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Perfectly hidden order and \mathbb{Z}_2 confinement transition in a fully packed monopole liquid

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We investigate a simple variant of spin ice whose degenerate ground states are densely packed monopole configurations. An applied field drives this model through a \mathbb{Z}_2 confinement transition, in absence of any local order parameter. Instead, this hidden order turns out to be diagnosed by a string order *invisible to any local probe*. We describe the transition in terms of a bosonic field theory with a pairing term, as well as a Kramers–Wannier duality into a 3D Ising model, which establishes its \mathbb{Z}_2 nature. This topological transition can be thought of as a variant of the celebrated U(1) Kasteleyn transition; but instead of the traditional ‘3/2’-order kink, the system shows critical scaling expected near a 3D Ising transition. Remarkably, however, the magnetic response scales with the critical exponent not of the susceptibility, but of the *specific heat*.

Frustrated magnetism has proven a fertile ground to realize many-body emergent phenomena as yet unobserved in high-energy physics [1]. The fine structure constant of quantum electrodynamics can be tuned [2], electromagnetism can become tensorial [3], magnetic monopoles and Majorana fermions can be stabilized [4–7]. This is because spin-liquid ground states can often be described by a gauge field, offering a variety of vacua for unusual quasiparticles bearing a gauge charge. Being excitations, these quasiparticles are usually studied at low density, since increasing the temperature populates excited states at the cost of transforming the system into a trivial paramagnet.

Here, we consider the opposite case, analyzing a three-

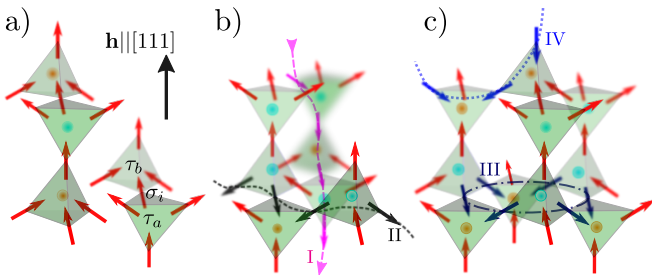


FIG. 1. (a) Ising pyrochlore lattice, saturated in a [111] magnetic field \mathbf{h} with single positive (orange) and negative (cyan) monopole charges, corresponding to configurations of 3 spins pointing in and 1 out, and vice versa. The centers of tetrahedra form a diamond lattice. Ising variables σ_i and τ_a sit respectively on the pyrochlore and diamond lattice. (b) When decreasing h/T , the system demagnetizes, constrained to retain a single charge in each tetrahedron. This may happen through string excitations spanning the whole system in any direction: for instance, strings I (magenta) and II (black) are respectively along and orthogonal to the [111] field direction. (c) Alternatively, finite loop excitations cost a finite energy and may appear at any temperature (III and IV).

dimensional spin-ice model with maximal monopole density [8–10]; in other words, a fully packed monopole liquid with a single-charge monopole at every lattice site (see Fig. 1). The presence of noninteracting monopoles does not introduce spin correlations, and offers a novel, constrained yet extensively degenerate set of magnetic configurations [8]. Very little is known about a dense liquid of gauge charges emerging from spin models.

We explore the phase structure of such a liquid when coupled to an external field \mathbf{h} . Despite the fact that the field completely lifts the monopole-liquid degeneracy in favour of a unique ground state, we show both analytically and numerically the presence of a topological transition. In particular, even though the monopoles are excitations of a U(1) gauge theory, this transition represents a rare example of \mathbb{Z}_2 (de)confinement in three dimensions (3D). We explain this connection from the co-existence of two types of excitations: (i) system-spanning strings, similar to those of the celebrated U(1) Kasteleyn transition [11–13], but running in *all* directions; and (ii) finite-size loops, present on both sides of the transition [14–16]. Remarkably, while this transition is driven by a magnetic field, its conjugate variable, the magnetization, and indeed any other local candidate order parameter, is smooth at the transition, making this an extreme example of hidden order [17–20].

