r) = \sum_{Q_r \in \mathbb{Z}} v Q_r^2 e^{iQ_r\theta_r}. \quad (34)$$

Because each diamond lattice vertex connects exactly four links, the local divergence Q_r is the algebraic sum of four spin variables. Even for half-integer spins, the sum of four half-integers is an integer, so $Q_r \in \mathbb{Z}$ for all S .

In the low-temperature regime $v \ll 1$, this sum is dominated by the fundamental monopole excitations $Q_r = \pm 1$. Truncating at leading order,

$$\begin{aligned} M(\theta_r) &\approx 1 + v e^{i\theta_r} + v e^{-i\theta_r} + \mathcal{O}(v^4) \\ &= 1 + 2v \cos(\theta_r) \approx \exp(2v \cos \theta_r). \end{aligned} \quad (35)$$

Taking the logarithm, we find that thermal monopoles generate a local sine-Gordon potential at every lattice vertex. For integer spins ($S \geq 1$), the effective action evaluates to

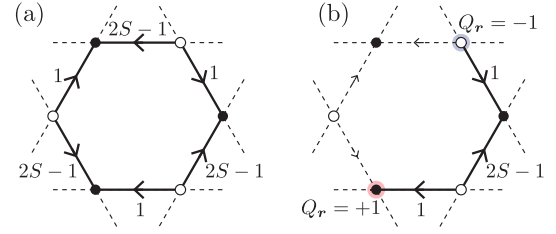


FIG. 5. Defect-string topology on the diamond lattice. Solid lines denote defect links carrying $\phi_\ell = 1$ or $2S-1$ (alternating with the sublattice convention); dashed lines denote vacuum links ($\phi_\ell = 0$ or $2S$); arrows indicate the bipartite $A \rightarrow B$ link orientation along which ϕ_ℓ is defined; open and filled circles denote A- and B-sublattice vertices. (a) At $v = 0$, defect strings form closed directed loops with $Q_r = 0$ at every vertex. (b) At $v > 0$, thermal monopoles ($|Q_r| = 1$) act as string end points, severing closed loops into open segments. The hexagonal loop is drawn schematically in two dimensions; on the actual lattice it is a chair-shaped six-membered ring.

$$S_{\text{eff}}[\theta] \approx -2w \sum_\ell \cos(\nabla\theta_\ell) - 2v \sum_r \cos(\theta_r). \quad (36)$$

The generated term $-2v \cos(\theta_r)$ acts as a uniform external magnetic field of strength $h \propto v$ applied along the $\theta = 0$ direction of the emergent 3D XY model. This field explicitly breaks the continuous U(1) symmetry and is a relevant perturbation that gaps the Goldstone modes and removes the thermodynamic singularity. Consequently, the 3D XY phase transition is rounded into a smooth crossover at any finite temperature $T > 0$ [18,23].

For half-integer spins ($S \geq 1/2$), where the unperturbed system resides in the U(1) Coulomb liquid phase, the effective action acquires the same term. This confirms the standard Debye-Hückel screening mechanism [29,53]: The monopole plasma introduces a screening length that exponentially cuts off the algebraic dipolar correlations, smoothly converting the Coulomb liquid into a trivial paramagnet without a phase transition.

B. Large- w regime: Generalized directed loop gas and topological string severing

We now symmetrically generalize the large- w directed loop-gas expansion to finite temperatures. The geometric consequence of thermally activating local monopoles ($Q_r \neq 0$) is that the defect strings are no longer topologically forced to form closed continuous loops. The directed strings can now terminate, creating open end points ∂G that correspond geometrically to the locations of the thermal monopoles [54,55] (Fig. 5).

The loop-gas partition function now expands over all directed graphs G on the diamond lattice, which include both closed loops and open string segments terminated by monopole end points. For $S \geq 3/2$, the end point vertex weight is computed as follows. At a monopole end point, one of the four links carries a fundamental defect ($\phi = 1$,

fixed), while the remaining three links are in the vacuum sector ($\phi \in \{0, 2S\}$). The monopole condition $\sum_{\ell \in r} \phi_\ell = 4S \pm 1$ (i.e., $|Q_r| = 1$) constrains how many of the three vacuum links carry $\phi = 2S$ versus $\phi = 0$. In the defect-free vacuum, each vertex has $\binom{4}{2} = 6$ valid ice-rule configurations (those with exactly two links at $\phi = 2S$ and two at $\phi = 0$). Of these 6 configurations, exactly $\hat{z}(1) = 3$ are compatible with one link being promoted to a defect while maintaining $|Q_r| = 1$ (see Sec. II of Supplemental Material [25]). The end point vertex weight is therefore $W_1 = \hat{z}(1)/6 = 1/2$. By the same normalization convention used for the junction and crossing weights ($\lambda_d = W_d/W_2^{d/2}$), the end point correction factor is $\lambda_1 = W_1/\sqrt{W_2} = (1/2)/\sqrt{1/3} = \sqrt{3}/2$. Including the monopole fugacity v , each end point contributes a factor $v\lambda_1 = \sqrt{3}v/2$, giving the generalized dilute loop gas partition function:

