Equilibrium Field Theory of Magnetic Monopoles in Degenerate Square Spin Ice: Correlations, Entropic Interactions, and Charge Screening Regimes

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We describe degenerate square spin as an ensemble of magnetic monopoles coupled via an emergent entropic field that subsumes the effect of the underlying spin vacuum. We compute their effective free energy, entropic interaction, correlations, screening, and structure factors that coincide with the experimental ones. Unlike in pyrochlore ices, a dimensional mismatch between real and entropic interactions leads to weak singularities at the pinch points and algebraic correlations at long distance. This algebraic screening can be, however, camouflaged by a pseudo-screening regime.

Introduction. Magnetic monopoles provide an emergent description of the low energy physics of rare earth spin ices and have raised considerable interest, in particular in regard to “magnetricity”.

Spin ices can be modeled as systems of Ising spins on a pyrochlore lattice, impinging on tetrahedra, such that their low energy state obeys the Bernal-Fowler ice rule: two spins point in, two out of each tetrahedron, realizing a degenerate manifold of constrained disorder and residual entropy. Then, violations of the ice rule can be described in terms of mobile, deconfined, magnetic monopoles, interacting via a Coulomb law, in a disordered spin vacuum. Spin ice is thus a prominent platform in which monopole physics can be investigated.

While experimental probes of monopoles in crystalline spin ice are necessarily indirect and at low temperature, magnetic monopoles can now be characterized directly in real time, real space at desired temperature and fields in artificial spin ices. These 2D arrays of magnetic, frustrated nanosheets are fabricated in a variety of geometries, often for exotic behaviors not found in natural magnets.

Here we study the monopoles of degenerate artificial square ice recently realized in nanopatterned pyrochlores and in a quantum annealer. Square ice provides a direct 2D analogue of 3D pyrochlore spin ice where monopole excitations can be directly characterized. Heuristic field theories of rare earth pyrochlores have dealt only with the ice manifold, via a coarse grained, solenoidal field that describes the spin texture. We propose instead a framework where magnetic monopoles are the constitutive degrees of freedom, while the underlying spin ensemble is subsumed into entropic forces among these topological defects.

We show that, in absence of physical interaction, monopoles interact entropically via a 2D-Coulomb, logarithmic law, leading to (2 + 1) electromagnetism, Bessel correlations of finite screening length for $T > 0$, and thus a conductive phase where monopoles are unbound. The correlation length diverges exponentially as $T \downarrow 0$, signaling the criticality of the ice manifold. Then, inclusion of the monopole-monopole 3D-Coulomb interaction, leads, unlike in 3D spin ice, to algebraic correlations and weak singularities in the structure factor at $T \neq 0$. Its interplay with the entropic interaction drives screening regimes of effectively bound and unbound monopoles.

1. Field Theory. Square ice is a set of $N_e$ classical, binary spins $\vec{S}_v$ aligned on the edges $e$ of a square lattice of unit vectors $\hat{e}_1, \hat{e}_2$, of $N_v = N_e/2$ vertices labeled by $v$. The 16 spin configurations of a vertex are classified by 4 topologies as t-I, ..., t-IV (Fig. 1). Of each vertex, the charge $Q_v = 2n - 4$ is equal to the number $n$ of spins pointing in minus the $4 - n$ pointing out. Then, $Q = 0$ for ice-rule obeying vertices (t-I, t-II). The following

$$\mathcal{H}[Q] = \frac{\epsilon}{2} \sum_v Q_v^2 + \frac{k}{2} \sum_{v \neq v'} Q_v Q_{v'},$$

is a suitable Hamiltonian for a variety of square ice realizations. $\epsilon$ is the cost of monopoles and $V_{vv'} = \epsilon/(2\pi|v - v'|)$ is their 3D-Coulomb interaction; we take the lattice constant $a = 1$ and thus $\mu$ is an energy. When $\mu/\epsilon < 2\pi/M\Box \simeq 3.9$ (where $M\Box \simeq 1.6155$ is our Madelung constant) the ground state is a disordered tessellation of the six ice rule vertices (Fig. 1) of known Pauling entropy. Above that threshold, the ground state becomes unstable toward the formation of a monopole ionic crystal.