Model.—We consider Ising spins $\mathbf{S}_i = \sigma_i \mathbf{e}_{\alpha(i)}$ on the pyrochlore lattice, where the \mathbf{e}_{α} point to the four local $\langle 111 \rangle$ easy-axis directions [21] and $\sigma_i = +1$ (–1) for spins pointing out of (into) “up” tetrahedra (see Fig. 1). The Hamiltonian is

$$\mathcal{H} = K \sum_t \sigma_1 \sigma_2 \sigma_3 \sigma_4 - \sum_i \mathbf{h} \cdot \mathbf{S}_i, \quad (1)$$

where t runs over all tetrahedra of the system, $\sigma_{1,\dots,4}$ are the four spins within each tetrahedron, and \mathbf{h} is the external magnetic field in reduced units. We shall work in the $K \rightarrow \infty$ limit, where every tetrahedron is in a “3-in-1-out” or “3-out-1-in” configuration, i.e., they host a single positive

or negative monopole, respectively. This defines the fully-packed monopole (FPM) model. A field applied along the [111] direction acts as a staggered field [22], distinguishing the sublattice $\alpha = 0$, whose spins are parallel to the field, from the other three, where $\mathbf{h} \cdot \mathbf{e}_\alpha = -1/3$; a strong field thus polarizes all spins to a unique monopole-crystal [23] ground state [Fig. 1(a)]. Along the field direction, the pyrochlore lattice can be seen as an alternating stack of triangular ($\alpha = 0$) and kagome ($\alpha = 1, 2, 3$) layers.

Simulations.—We simulated a system of rhombohedral shape with $N = 4L^3$ spins and periodic boundary conditions within each kagome layer and along the [111] direction [21], and developed a loop Monte Carlo algorithm [21, 24, 25]; non-local loop updates are necessary to move between the spin configurations compatible with the constraint imposed by $K \rightarrow \infty$. The magnetisation and heat capacity from these simulations are plotted in Fig. 2. The former appears very smooth and does not saturate at any finite field [Fig. 2(a)], although it does show non-analytic behaviour at a critical value of $x_c = h/T \approx 1.14$, as shown in the inset. Criticality at this point becomes manifest as a peak in the specific heat that grows with system size [Fig. 2(b)]. Remarkably, as the energy is entirely of Zeeman origin, the susceptibility also diverges *with the heat capacity critical exponent*. Our results show finite-size scaling consistent with the 3D Ising universality class (see insets).

Kramers–Wannier duality.—This behaviour suggests a second-order phase transition, in violation of the Landau–Ginzburg–Wilson paradigm. Since the magnetic field selects a unique ground state, the magnetization should either smoothly approach saturation or undergo a first-order transition. In the following, we explain this unconventional transition in terms of a duality, which gives rise to criticality with a nonlocal, topological order parameter [26].

For convenience, we flip the sign convention of all spins σ_i in the (111) triangular layers ($\mathbf{e}_0 \rightarrow \mathbf{e}'_0 = -\mathbf{e}_0$), such that the local fields favor $\sigma' = +1$ on every site and the $K \rightarrow \infty$ constraint requires an *even* number of $\sigma' = \pm 1$, corresponding to the eight-vertex model on the diamond lattice. The Hamiltonian (1) becomes

$$\mathcal{H}_0 = -K \sum_{\uparrow} \sigma'_1 \sigma'_2 \sigma'_3 \sigma'_4 - \sum_i h_i \sigma'_i, \quad (2)$$

where $h_i = h$ for spins in the triangular and $h/3$ in the kagome (111) layers. Now, we establish a Kramers–Wannier duality between (2) and the nearest-neighbor Ising ferromagnet ($\tau_a = \pm 1$) on the diamond lattice,

$$\mathcal{H}^* = - \sum_{\langle ab \rangle} J_{ab} \tau_a \tau_b, \quad (3)$$

where the diamond sites a, b are the tetrahedron centers of the original pyrochlore lattice [Fig. 1(a)]. Following Ref. [26], we consider the high-temperature expansion of (3) and the low-temperature expansion of (2). With N_τ diamond sites, the