$$\frac{Z_{v>0}}{Z_{\text{vac}}} = \sum_{\{G\}} 2^{N_{\text{comp}}(G)} \tilde{x}_1^{|G|} \left(\frac{\sqrt{3}v}{2} \right)^{|\partial G|}, \quad (37)$$

where $|G|$ is the total number of edges, $|\partial G|$ is the number of monopole end points (string termination sites with $|Q_r| = 1$), and $N_{\text{comp}}(G)$ is the number of strands—both closed loops and open strings—each carrying two chiral orientations on the directed diamond lattice. This graphical expansion maps exactly to the high-temperature expansion of a classical O(2) (i.e., 3D XY) spin model in the presence of a uniform external magnetic field h . In the standard O(2) high-temperature expansion, an external field h assigns a weight $h/2$ to each string end point. Equating $h/2 = \sqrt{3}v/2$ immediately yields the effective field strength:

$$h_{\text{eff}} \approx \sqrt{3}v. \quad (38)$$

This result extends to $S = 1$ ($n = 1$, undirected loops mapping to the 3D Ising model). Unlike directed loops at $S \geq 3/2$, the $S = 1$ defect $S_\ell^z = 0$ is directionless: $\phi = 1$ is its own conjugate under $\phi \rightarrow 2S - \phi$, so a single defect link can terminate at either a $Q = +1$ or $Q = -1$ monopole. This doubles the valid vacuum configurations at each end point from $\hat{z}(1) = 3$ to $3 + 3 = 6$, and hence the end point weight from $W_1 = 1/2$ to $W_1 = 1$ (see Ref. [18] for the detailed $S = 1$ derivation). The resulting end point factor $\sqrt{3}v$ (doubled relative to the directed case $\sqrt{3}v/2$) precisely compensates for the halved magnetic coupling in the Ising convention [$\exp(h\sigma) \propto 1 + \tanh(h)\sigma$], yielding the same universal effective field: $h_{\text{eff}} \approx \sqrt{3}v$.

Thus, irrespective of S , thermal monopoles act as a uniform external magnetic field applied to the emergent gauge variables. This field severs the defect strings, allowing the confined topological loops to terminate in the bulk. The macroscopic flux quantization laws

established in Sec. III are thereby destroyed, rendering all topological sectors adiabatically connected [18,56].

C. Order-dependent fate of topological transitions

The thermodynamic consequence of this string-severing field depends on the order of the monopole-free phase transition. On the one hand, for continuous transitions ($S = 1$ and $S \geq 2$), any finite symmetry-breaking field conjugate to the order parameter destroys a second-order critical point [33,57]; the continuous deconfinement transitions are therefore rounded into smooth crossovers for any $v > 0$. On the other hand, for the first-order transition ($S = 3/2$), the situation is qualitatively different: Because the transition involves a discontinuous jump between two macroscopic minima separated by a free-energy barrier (driven by the relevant cubic invariant), a coexistence line is expected to persist under a weak symmetry-breaking field.

Therefore, the first-order transition unique to $S = 3/2$ is predicted to survive at finite temperatures as a genuine thermodynamic phase boundary [Fig. 1(b)]. The situation is analogous to the liquid-gas transition: At zero external field ($v = 0$), the free energy has two degenerate minima (ordered and disordered phases) separated by a barrier. A weak symmetry-breaking field ($v > 0$) tilts the free-energy landscape but cannot eliminate the barrier, so the coexistence line should persist. As the monopole fugacity v increases, the free-energy barrier shrinks and vanishes at a finite critical monopole density v_c , where the two minima merge into one. At this point, the first-order line terminates at a critical end point, analogous to the liquid-gas critical point and expected to belong to the 3D Ising universality class.

To estimate v_c , we extend the Bethe-Peierls analysis of Sec. VB by including the monopole-induced symmetry-breaking field h , which enters as $s = (e^h - 1)/(e^h + 2) = \sqrt{3}v/2$ [cf. Eq. (37)]. The external field modifies the cavity recursion to $r = e^h[(e^K r + 2)/(r + e^K + 1)]^b$, where the prefactor e^h biases the cavity message toward the field-favored state. The critical end point—the point at which the free-energy barrier just vanishes—is determined by three simultaneous conditions on the iterative map $g(r)$: (i) $g(r) = r$ (self-consistency of the cavity message), (ii) $g'(r) = 1$ (the ordered and disordered fixed points have merged, i.e., marginal stability), and (iii) $g''(r) = 0$ [the inflection point of $g(r) - r$ vanishes, signifying the disappearance of the intervening barrier]. These three equations for the three unknowns (K_c, h_c, r_c) can be solved in closed form, yielding $e^{K_c} = (\sqrt{33} - 1)/2$ and $h_c \approx 0.010$, corresponding to $v_c \approx 0.004$ or $T_c/J \approx 0.09$ (see Sec. VIII of Supplemental Material [25] for the complete algebraic derivation).