In magnetic realizations, Eq. (1) corresponds to the dumbbell model of ref2 (then $\epsilon$ is the coupling of the dumbbell charges in the vertex) with the 3D-Coulomb interaction comes from the usual truncated multipole expansion, and therefore $\mu = \mu_0 \epsilon^2/\ell^2$, with

![FIG. 1. Left: the four vertex configurations, ice-rule ones at the top (Q = 0) and monopole at the bottom (multiplicities in parenthesis). Right: portion of spin ice with monopoles of different charge circled.](image-url)
\( p \) the magnetic moment, \( l_d < a \) the dumbbell length. Then, \( \mu/\epsilon \simeq 1 - l_d/a < 1 \). Equation (1) does not describe the standard, non-degenerate square ice\(^{18,21,39-42}\) in which monopoles are confined by the tension of magnetic Faraday lines.\(^{43,47,48-45}\) Finally, even in realizations where ice-rule vertices are degenerate\(^{30-34}\), the long ranged dipolar interaction favors antiferromagnetic ordering\(^{32}\) at \( T \ll \epsilon \), an effect that we consider here elsewhere.

The partition function is

\[
Z[H] = \sum_q \exp \left( -\beta \mathcal{H} + \beta \sum_e \mathcal{S}_e \cdot \mathcal{H}_e \right), \tag{2}
\]

(\( \beta = 1/T \)) such that \( \langle \mathcal{S}_e \rangle = \partial \mathcal{R}_\mathcal{A} \mathcal{R}_n \ln Z \). To sum over the spins, we insert the tautology\(^7 \) 1 = \( \prod_v \int dq_v \phi_v \exp \left[ i \phi_v(q_v - Q_v) \right] / (2\pi) \) obtaining

\[
Z[H] = \int [dq] e^{-\beta \mathcal{H}[\phi]} \Omega[q], \tag{3}
\]

where \( [dq] = \prod_v dq_v / (2\pi)^N \), and the density of states

\[
\Omega[\phi] = 2^{N_v} \prod_{\langle vv' \rangle} \cosh (-i \nabla_{vv'} \phi + \beta H_{vv'}), \tag{4}
\]

is the Fourier transform of the partition function for \( \phi \)

\[
\Omega[\phi] = 2^{N_v} \prod_{\langle vv' \rangle} \cosh (-i \nabla_{vv'} \phi + \beta H_{vv'}), \tag{5}
\]

(edges \( \langle vv' \rangle \) are counted once, \( \nabla_{vv'} \phi := \phi_v - \phi_{v'}, H_{vv'} := \mathcal{H}_v \cdot \mathcal{H}_{v'} \)). By construction, \( \langle Q_v \rangle = \langle q_v \rangle \). We have obtained a theory of continuous charges coupled to an entropic field\(^{16} \) \( V_e = i T \phi \), of “free energy”

\[
\mathcal{F}[\phi] = -T \ln \Omega[\phi]. \tag{6}
\]

From Eqs. (3-5) we have

\[
\langle S_{vv'} \rangle = \langle \tanh (\beta H_{vv'} - i \nabla_{vv'} \phi) \rangle, \tag{7}
\]

implying that while \( V_e = i T \phi \) correlates charges, \( B_e = i T \nabla \phi \) correlates spins that would be trivially paramagnetic in its absence. Note that \( \nabla_{vv} \phi := \langle V_v \rangle = i T \langle \phi \rangle \) is real\(^7\). In fact, standard Gaussian gymnastics\(^7\) shows

\[
\begin{align*}
\nabla_{vv} \phi &= \mu \pi \sum_{\alpha=x,y} \frac{\bar{q}_{\alpha}}{|v - v'|} \\
\bar{q} &= \sum_{\alpha=x,y} \partial \tanh (\beta \partial_\alpha V_e - \beta H_\alpha),
\end{align*} \tag{8}
\]

with the second equation following from the definition of \( \Phi \) and from Eq. (7) in the continuum limit.

2. Approximations. Eqs. (8) allow to compute the charge under boundary conditions in various approximations. For \( \mu = 0 \) their linearization returns screened-Poisson equations for \( q, V_e \), of screening length

\[
\xi_0 = \sqrt{\epsilon / T}. \tag{9}
\]

(A similar screening length had been found in different geometries via other methods\(^9,48,49\), and, we show elsewhere, holds for a general graph\(^7 \). ) This approximation corresponds to a high \( T \) limit. From Eqs. (3,4), by integrating over \( q \), one obtains \( \langle q^2 \rangle \simeq \epsilon / T \); as \( T \) increases the system loses correlation and the entropic field decreases.