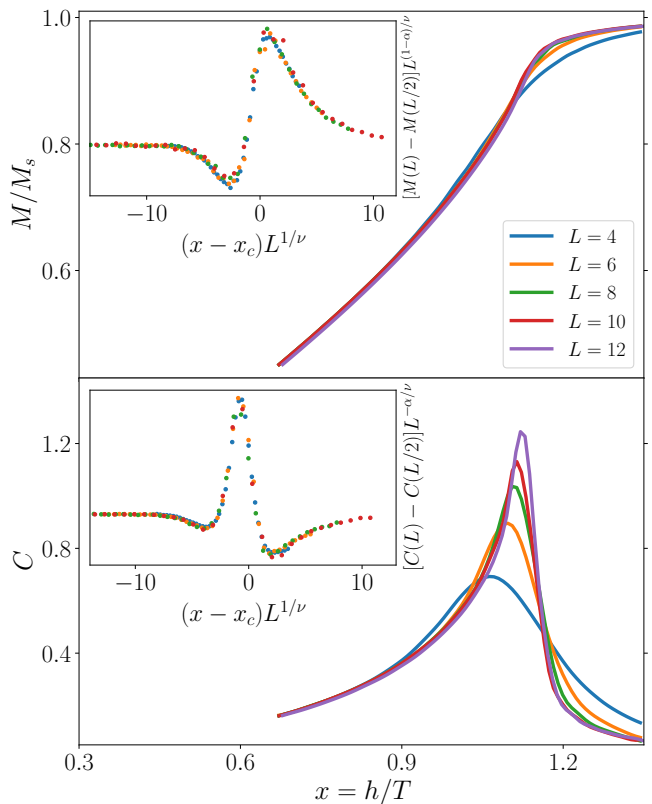


FIG. 2. Magnetization M (top panel) and specific heat C_h (bottom panel) as a function of $x = h/T$ for the FPM model in a [111] field. The heat capacity shows a diverging peak which obeys a finite-size scaling form with the critical exponents α, ν of the 3D Ising universality class (inset). The magnetic susceptibility is proportional to the heat capacity, so it diverges with the same exponents; therefore, the finite-size anomaly in the magnetisation scales with critical exponent $1 - \alpha$ (inset). To eliminate nonsingular contributions, finite-size scaling was performed on the difference between measurements at system sizes L and $L/2$, see [21].

former takes the form

$$\begin{aligned} Z^* &= 2^{N_\tau} \left\langle \prod_{\langle ab \rangle} e^{\beta J_{ab} \tau_a \tau_b} \right\rangle \\ &= 2^{N_\tau} \prod_{\langle ab \rangle} \cosh(\beta J_{ab}) \left\langle \prod_{\langle ab \rangle} [1 + \tanh(\beta J_{ab}) \tau_a \tau_b] \right\rangle, \end{aligned} \quad (4)$$

where the expectation value is taken over the infinite-temperature ensemble. Upon expanding the second product in the latter form, we get a term for every set of diamond-lattice bonds $\langle ab \rangle$ or, equivalently, pyrochlore sites i [Fig. 1(a)]. The expectation value $\langle \tau_a \tau_b \dots \rangle$ in these terms vanishes, unless every τ_a appears an even number of times. Therefore,

$$Z^* = 2^{N_\tau} \prod_i \cosh(\beta J_i) \sum'_{\{i\}} \prod_i \tanh(\beta J_i), \quad (5)$$

where the prime indicates that the sum is taken over all sets $\{i\}$ of pyrochlore sites i with an even number of them on each tetrahedron; in other words, all sets $\{i\}$ of closed loops on

the pyrochlore lattice. The eight-vertex constraint ($K \rightarrow \infty$) imposes the same structure on the low-temperature expansion of (2):

$$Z_0 = \prod_i e^{\beta h_i} \sum_{\{i\}} \prod_i e^{-2\beta h_i}. \quad (6)$$

Since $h_i > 0$, a Kramers–Wannier duality follows: if $\tanh(\beta J_i) = e^{-2\beta h_i}$, the partition functions of (2) and (3) are the same up to an overall analytic prefactor. Furthermore, as $J > 0$ on all bonds of the diamond lattice, the Hamiltonian (3) has a single ferromagnetic transition, which belongs to the 3D Ising universality class.