The small value of h_c reflects the weakness of the first-order transition at $q = 3$: Since $q = 3$ is the smallest integer for which the Potts model exhibits a first-order transition in

three dimensions, the free-energy barrier is intrinsically shallow and easily destroyed by a weak perturbation. Indeed, the Bethe-Peierls approximation systematically overestimates the barrier height because it neglects the long-wavelength fluctuations that further erode the shallow free-energy landscape. Monte Carlo simulations of the 3D three-state Potts model in an external ordering field on the simple cubic lattice [58,59] have established that the first-order coexistence line terminates at a critical end point in the 3D Ising universality class at a critical field $h_c = 7.75(10) \times 10^{-4}$ —more than an order of magnitude smaller than the Bethe-Peierls estimate $h_c \approx 0.010$. On the diamond lattice relevant to the present pyrochlore problem, where the lower coordination number ($z = 4$ vs $z = 6$) amplifies thermal fluctuations, the true critical field is expected to be smaller still.

This critical end point provides a distinctive experimental signature: In candidate $S = 3/2$ pyrochlore materials, the specific heat and susceptibility should exhibit Ising-like critical scaling at an isolated temperature, offering a direct thermodynamic probe of the underlying string-fusion physics. Notably, unlike the liquid-gas-type critical end points in conventional $S = 1/2$ spin ice, which require a finely tuned external magnetic field [8], this critical end point occurs at strictly zero external field. The symmetry-breaking field is intrinsically generated by the thermal monopole plasma, making the $S = 3/2$ pyrochlore spin ice a rare example of a system that spontaneously generates its own topological critical end point through thermal fluctuations alone.

VII. MONTE CARLO SIMULATIONS AT FINITE TEMPERATURE

To test the analytical predictions of the preceding sections at finite temperatures, we perform classical Monte Carlo simulations of the Hamiltonian Eq. (1) on finite pyrochlore lattices comprising $2N = 16L^3$ spins (where $N = 8L^3$ is the number of diamond-lattice vertices) and periodic boundary conditions. Throughout this section we fix $J = 1$ as the energy unit.

A. Simulation method

A standard Monte Carlo sweep consists of $2N$ single-spin heat-bath updates. After 10^6 thermalization sweeps, measurements are accumulated over 5×10^6 sweeps.

The primary thermodynamic observable is the specific heat per spin,

$$c := \frac{1}{2N} \frac{\langle E^2 \rangle - \langle E \rangle^2}{T^2}, \quad (39)$$

whose peaks trace the crossover scales. To unambiguously distinguish collective topological phenomena from noncooperative local single-ion physics, we systematically

compute the thermal occupancy fraction of each spin amplitude,

$$n_s := \frac{1}{2N} \sum_{\ell} \langle \delta_{|S_{\ell}^z|, s} \rangle, \quad (40)$$

i.e., the fraction of links carrying amplitude $|S_{\ell}^z| = s$, averaged over all $2N$ links and Monte Carlo configurations.

B. Integer spins ($S = 1, 2, 3$)

We compute the specific heat as a function of μ at low temperatures ($T = 0.2$) for $S = 1, 2$, and 3 with system sizes $L = 2, 4$, and 8 ; Figs. 6(a) and 6(b) show the results for $S = 2$ and $S = 3$, respectively. In all three cases, c exhibits prominent peaks whose positions are in reasonable agreement with the analytically predicted crossover scales $\mu = -T \ln w_{c1}$ and $\mu = -T \ln w_{c2}$, where w_{c1} and w_{c2} are the monopole-free critical fugacities estimated in Secs. IV and V, respectively. Notably, the peak heights do not diverge with increasing L , confirming that the monopole-free phase transitions are rounded into smooth crossovers at finite temperature, as predicted by the monopole-screening analysis of Sec. VI. For $S = 1$, the results are fully consistent with the detailed numerical study of Ref. [18], which demonstrated that the specific-heat peaks saturate to finite values in the thermodynamic limit and that the $\mathbb{Z}_2$ deconfinement transition (which maps onto the ice-VII to ice-X transformation in high-pressure water ice) is a continuous crossover driven by Debye-Hückel monopole screening.

For $S \geq 2$, in addition to the cooperative crossover peaks, the specific heat exhibits a broad secondary shoulder near $\mu \approx 0.1$, which is absent for $S = 1$ (because $S = 1$ hosts only two amplitudes, $|S_{\ell}^z| = 0$ and 1 , so no intermediate depopulation step exists). As established by the completeness argument of Sec. III, this feature does not correspond to an intermediate thermodynamic phase. Rather, it is a noncooperative *Schottky anomaly* driven by the single-ion anisotropy. The single-ion energy splitting between the two highest-amplitude states, $|S_{\ell}^z| = S$ and $|S_{\ell}^z| = S - 1$, is $\Delta E = \mu[S^2 - (S - 1)^2] = \mu(2S - 1)$. For $\mu > 0$, the maximal-amplitude state $|S_{\ell}^z| = S$ is the excited (higher-energy) state of this two-level system. Approximating this as an independent two-level system whose excited state $|S_{\ell}^z| = S$ is thermally depopulated as μ increases, the Schottky specific heat peaks at $\Delta E/T \approx 2.4$, yielding an estimated peak position $\mu_{\text{Schottky}} \approx 2.4T/(2S - 1)$. This analytical estimate accurately captures the position and the $1/(2S - 1)$ scaling of the secondary humps observed in the Monte Carlo data: As S increases, the hump shifts closer to $\mu = 0$ [Fig. 6(e)]. Furthermore, the explicitly computed microscopic spin occupancies n_s [Figs. 6(c) and 6(d)] reveal that this shoulder coincides precisely with the continuous thermal depopulation from the maximal-amplitude state $|S_{\ell}^z| = S$ ($n_S \rightarrow 0$) to the lower spin amplitudes