We can therefore legitimately expand \( \mathcal{F}[\phi] \) in small \( \phi \). Then, Fourier transforming on the Brillouin Zone (BZ)\(^{49}\), we obtain the approximate partition function

\[
Z_{\text{eff}} = \int [dq d\phi] \exp \left( -\int_{\text{BZ}} \beta \mathcal{F}_{\text{eff}}[q, \phi](\mathbf{k}) \frac{d^2 \mathbf{k}}{(2\pi)^2} \right), \tag{10}
\]

of free energy functional at second order

\[
\mathcal{F}_{\text{eff}}[q, \phi] = \frac{\epsilon + \mu \tilde{V}}{2} |q|^2 + \frac{T}{2} \gamma^2 |\tilde{\phi}|^2 - iT \tilde{q} \tilde{\phi} \tag{11}
\]

\[
- \tilde{\phi} \gamma \cdot \tilde{H} - \beta \frac{T}{2} |\tilde{\mathbf{H}}|^2,
\]

where \( \gamma = \frac{2 \sin (k_a / 2)}{\tilde{V}(\tilde{k})} is the Fourier transform of \( V \) on the lattice. Integrating \( Z_{\text{eff}} \) over \( \phi \) returns the effective free energy for monopoles

\[
\mathcal{F}_{\text{eff}}[q] = \frac{1}{2} \left( \epsilon + \mu \tilde{V} + \frac{T}{\gamma^2} \right) |q|^2. \tag{12}
\]

The last term implies an entropic interaction among charges that at large distances \( (\gamma^2 \simeq k^2) \) is i.e. 2D-Coulomb. Instead, from Eq. (12) the entropic interaction would be 3D-Coulomb, or \( \sim 1/r \); thus merely altering the coupling constant \( \mu \to \mu + T \) of the real interaction, as indeed found numerically\(^{50,51}\). A charge assignment changes the degeneracy of the spin configurations compatible with it and thus the entropy. That the change in entropy can be written as the sum of pairwise logarithmic interactions is not obvious.

Equation (12) implies the charge correlations in \( k \) space

\[
\langle \tilde{q}(\tilde{k}) | \langle \tilde{q}(\tilde{k})^2 = \gamma^2 |\tilde{k}|^2 \phi_{\|}(\tilde{k}) \tag{14}
\]

with \( \phi_{\|}(\tilde{k}) \) given by

\[
\phi_{\|}(\tilde{k}) = \frac{1}{\xi_0^2} - \frac{\xi_0^2}{\gamma^2} \left[ 1 + \frac{\mu}{\epsilon} \tilde{V}(\tilde{k}) \right]. \tag{15}
\]

Note that \( \langle |\tilde{q}(\tilde{k})|^2 \rangle \) peaks on the \( K \) points of the BZ. These peaks diverges when \( \mu \uparrow (2\pi / M_c)(\epsilon + T / 8) \), signaling the aforementioned instability toward an ionic crystal of \( \pm 4 \) monopoles.\(^{52}\) Note also that \( \langle q^2 \rangle = \int_{\text{BZ}} \langle |\tilde{q}(\tilde{k})|^2 \rangle d^2 \mathbf{k} / (2\pi)^2 \uparrow 4 \) as \( T \uparrow \infty \), which is correct, as it can be verified by considering only vertex multiplicities \((2^2 / 2 + 4^2 / 8 = 4)\).