By duality, therefore, the transition in our FPM model (1) belongs to the same universality class, as confirmed by the finite-size scaling of magnetization and specific heat in the insets of Fig. 2. The high- and low- h phases are dual to the low- J paramagnet and the high- J ferromagnet, respectively.

Kasteleyn mechanism.—In the following, we show that this hidden Ising transition is in fact a \mathbb{Z}_2 topological variant of the Kasteleyn transition [11–16], i.e., it is driven by system-spanning strings of flipped spins.

Consider the [111] field-polarised state, in which each up (down) tetrahedron hosts a positive (negative) monopole. Conventional Kasteleyn transitions occur in systems with a zero-divergence constraint, e.g. in hard-core dimer models or emergent U(1) gauge theories [11, 13]. In our FPM model, this additional constraint would impose a local charge conservation on all tetrahedra [27]. The resulting elementary excitations would be system-spanning strings of spins along the [111] field direction [e.g., string I in Fig. 1(b)]. Such a string costs a Zeeman energy proportional to its length (the system size L). However, it also leads to an entropic gain proportional to its length, since it can enter each (111) kagome layer (sublattices $\alpha = 1, 2, 3$) in three different ways from the triangular layer ($\alpha = 0$) above it. In the thermodynamic limit, both terms diverge, but their ratio remains fixed; system-spanning strings are thus exponentially unlikely to appear at high field, resulting in perfectly saturated magnetization down to a finite value of $x \equiv \beta h = h/T$, followed by a sudden kink in the magnetization [11].

This picture of a standard Kasteleyn transition is, however, qualitatively incorrect in our case. The magnetization does not saturate at high fields and does not show such a “3/2-order” kink at the transition point (Fig. 2) [11, 28]. Furthermore, the entropy–energy balance argument given above leads to an estimate of the transition point at $x_K = (3/8) \ln 3 \approx 0.412$ [11, 21], very far from the numerically obtained $x_c \approx 1.14$.

The reason for this discrepancy is that in the FPM model, monopole charges are not locally conserved, only their *parity* is. Crucially, the $K \rightarrow +\infty$ limit in (1) is *not* a zero-divergence constraint, since flipping *any* two spins in a tetrahedron is allowed. This means that *any* closed loop of spins can be flipped without violating the constraint. For example, a system-spanning string entirely within a (111) kagome layer [string II in Fig. 1(b)] becomes flippable. Since the Zeeman energy of these spins is only a third of those in