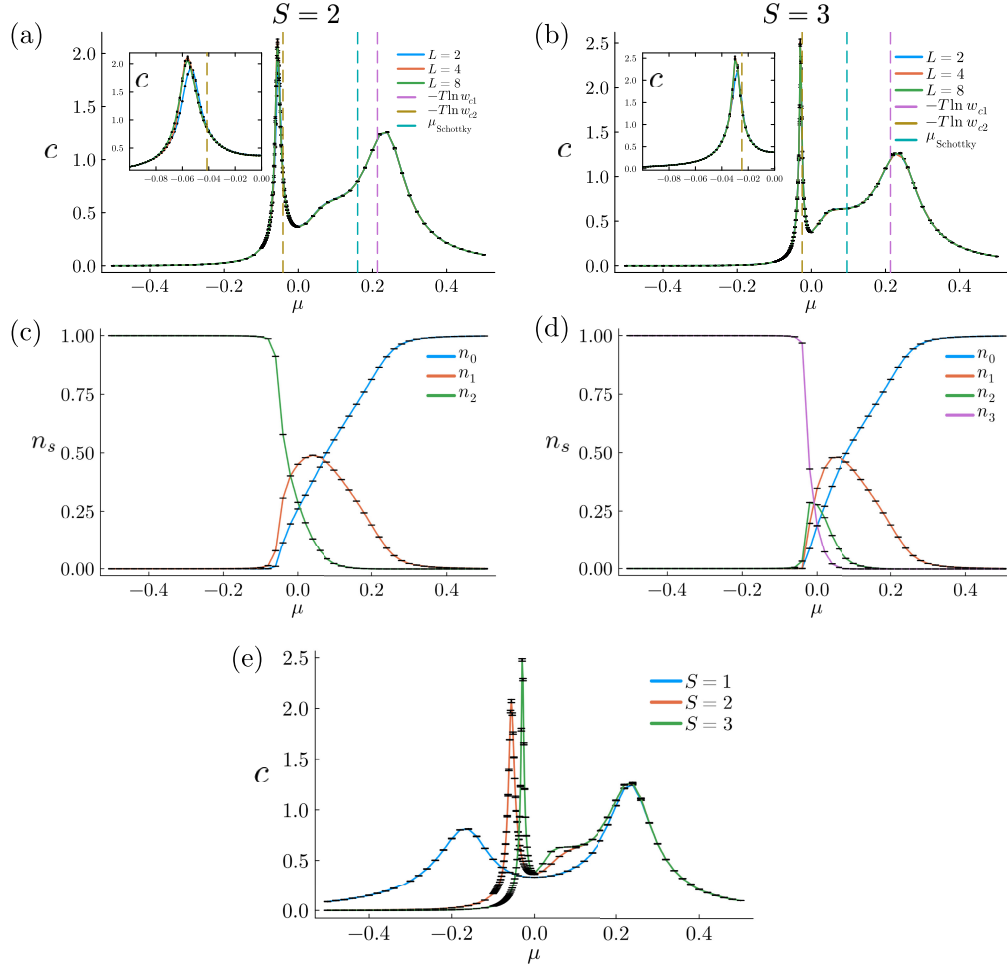


FIG. 6. Monte Carlo results for integer spins at $T = 0.2$ with $L = 2, 4, 8$; the exchange coupling is fixed to $J = 1$, and μ and T are quoted in units of J . (a),(b) Specific heat per spin c for $S = 2$ and $S = 3$; insets enlarge the $\mu < 0$ peak region. Vertical dashed lines mark the predicted crossover scales $-T \ln w_{c1}$ (purple) and $-T \ln w_{c2}$ (dark yellow) and the Schottky position $\mu_{\text{Schottky}} = 2.4T/(2S-1)$ (cyan). (c),(d) Thermal occupancy fractions $n_s = \langle \delta_{|S^z|,s} \rangle$ for $S = 2$ and $S = 3$ ($L = 8$). (e) Specific heat across $S = 1, 2$, and 3 ($L = 8$).

($n_{S-1} \rightarrow 1$). The absence of finite-size scaling for this shoulder, combined with the occupancy data, clearly decouples the local single-ion entropy release from the collective topological phenomena.

