Dumping topological charges on neighbors: ice manifolds for colloids and vortices

Cristiano Nisoli
Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA
E-mail: cristiano@lanl.gov and cristiano.nisoli@gmail.com

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Abstract
We investigate the recently reported analogies between pinned vortices in nanostructured superconductors or colloids in optical traps, and spin ice materials. It has been found experimentally and numerically that both colloids and vortices exhibit ice or quasi-ice manifolds. However, the frustration of colloids and vortices differs essentially from spin ice at the vertex level. We show that the effective vertex energetics of the colloidal/vortex systems is made identical to that of spin ice materials by the contribution of an emergent field associated to the topological charge of the vertex. The similarity extends to the local low-energy dynamics of the ice manifold, where the effect of geometric hard constraints can be subsumed into the spatial modulation of the emergent field, which mediates an entropic interaction between topological charges. There, as in spin ice materials, genuine ice manifolds enter a Coulomb phase, whereas quasi-ice manifolds possess a well defined screening length, provided by a plasma of embedded topological charges. We also show that such similarities break down in lattices of mixed coordination because of topological charge transfer between sub-lattices. This opens interesting perspective for extensions beyond physics, to social and economical networks.

Keywords: spin ice, frustration, optically trapped colloids, superconductive vortices, statistical mechanics
1. Introduction: (artificial) frustrated materials

A recent multidisciplinary effort in the creation and study of artificial frustrated nano-materials [1–37] has provided mesoscale realizations accessible to direct visualization. These systems have led to the exploration of new of exotic states [20, 21, 27, 28, 38], including dynamics of magnetic charges and monopoles [39]. While these results suggest possible applications to superconductivity, sensing, and information storage, they more importantly represent an attempt to design, rather than discover, desired emergent phenomena in the low-energy physics of interacting meso-structures, whose realization is now afforded by recent advances in synthesis and integration.

Among these materials, the so-called artificial spin ice [9, 11] has now reached a certain maturity and has attracted physicists from a variety of backgrounds [11]. The system is composed of magnetically interacting nano-structures that behave as single-domain macrospins. Their mutual geometric arrangement can be engineered and underlies potential emergence from their low-energy collective behavior. Thus, although devised initially [9, 10] as a mesoscale analogue of the frustration of natural pyrochlore magnets [40], artificial spin ice has then raised its own interesting issues. There is now growing awareness that this kind of program might lead to a bottom-up engineering of new magnets with desired emergent properties, whose functional units could be delocalized monopolar degrees of freedom, rather than the localized dipolar magnetic domains of nature-given materials.

Proposals for realizations of frustrated analogues of spin-ice materials are not, however, limited to magnetic systems. In numerical works, Libal et al have proposed systems of colloids held in place by elongated optical traps arranged along the sides of a two-dimensional (2D) lattice (typically square [3], or hexagonal). Each trap has a double-well potential forcing the colloids to be in the proximity of one of the two vertices connected by the trap (figure 1). When Brownian dynamics is performed on these systems they obey the ice rule (for a square lattice) or quasi-ice rule (for an hexagonal lattice) in the strong interaction regime. While the same ice rule has also been observed in natural and artificial spin ice materials, its origin is different, as we shall see.
The ice rule has also been proposed, by the same authors, in the context of pinned quantum vortices [4, 8] in properly nano-structured superconductors, and unsurprisingly so. Clearly the model is the same: whether colloids or vortices, we have in both cases certain objects subjected to hard constraints (a link with half occupation) and repulsive interactions, which are the strongest in the vertices on which the links impinge.

Some of these predictions were recently realized experimentally [6, 7]. Naturally, research in pinning superconductive vortices to a substrate nano-patterned with holes had been conducted since the late 1970s [41] with the goal of increasing critical currents. Latimer et al., however, arranged the pinning with the intention of reproducing the frustration of an ice-like material [6]. They fabricated superconducting thin films of MoGe containing pairs of circular holes arranged as in figure 1: a square lattice whose vertices can accommodate in principle four vortices each. Then, if the applied magnetic field is at half the matching value, only half of the holes are occupied. They found that at each vertex only two holes are occupied, and two are not, following the ice rule, as predicted numerically [4].

These most interesting results need now to be placed on some more solid theoretical footing. First of all one immediately notices that the models of Libal, Olson, Reichhardt and collaborators are over-constrained compared with the experimental realization of Latimer et al: in the latter there are no semi-occupied link-shaped traps and the vortices can simply pin to the holes in a ratio of vortices to hole dictated by the field (here, as in their work, we consider that ratio to be $\frac{1}{2}$). More relevantly, it cannot be escaped that while an ice manifold appears both in colloids/vortex systems and in magnetic spin ice materials, its origin is rather different because the energetics and frustrations involved are different.