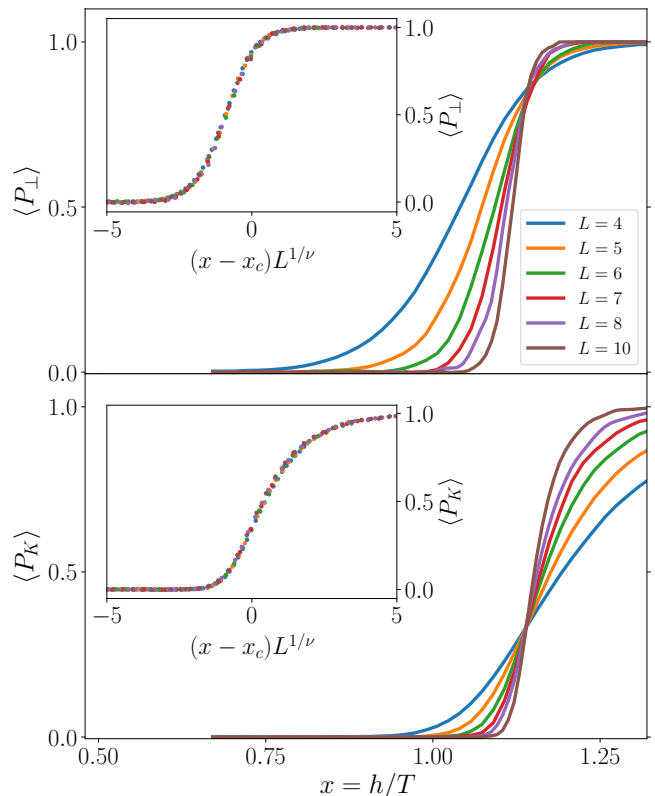


FIG. 3. \mathbb{Z}_2 topological order parameter $\langle P \rangle$ for the FPM model in a [111] field. The upper and lower panels show the order parameter for kagome planes respectively perpendicular, $\langle P_\perp \rangle$, and at an angle $\arccos(-1/3)$ to the [111] field, $\langle P_K \rangle$. The insets show the finite-size scaling with 3D Ising critical exponents; the best visual collapse is achieved at $x_c = 1.1415$.

triangular layers, they exhibit a Kasteleyn instability around $x'_K = (3/2) \ln 2 \approx 1.040$ [21], much closer to the numerical result.

Order parameters.—More importantly, we can also flip *closed* loops as short as six spins [e.g., loops III and IV in Fig. 1(c)]. Since their energy cost is finite, there is always a finite density of them at any temperature $T > 0$. This prevents the magnetization M from saturating in either phase, which is why M ceases to be a good order parameter. By contrast, the *parity* of flipped spins, $P = \prod_i \sigma_i$ in any (111) plane can only be changed by system-spanning strings; closed loops always flip an even number of spins in any (111) plane. Similar to the standard Kasteleyn transition, these strings are exponentially suppressed in the high- h phase, so $\langle P \rangle \rightarrow 1$ in the thermodynamic limit. Below the transition, the proliferation of strings causes $P = \pm 1$ to be equally likely, so $\langle P \rangle \rightarrow 0$. This expectation is confirmed by the Monte Carlo simulation results plotted in Fig. 3.

The model thus exhibits a \mathbb{Z}_2 topological version of the Kasteleyn transition [14, 15], with $\langle P \rangle$ as a strictly non-local order parameter. In fact, the Kramers–Wannier duality guarantees that the \mathbb{Z}_2 Kasteleyn transition does not have a lo-

cal order parameter, since correlation functions in one model correspond to the free energy cost of nonlocally deforming boundary conditions in its dual [26]. In particular, the topological order parameter $\langle P \rangle$ is equal to the ratio of the partition function of the dual model (3) with antiperiodic and periodic boundary conditions [21]. The paramagnet is insensitive to these boundary conditions, so the partition function in the thermodynamic limit is equal for both, leading to $P = +1$ in the dual high- h phase. By contrast, ferromagnetic ordering is frustrated by the antiperiodic boundary conditions, so $\langle P \rangle$ is suppressed exponentially in the low- h phase. Even if the system is anisotropic, this duality argument shows that $\langle P \rangle$ is a proper order parameter for all (111) planes, whether perpendicular to the field direction axis or not. We confirmed this using Monte Carlo simulations (Fig. 3).

Likewise, the ferromagnetic order parameter of the dual model (3) becomes a string order parameter upon the duality transformation:

$$\langle \tau_a \tau_b \rangle_{\text{dual}} = Z'_{ab} / Z = e^{-\beta F_{ab}}, \quad (7)$$

where Z'_{ab} is the partition function of (2) with two defects on tetrahedra a and b , where $\sigma'_1 \sigma'_2 \sigma'_3 \sigma'_4 = -1$ rather than $+1$. While this might appear local, inserting such a pair of topological defects requires flipping a string of spins between a and b . In the paramagnet, $\langle \tau_a \tau_b \rangle$ decays exponentially with the a - b distance: that is, the free-energy cost F_{ab} of the defects in the high- h dual phase grows linearly, i.e., they are confined. By contrast, $\langle \tau_a \tau_b \rangle$ tends to the magnetic order parameter in the ferromagnet, so in the dual low- h phase, their free-energy cost is finite at any separation. The \mathbb{Z}_2 Kasteleyn transition is thus a deconfinement transition of loops of flipped spins: In the high- h phase, their string tension (measured by F_{ab}) is finite, so only finite, closed loops are thermally allowed. Upon approaching the transition, this string tension vanishes, causing the size of the loops to diverge. This results in arbitrarily long strings, including system-spanning ones, proliferating at the transition, in agreement with the Kasteleyn argument explained previously.