By performing the integral in Eq. (10) we obtain

\[
\ln Z_{\text{eff}} = \frac{1}{2} \left( \beta \mathcal{H} \right) \cdot \left( \tilde{\gamma} \phi_{\|} + \frac{1}{\gamma} \frac{\partial}{\partial \phi_{\|}} \phi_{\|} \right) \cdot \left( \beta \mathcal{H} \right) \tag{16}
\]
(\hat{\gamma} := \frac{\gamma}{\gamma}, \check{\gamma} := \hat{\gamma}_3 \wedge \hat{\gamma})$, showing that \( \hat{\chi}_l(k) \) is the longitudinal susceptibility (multiplied by \( T \)). Thus,

\[
(\hat{S}_\alpha(k)\hat{S}_{\alpha'}(\check{k})) = \hat{\gamma}_\alpha \hat{\gamma}_{\alpha'} \hat{\chi}_l + \check{\hat{\gamma}}_\alpha \check{\hat{\gamma}}_{\alpha'}, \tag{17}
\]

are the spin correlations, whose structure factor \( \Sigma_m(k) := \frac{1}{2} \cdot \hat{\bar{S}}(k) \hat{S}(k) \cdot \check{k} \) we plot in Fig. 2. In the limit \( T \downarrow 0 \) and thus \( \epsilon_0 \uparrow \infty \), correlations in Eq. (17) become purely transversal. When \( T > 0, \mu = 0 \), pinch points are smoothened by a Lorentzian of width \( \xi \). Instead, for \( \mu \neq 0 \) the profile is sharper, with weak singularities controlled by the Bjerrum length \( 2l_B := \mu/T \),

\[
\Sigma_m(2\pi, k_y) \approx 1 - 2b|k_y| \quad \text{at} \quad k_y \approx 0, \tag{18}
\]

due to the aforementioned dimensional mismatch.

To gain insight on how to proceed at low \( T \), one can perturbatively expand \( \hat{F}[\phi] \). Instead, we make the reasonable ansatz that the effective theory has the same functional form as \( \hat{F}_{eff} \) in Eq. (12) but with constants “dressed” by the interactions among fluctuations at low \( T \). Note that \( \epsilon_0 \uparrow \infty \) as \( T \downarrow 0 \) and Eq. (14) implies

\[
\epsilon_0 \approx 1/\sqrt{(q^2)} \quad \text{for} \quad T \downarrow 0, \tag{19}
\]

and therefore \( \epsilon \) is dressed as \( \epsilon \rightarrow \epsilon(T) \sim T/(q^2) \). Then, if we approximate \( \langle q^2 \rangle \) by assuming uncorrelated vertices, we obtain \( \epsilon_0 \approx \exp(\epsilon/T) \). This exponential divergence of the correlation length (consistent with experimental findings\(^{54}\)) points to the topological nature of the critical ice manifold at \( T = 0 \). Note that \( \epsilon_0 \) in Eq. (19) is exactly the Debye-Hückel\(^{55}\) length for a Coulomb potential of coupling constant proportional to \( T \), as is the case of the entropic potential. In Supp. Mat.\(^{7}\), a Debye-Hückel\(^{50,56}\) approach inclusive of the entropic field\(^{40}\) leads to the very Eq. (13) yet with \( \epsilon_0 \) given by Eq. (19), corroborating our ansatz.

When \( \mu = 0 \), Eq. (12) reduces to a 2D Coulomb gas and from Eq. (14,15) the charge correlations at large distance are

\[
\langle q_{r_1}q_{r_2} \rangle \approx -\frac{1}{2\pi \epsilon_0^2} K_0(\|r_1 - r_2\|/\epsilon_0), \tag{20}
\]

as recently experimentally verified\(^{34}\), showing that \( \epsilon_0 \) is indeed the correlation length. \( \epsilon_0 \) is also the screening length: a charge \( Q_{\text{pin}} \) pinned in \( v_0 \) elicits a charge

\[
\bar{q}_v = Q_{\text{pin}}(q_{v_0})/\langle q^2 \rangle. \tag{21}
\]

A finite screening length implies that the system is conductive. There is no BKT transition\(^{35,57}\) to an insulating phase (i.e., algebraic correlations, bound charges) because the interaction among charges is purely entropic, has coupling constant proportional to \( T \), and thus no interplay between entropy and energy can drive a transition. The lack of such transition can be shown in general from the model, regardless of our formalism.\(^{57}\) Yet, when \( \mu > 0 \) the system is always insulating, as we show now.