C. Half-integer spins ($S=3/2, 5/2, 7/2$)

For half-integer spins, the analytical framework of Sec. IV predicts no transition in the small- w regime because the half-integer link weights map directly onto the $S = 1/2$ Coulomb liquid. The only nontrivial topological crossover is therefore the large- w deconfinement crossover, whose monopole-free scale is set by $w_c \approx 1.44$ for $S = 3/2$ (our closed-form Bethe-Peierls estimate, Sec. VB; the transition point measured in Ref. [19] is $w_c \approx 1.42$) and $w_c \approx (1.859)^{1/(2S-1)}$ for $S \geq 5/2$ [Eq. (32)].

The Monte Carlo specific heat at $T = 0.15$ ($S = 3/2$) and $T = 0.2$ ($S = 5/2$) confirms this picture [Figs. 7(a) and 7(b)]: A sharp dominant peak associated with the topological

crossover appears near $\mu = -T \ln w_c$, and its height saturates with increasing L ; the corresponding peak for $S = 7/2$ at $T = 0.2$ is shown in Fig. 7(f) ($L = 8$). In the large-positive- μ (small- w) limit, where the single-ion anisotropy $\mu(S^z)^2$ confines every spin to its minimal doublet $S^z = \pm 1/2$, the model reduces to an effective $S = 1/2$ Ising spin ice whose exchange coupling is rescaled by $(1/2)^2 = 1/4$, yielding an effective temperature $T_{\text{eff}} = 4T$. The horizontal dashed lines in Figs. 7(a) and 7(b) show the specific heat of this effective $S = 1/2$ model computed independently, and the Monte Carlo data converge to these values at large μ for all half-integer spins, providing direct numerical confirmation of the effective Hamiltonian mapping. Furthermore, similar to the integer-spin case, a broader secondary hump is clearly visible on the large- μ side for all $S \geq 3/2$. As confirmed by the fractional occupancies n_s [Figs. 7(c) and 7(d)], which track the thermal depopulation cascade, this is the identical noncooperative Schottky anomaly driven by $\Delta E \sim T$. As predicted by our scaling formula