Quantum-classical mapping.—We can also capture this transition using a field theory similar to the one developed for the Kasteleyn transition in Ref. [29], where strings of flipped spins are world-lines of hard-core bosons in (2+1)-dimensional spacetime, and the [111] field direction plays the role of imaginary time. However, the number of bosons (strings) is no longer conserved between imaginary-time slices: at the ends of closed loops (e.g., loop III in Fig. 1), they can be created or removed, but only *in pairs*, requiring pairing terms in the effective action. In terms of the boson field ψ , the most general quadratic Lagrangian thus reads

$$L = \sum_k \psi_k^* \partial_\tau \psi_k + r(k) \psi_k^* \psi_k + \frac{1}{2} [\Delta(k) \psi_k^* \psi_{-k}^* + \text{c.c.}], \quad (8)$$

which can be Bogoliubov transformed into

$$L = \sum_k \phi_k^* \partial_\tau \phi_k + \varepsilon(k) \phi_k^* \phi_k, \quad (9)$$

where $\varepsilon(k) = \sqrt{r^2(k) - \Delta^2(k)}$. For a gapped dispersion of $\varepsilon(k)$, finite loops may appear due to the pairing term, but none of these span the system so that the topological order parameter $P = +1$. The transition corresponds to $\varepsilon(k=0) \rightarrow 0$: $\phi_{k=0}$ condenses, and system-spanning loops appear. For generic dispersions $r(k), \Delta(k), \varepsilon(k) \propto |k|$ at the transition, so the dynamical exponent of the transition is $z = 1$, rather than the Kasteleyn value $z = 2$ [29]. More importantly, the action (9) and the Bogoliubov transformation from ψ to ϕ becomes nonanalytic, thus $\langle \phi \rangle$ becomes a hidden, nonlocal order parameter.

Discussion.—We have shown how a magnetic field can induce a \mathbb{Z}_2 topological phase transition in a variant of spin ice. It is an extreme case of hidden order: while the transition itself is detectable through a divergence in the heat capacity, there is no local order parameter to distinguish the two phases. We demonstrate these properties through a Kramers–Wannier duality with the diamond-lattice Ising ferromagnet. This duality shows that the topological transition belongs to the 3D Ising universality class.

Remarkably, a straightforward measurement of the magnetization in our model would find standard trappings of critical phenomena with scaling behavior etc. However, it would determine the critical exponent for the susceptibility to be that of the specific heat, $\alpha \approx 0.110$, rather than the susceptibility exponent of the Ising ferromagnet, $\gamma \approx 1.237$.

The duality also makes the hidden nature of the order explicit [26]; the conventional order parameter of the dual ferromagnet maps onto a string order parameter directly related to the tension of strings that drive the transition. System-spanning string excitations of flipped spins appear and proliferate at the transition; this can be thought of as a *deconfinement* transition of defects in the \mathbb{Z}_2 constraint, and is a rare example of a \mathbb{Z}_2 Kasteleyn transition. In contrast to its U(1) counterpart, the single-monopole constraint in our model allows for finite loops at any field strength, leading to a gradual approach to saturation. This is strikingly different to the U(1) Kasteleyn transition [13], where the local susceptibility can be used as a diagnostic of the high-field phase, throughout which it vanishes exactly, while it is nonzero at fields below the transition. As behooves a system with \mathbb{Z}_2 invariants, the order parameter is the parity of these system-spanning strings. The hidden nature of the order is a result of the intrinsic non-locality of this parity.

Years of research on spin-ice materials have brought to light a variety of mechanisms to stabilize gauge-charged excitations at low temperatures – magnetic field [30], further neighbor exchange [31, 32], magneto-elastic coupling [9, 33–35], material design [10, 23, 36, 37], etc. This, as well as progress in constructing constrained models on versatile AMO [38, 39] and NISQ [40, 41] platforms, makes us optimistic about a future experimental realization of our model. The present work is just one example of the rich physics that can arise in systems where emergent gauge charges are fundamental building blocks rather than rare excitations.

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