3. Monopole Interactions and Algebraic Correlations. Consider now \( \mu > 0 \). At small \( k \), \( V(k) \sim 1/k \) and Eq. (21) reads

\[
\bar{q}(k) \approx \frac{k^2}{1 + 2l_Bk + \epsilon_0^2k^2} \frac{Q_{\text{pin}}}{\langle q^2 \rangle}, \tag{22}
\]

which is not analytical at \( k = 0 \), leading to the aforementioned weak singularities at the pinch points. In 3D it would be analytical, because \( V(k) \sim 1/k^2 \), the poles of \( \bar{q}(k) \) would be purely imaginary \(|k_\pm = \pm i/\xi_3\) with \( \xi_3 = \epsilon_0^{-2}(1 + \mu/T) \), and thus \( \xi_3 \) would be a screening length. But in 2D the poles are \( k_\pm = -k \pm i/\xi_\mu \) with

\[
\frac{\xi_\mu^2}{\xi_0^2} = \frac{\xi_0^2 - l_B^2}{T - T_x} = \frac{T}{T - T_x}. \tag{23}
\]

and they always have a real part \( \bar{k} = l_B/\xi_0^2 = \mu/2\epsilon \).

Above the crossover temperature \( T_x = \mu^2/4\epsilon \), \( \xi_0 > l_B \), \( \xi_\mu \) is real, and poles have imaginary parts \(|q_\mu|\). Thus, one could heuristically consider \( \xi_\mu \) a screening length, and above \( T_x \) monopoles are unbound, and the phase is conductive. Below \( T_x \), \( \xi_\mu \) is imaginary, and one could say that there is no screening length, and monopoles are bound by the strength of the magnetic interaction \((\xi_0 < \xi_\mu) \).
l_B), in an insulating phase. However, things are more complicated than this naive picture.

In fact, mathematically speaking, there is never a finite screening length. To demonstrate it, consider a charge \( Q_{\text{pin}} \) pinned in the origin. From Eqs. (12,13), \( V_c(k) = Tq(k)/k^2 \), and thus we obtain

\[
\beta V_c(k) = \frac{\xi_\mu}{2k_0^2} \left( \frac{1}{k - k_+} - \frac{1}{k - k_-} \right) Q_{\text{pin}}. \tag{24}
\]

Using \( 2/c = \int_0^\infty \exp(-|z|c)dz \) for \( R(c) > 0 \) on each fraction in Eq. (24) and Fourier transforming, we have

\[
\beta V_c(r) = \frac{l_B}{2\pi (q^2)} \int_{-\infty}^{+\infty} \frac{\lambda(z)}{(r^2 + z^2)^3/2}dz \tag{25}
\]

where \( \lambda(z) \) can be interpreted as a linear charge density

\[
\lambda(z) = \frac{\xi_\mu}{2k_0^2 l_B} |z| \sin(|z|/\xi_\mu) e^{-k_0 |z|} Q_{\text{pin}}, \tag{26}
\]

for which \( \int \lambda(z)dz = Q_{\text{pin}} \). Therefore, the entropic potential can be represented as if generated by an image charge\(^\dagger\), spread along a line (of coordinate \( z \)) perpendicular to the 2D system, and of total charge \( Q_{\text{pin}} \).

Crucially, \( \lambda(z) \) is exponentially confined by a length \( l \). When \( T > T_x, l = 1/k_+ \). When \( T < T_x \), the sine in Eq. (26) becomes hyperbolic and \( l = 1/k_+ \). For \( r \gg l \) the charge is seen as point-like, the potential scales as

\[
V_c(r) \simeq \frac{l_B}{2\pi (q^2)} \frac{Q_{\text{pin}}}{r^3}, \tag{27}
\]

and, by taking its Laplacian, \( \overline{\nabla}^2(r) \) scales as

\[
\overline{\nabla}^2(r) \simeq -\frac{9l_B}{2\pi (q^2)} \frac{Q_{\text{pin}}}{r^5}. \tag{28}
\]

Remarkably, long distance screening—and thus spin correlations—are algebraic at any \( T \) (Fig 3a,b). In 3D spin ice, instead, spin correlations are only at \( T = 0 \), even with monopole interaction. Algebraic screening from a 3D-Coulomb potential in the polarizability of quantum or classical 2D charge systems has been rediscovered multiple times\(^\ddagger\)\(^\ddagger\). In fact, it is not merely a 2D feature, but can happen in any dimension for the same dimensional mismatch in the Coulomb interaction\(^2\). Importantly, unlike electrical charges, magnetic monopoles are emergent particles of a spin ensemble, and interact entropically. The interplay between the correlation length at zero interaction (\( \xi_0 \)) and the Bjerrum length \( (l_B) \) leads to a crossover at \( T_x \) between effectively conductive and insulating regimes.