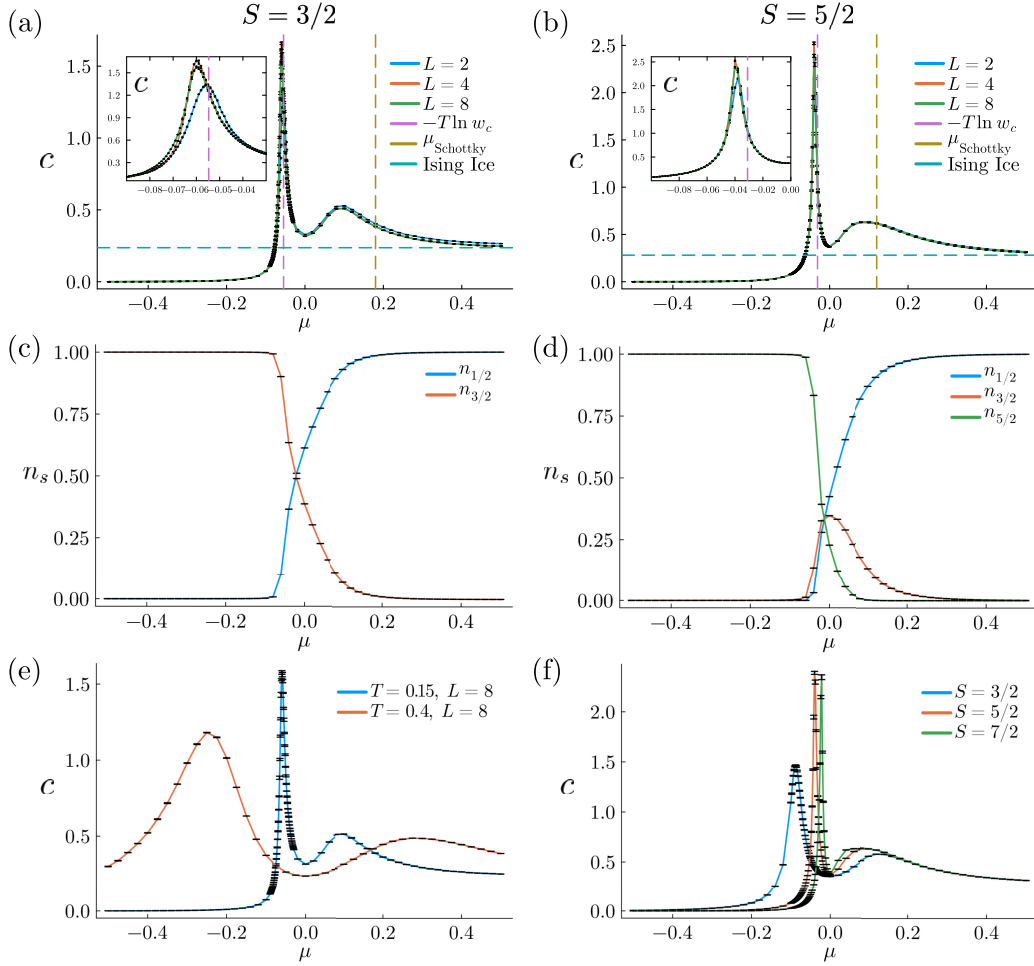


FIG. 7. Monte Carlo results for half-integer spins; the exchange coupling is fixed to $J = 1$, and μ and T are quoted in units of J . (a) Specific heat per spin c for $S = 3/2$ at $T = 0.15$ and (b) for $S = 5/2$ at $T = 0.2$, with $L = 2, 4, 8$; insets enlarge the peak region. Vertical dashed lines mark the predicted crossover scale $-T \ln w_c$ (purple; for $S = 3/2$, $w_c \approx 1.44$ from Table II) and the Schottky position μ_{Schottky} (dark yellow); the horizontal dashed line (cyan) marks the specific heat of the effective $S = 1/2$ Ising spin ice at $T_{\text{eff}} = 4T$. (c),(d) Thermal occupancy fractions n_s for $S = 3/2$ and $S = 5/2$ ($L = 8$). (e) The $S = 3/2$ specific heat at $T = 0.15$ and 0.4 ($L = 8$). (f) Comparison across $S = 3/2, 5/2$, and $7/2$ at $T = 0.2$ ($L = 8$).

$\mu_{\text{Schottky}} \approx 2.4T/(2S - 1)$, this Schottky peak gradually shifts toward $\mu = 0$ and merges with the topological crossover peak as S increases [Fig. 7(f)].

For $S = 3/2$, the monopole-free limit ($T/J \rightarrow 0$) predicts a first-order transition driven by the symmetry-allowed $\mathbb{Z}_3$ Potts cubic invariant. At the finite temperatures accessible to our simulations, however, the specific-heat peak shows no sign of thermodynamic divergence with L , and the energy Binder cumulant exhibits no negative dip characteristic of a first-order transition. This implies that the first-order coexistence line has either terminated at a critical end point below the simulated temperatures or that exponentially larger system sizes are needed to resolve a weakly first-order nature. Indeed, a comparison of the specific heat at $T = 0.15$ and $T = 0.4$ [Fig. 7(e)] reveals that while the peak sharpens upon cooling, it remains a crossover. Quantitatively, at

$T = 0.15$, the monopole fugacity $v = e^{-J/(2T)} \approx 0.036$ is an order of magnitude larger than the critical end point value $v_c \approx 0.004$ estimated from the Bethe-Peierls analysis in Sec. VI (see Sec. VIII of Supplemental Material [25])—and likely 2 orders of magnitude larger than the true lattice value, given that the Bethe-Peierls approximation overestimates h_c by more than a factor of 10 relative to the exact Monte Carlo result for the 3D three-state Potts model [58]. The simulation therefore unambiguously places the system well inside the crossover regime, confirming that thermal monopoles have completely washed out the macroscopic phase coexistence. We stress the corresponding limitation: Because all accessible temperatures lie above the estimated critical end point, the present simulations test the crossover regime but do not directly verify the predicted survival of the first-order line at lower temperatures.

Prompted by this limitation, we have additionally performed parallel-tempering simulations of the physical ($v > 0$) model at smaller anisotropies, for which the predicted transition temperature lies *below* the estimated critical end point; the question probed is not the existence of the first-order transition—established at $v = 0$ in Ref. [19]—but its predicted survival at $v > 0$. These runs show signatures consistent with a weakly first-order transition—a specific-heat peak that sharpens and grows with system size at the predicted location, a negative minimum of the energy Binder cumulant, and an incipient bimodal energy distribution—and the signatures become clearer as $\mu \rightarrow 0^-$, where the monopole fugacity at the transition is smaller. The finite-size hallmarks that would make the identification definitive are, however, not yet resolved at the accessible sizes; a conclusive test requires more sophisticated sampling and is left for future work.

We close this section by commenting on the prospects for simulating the monopole-free limit directly. For $S = 1/2$ spin ice, it is standard to sample the ice-rule manifold at $v = 0$ using nonlocal loop updates [9], and worm algorithms of exactly this type were used in Refs. [16,19] to map out the $v = 0$ phase diagram at $S = 1$ —including finite-size-scaling analyses consistent with the 3D XY and 3D Ising universality classes of the two transitions—and to establish the first-order transition at $S = 3/2$. The same strategy generalizes to arbitrary S : A worm-type update that shifts S_ℓ^z by ± 1 along a closed loop (respecting $|S_\ell^z| \leq S$) is ergodic within the ice-rule manifold. For $S \geq 2$, where our theory predicts 3D XY criticality at the couplings $w_c(S)$ of Eq. (32) and an S -independent small- w transition at w_{c1} for integer S , no such simulations have yet been performed; they would provide a direct test of these predictions and are deferred to a separate study. The finite-temperature fate of the $S = 3/2$ coexistence line near the predicted critical end point ($T/J \approx 0.09$, where $v \approx v_c$) could likewise be probed by loop-based sampling supplemented with monopole insertions.

VIII. EXPERIMENTAL OUTLOOK

Before concluding, we discuss experimental contexts for the model, Eq. (1), and for our predictions.

A. Higher-spin pyrochlore magnets

The single-ion term in Eq. (1) is not a theoretical idealization: The magnetic site of every pyrochlore magnet has D_{3d} point symmetry with its trigonal axis along the local $\langle 111 \rangle$ direction, so for any ion with $S \geq 1$, the leading symmetry-allowed single-ion anisotropy is precisely $\mu(S^z)^2$ with S^z along the local axis. Anisotropies comparable to the exchange coupling are documented on both sides of $\mu = 0$: Electron-paramagnetic-resonance measurements for the $S = 7/2$ gadolinium pyrochlores find an easy-plane single-ion term ($\mu > 0$) of about $0.75J$ in $\text{Gd}_2\text{Ti}_2\text{O}_7$ [60],

while for the $S = 3/2$ pyrochlore $\text{Cd}_2\text{Os}_2\text{O}_7$, an easy-axis term ($\mu < 0$) with $|\mu| \approx J$ has been obtained by *ab initio* quantum-chemistry calculations and adopted in the resonant inelastic x-ray scattering analysis of the magnetic excitations [61,62]. Higher-spin pyrochlore magnets now exist across the full range of spin values—most systematically in the fluoride family, which realizes effective $S = 1/2$ ($\text{NaCaCo}_2\text{F}_7$ [63]), $S = 1$ ($\text{NaCaNi}_2\text{F}_7$ [64]), $S = 2$ ($\text{NaCaFe}_2\text{F}_7$, $\text{NaSrFe}_2\text{F}_7$), and $S = 5/2$ ($\text{NaSrMn}_2\text{F}_7$) [65] on the same lattice [66]. We stress that none of these compounds is currently placed at the transitions studied here: The Ni and Mn members of the fluoride family are nearly Heisenberg-like (for $\text{NaCaNi}_2\text{F}_7$, polarized neutron scattering bounds the single-ion anisotropy to a small fraction of the exchange [67]), the single-ion anisotropy of the $S = 2$ iron members has not yet been determined experimentally, and materials with dominant easy-axis exchange typically sit deep inside one phase. Rather, the present model provides the organizing phase diagram for this growing materials landscape—with the canonical spin ices $\text{Ho}_2\text{Ti}_2\text{O}_7$ and $\text{Dy}_2\text{Ti}_2\text{O}_7$ occupying the extreme easy-axis limit $w \rightarrow \infty$, in which the crystal field isolates the largest- $|m_J|$ doublet—and identifies which single-ion parameters, tunable by chemical substitution, strain, or pressure, would drive a material across the crossover ridges—and, for $S = 3/2$, across the first-order line—classified here.

B. High-pressure ice

Outside magnetism, the $S = 1$ member of Eq. (1) describes the hydrogen-bond network of high-pressure water ice, with $S_\ell^z = \pm 1$ representing the two off-center proton positions on a hydrogen bond, $S_\ell^z = 0$ the bond-centered position, μ the pressure-tuned centering energy, and ionic defects ($\text{H}_3\text{O}^+/\text{OH}^-$) playing the role of monopoles. In this language, proton-disordered ice VII corresponds to the $\mathbb{Z}_2$ -confined Coulomb phase at large w , bond-symmetrized ice X to the trivial paramagnet at small w , and the monopole-induced rounding derived in Sec. VI explains why the ice VII–X transformation is observed as a broad, probe-dependent crossover rather than a sharp transition; a companion paper develops this application in detail [23]. Notably, the competition $\mu \sim J$ is realized there directly by the proton coordinate, without fine-tuning, and the isotope effect (H_2O versus D_2O) shifts the crossover pressure by about 10 GPa [68], making the model parameters experimentally scannable.

C. Engineered platforms

Blume-Capel ($S = 1$) degrees of freedom have recently been realized in an artificial nanomagnet array with lithographically tunable anisotropy [24], and programmable platforms—superconducting-flux-qubit annealers realizing artificial spin ice [69] and proposed three-dimensional

Rydberg-atom arrays on the pyrochlore lattice [70]—offer settings in which both fugacities w and v can, in principle, be controlled independently. The quantitative phase boundaries of Tables I and II and the predicted zero-field critical end point provide concrete targets for such platforms.

D. Measurable signatures

Three predictions of this work are directly testable. First, for $S = 3/2$ realizations, the first-order line should terminate at a critical end point at strictly zero external field, at which the specific heat and susceptibility exhibit 3D Ising critical scaling at an isolated temperature $T \lesssim J/10$ (Sec. VI). Second, the crossover ridges of the specific heat trace the straight lines $\mu_c = -T \ln w_c$ with the S -dependent slopes of Tables I and II (for $S = 1$ and $S = 3/2$, the corresponding experimental temperature scales were already emphasized in Refs. [16,19]). Third, the Schottky anomaly at $\mu_{\text{Schottky}} \approx 2.4T/(2S - 1)$ provides a practical protocol for separating single-ion features from the collective crossovers in candidate higher-spin pyrochlore magnets (Sec. VII).