To see that, consider

\[
Q_{\text{alg}}/Q_{\text{pin}} \simeq -3l_B/(q^2)^3, \tag{29}
\]

the fraction of the charge screened algebraically, obtained by integrating Eq. (28) for \( x \gg l \). When it is very small, and \( l \) is large, the algebraic nature of the screening might not be detectable.

When \( T \gg T_x \), \( Q_{\text{alg}}/Q_{\text{pin}} \simeq 10^{-2} \) or less, and thus the algebraic screening might not be experimentally detectable. Moreover, as Fig 3c shows, the screening within \( l \) is well fitted by an exponentially screened function. Above \( T_x \), there is a “pseudo screening length” \( \xi_\mu > l_B \).

When \( T \ll T_x \) we can take \( k_+ \approx 0 \) and from Eq. (24)

\[
V_c(k) \sim 1/k, \quad \text{and thus } \overline{V}_c(r) \sim 1/r \quad \text{for } r \ll l = 1/k_+ \quad \text{(as confirmed by the numerical plot in Fig 3b). In this regime the insulating phase is easily detectable.}
\]

Considering \( l, T_x, \) and \( Q_{\text{alg}} \), we can sketch heuristic regime diagrams, which are necessarily somehow arbitrary as they depend on practical specifications. Clearly, when \( l \) is smaller than, say, 2 the behavior is completely algebraic. When \( l \) is instead large, there might be pseudo-screening for \( x < l \) if \( T > T_x \) and if most (we choose 99\% in figure) of the charge is screened within a radius \( l \) (left side of the dashed line in Fig. 4). If \( l \gg 2 \) and \( Q_{\text{alg}}/Q_{\text{pin}} \)
FIG. 4. Heuristic regime diagram. The solid line is $T_x(\mu)$. The dashed line corresponds to 99% of the charge being screened within the radius $l$. On the right of the dotted line, $l \leq 2$ and there is therefore \textit{algebraic} screening, $\langle q(r)q(0) \rangle \sim r^{-3}$. On the left of the dashed line 99% of the charge is screened within $l$, and, because $T > T_x(\mu)$, the regime is \textit{pseudo screened}. In the \textit{pseudo screened}, \textit{then algebraic} regime the behavior is effectively screened for $x < l$ but more than 1% of the charge is algebraically screened at $x > l$. In the \textit{double algebraic} region $\langle q(r)q(0) \rangle \sim r^{-3}$ for $x < l$ and $\langle q(r)q(0) \rangle \sim r^{-5}$ for $x \gg l$. Note that in nanomagnetic realizations the dumbbell model imposes $\mu/\epsilon < 1$.

is not small, an initial exponential screening for $r < l$ is followed by algebraic screening for $r \gg l$. Finally, note that $\epsilon$ gets dressed at low temperature. At low $\mu/\epsilon$, the algebraic screening might be extremely hard to detect.

\textbf{Conclusion.} We have developed a field theory for monopoles in degenerate square ice. In absence of a real monopole interaction the system is a 2D-Coulomb gas where monopoles interact entropically, are always screened, and thus in an unbound, conductive phase. This case has been recently realized in quantum dots\textsuperscript{34}. When the 3D-Coulomb interaction among monopoles is considered, reduced dimensionality prevents full screening, and a dimensional mismatch between Green functions of the Laplace operator drive different effective screening regimes.

Our results, obtained via approximations on a simplified mode, invite experimental tests which are however non-trivial: the algebraic behavior can be camouflaged by pseudo-screening if the monopole-monopole interaction is small, and detection might require large real-space characterization. Algebraic correlations might be experimentally detectable in weak singularities near the pinch points, from which the Bjerrum length can be extracted.

In the future, more precise expressions for various quantities can be computed by Feynman diagram expansion of $F[\phi]$. The spirit of our approach can be applied also to 3D spin ice and to honeycomb/Kagome spin ice\textsuperscript{18,62}, and can be extended to include topological currents beside charges, thus underscoring the gauge-free duality of the square geometry.

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