IX. CONCLUSION AND OUTLOOK

In this work, we have developed a self-contained theoretical framework that classifies the macroscopic topological phases, emergent gauge theories, and critical phenomena of classical spin- S pyrochlore magnets for arbitrary S . The framework combines thermodynamic energy convexity, the microscopic lattice geometry ($z = 4$), exact graphical mappings, and RG analysis.

In the monopole-free limit, we established the completeness of the phase diagram: Uniform backgrounds of intermediate spin amplitude are excluded by the convexity of the single-ion energy, and partial-deconfinement scenarios are excluded by a free-energy comparison of the competing defect strings. A spin parity dichotomy emerges in the small- w limit: half-integer spins reduce to the divergence-free Coulomb fluid, whereas integer spins map onto the 3D XY model. In the large- w limit, we proved geometrically that the macroscopic polarization flux is quantized to multiples of $2S$, establishing an emergent $\mathbb{Z}_{2S}$ -confined Coulomb phase. The resulting classification in this limit is summarized in Tables I and II.

The nature of the deconfinement transitions reveals a further dichotomy. While $S = 1$ defects map to the 3D Ising class, all $S \geq 3/2$ defects generate chiral, directed loops. The ice-rule compatibility criterion shows that the $\mathbb{Z}_{2S}$ Gauss law is compatible with the physical ice rule at the vertex level if and only if $S \leq 3/2$. Exploiting this geometric property, we mapped the $S = 3/2$ defect gas to the three-state Potts model, whose symmetry-allowed cubic invariant drives a first-order transition.

For $S \geq 2$, this discrete clock mapping breaks down: The modular $\mathbb{Z}_{2S}$ conservation law is no longer equivalent to

the physical ice rule. The system is instead forced into hierarchical fusion processes with exponentially suppressed intermediate defects. Using a decomposition of the partition function, we showed that the macroscopic graph ensemble reduces to the continuous U(1) 3D XY model at leading order. The residual fusion cascade acts as a dangerously irrelevant operator at the 3D XY fixed point; its exponentially small bare weight places the system deep inside the basin of attraction of that fixed point, where its irrelevance fixes the universality class and guarantees an early onset of the asymptotic critical behavior, placing all $S \geq 2$ deconfinement transitions in the 3D XY universality class.

Finally, by relaxing the strict ice rules, we showed that thermally excited monopoles act as an explicit symmetry-breaking field $h_{\text{eff}} \approx \sqrt{3}v$ in the emergent gauge theory. This field severs the topological defect strings and renders all topological sectors adiabatically connected. The consequences are order dependent: The continuous 3D Ising ($S = 1$) and 3D XY ($S \geq 2$) transitions are rounded into crossovers for any $v > 0$, while the first-order $S = 3/2$ transition is predicted to survive at finite temperatures, protected by a macroscopic free-energy barrier, and to terminate at a critical end point. Classical Monte Carlo simulations for integer ($S = 1$ –3) and half-integer ($S = 3/2$ – $7/2$) spins confirm this crossover picture at the accessible temperatures: The specific-heat peaks saturate to finite values with increasing system size, and the crossover scales are in quantitative agreement with the analytically predicted fugacities. We emphasize, however, an important limitation of the numerical part of this work: The accessible temperatures lie above the estimated critical end point of the $S = 3/2$ coexistence line ($v \approx 0.036$ at $T = 0.15$, versus $v_c \approx 0.004$ from the Bethe-Peierls estimate), so the predicted survival of the $S = 3/2$ first-order transition—and, more generally, the universality classes of the monopole-free transitions—are not directly verified by the present simulations. Direct tests would require sampling the $v = 0$ manifold with loop algorithms, as discussed in Sec. VII, and constitute an important direction for future work. Preliminary parallel-tempering simulations at smaller $|\mu|$, reaching below the estimated end point, already show signatures consistent with the predicted survival (Sec. VII), though not yet its definitive demonstration. The spin-amplitude occupancies n_s further identify a noncooperative Schottky anomaly for $S \geq 2$, clearly separating local single-ion physics from collective topological phenomena. This clear decoupling, governed by the analytically predicted $1/(2S - 1)$ scaling of the Schottky peak position, provides a practical diagnostic for experimentalists seeking to disentangle broad specific-heat anomalies in candidate higher-spin pyrochlore magnets from the signatures of collective topological phenomena.

Extending this framework to the quantum regime is a natural direction for future work. The interplay between

quantum fluctuations, emergent discrete $\mathbb{Z}_{2S}$ gauge fields, and the geometric properties unique to $S = 3/2$ may give rise to novel fractionalized quantum spin liquids and higher-spin topological phases [2,30,71–74]. More broadly, the mechanism identified here—in which the microscopic real-valued constraint keeps the model $U(1)$ symmetric while the lattice geometry exponentially suppresses the processes that would single out a discrete subgroup—may apply to other frustrated lattice models where discrete gauge symmetries compete with continuous gauge symmetries, including dimer models on nonbipartite lattices and higher-rank tensor gauge theories.

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DATA AVAILABILITY

The data that support the findings of this study, including the Monte Carlo simulation data shown in Figs. 6 and 7, are available from the corresponding author upon reasonable request.

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