In this paper we discuss similarities and differences between these systems and (artificial) spin ice. We investigate when, why, and how colloids/vortices can access an ice manifold, and when their ice manifold disappears. We show how their collective behavior leads to an effective energetics that replicates the energetics of spin ice materials. This is obtained by including an emergent field conjugated to the topological charge of the vertex. We then investigate spatial modulations, and we show that the equivalence extends to the low-energy physics above the ice manifold, where the emergent field mediates an entropic interaction between topological charges. Similar to spin ice materials, the ice manifold (for lattices of even coordination) is in a Coulomb phase, whereas the quasi-ice manifold (for lattices of odd coordination) possesses a finite screening length provided by its overall neutral plasma of embedded charges. Finally, because the similarity between the two models is a consequence of conservation of topological charge, we show that it breaks down in lattices of mixed coordination. There, a net transfer of topological charge between differently coordinated nodes must occur—something inherently impossible in magnetic spin ice materials [30, 31]. We also hint at extensions to networks and trees, which might be relevant in social settings, and on which we will report elsewhere.

2. Scalar constraint: ice manifolds

The ice rule is so named because in water ice each oxygen atom sits at the center of a proton-sharing tetrahedron. Two protons are close and covalently bonded to the oxygen, whereas the two others are close to a neighbor. The resulting 2-in/2-out ice rule thus originates in the stoichiometry of water. Famously, Pauling showed [42] the exponential freedom in choosing
configurations within the ice manifold allows it to retain a finite density of residual entropy at very low temperatures, thus explaining the zero-point entropy of water ice.

In spin ice materials (natural [40] or artificial [11]) protons are replaced by classical macrospins, and the ice rule (two spins pointing in, two spins pointing out for a \( z = 4 \) coordination lattice [9, 11, 40]) or quasi-ice-rule (1-in/2-out, and 2-in/1-out for \( z = 3 \) lattices [11, 15, 24]) is dictated by minimization of the frustrated energies of the vertices. Thus, for (artificial) spin ice, it is the pairwise interaction between nearest-neighbor spins converging in the same vertex that is frustrated. Indeed, if one describes these material in terms of a vertex-model [43, 44], as is often done [15, 16, 18, 30], then the ice-rule vertices have the lowest energy. Instead, the frustration of colloidal systems presented by Libal et al is of the emergent kind, a collective effect of the entire lattice.

2.1. Nature of the constraints

The model of Libal et al for colloids and vortices is over-constrained compared to the experiment of Latimer et al for vortices. In the experiment of Latimer et al, where holes are nano-patterned in a MoGe thin film, at half matching field only half of the holes are pinning a vortex. This introduces a scalar constraint on the total number of pinned vortices. With respect to this experimental reality, the systems typically studied by Libal, Olson, Reichhardt and collaborators introduce an additional, geometric hard constraint: each vertex of the lattice is connected by links, and each link contains only one colloid/vortex, which can occupy only the extremities. Obviously this geometric hard-constraint implies the scalar constraint whereas the opposite is not true. For instance, in the experimental arrangement it is not impossible for two neighboring vertices to both harbor \( z \) colloids \(^1\) without violating the half-occupation constraint —unfavorable energetics notwithstanding—yet the same is ‘kinematically’ forbidden in the linked models considered by Libal and collaborators.

We show here that the ice rule follows simply from the scalar constraint that enforces half-occupation only—which is why it is observed in Latimer’s experiment [6]. In section 3 we will show that the stricter, hard constraint implied by links is instead responsible for emergent interactions between topological charges.

2.2. Mean field

Consider a lattice of vertices connected by links with coordination \( z \). On each link sits a colloid (or a vortex) which can only occupy the extreme ends (figure 1). This situation reproduces the system treated numerically in [3, 4, 8]. The colloids (or vortices) considered in these works repel each other, via screened Coulomb (or modified Bessel) interaction. We assume that these objects repel each other with an energy \( \mathcal{E} \), and we neglect interactions between colloids belonging to different nodes, thus treating the system as a vertex-model\(^2\). Then, since each node can have \( n = 0, 1, \ldots, z \) close colloids, we can write

\(^1\) \( z \) being the coordination of the lattice.

\(^2\) Numerical results have shown that the ice manifold emerges in regimes in which the screening length of colloids or the London penetration length is much smaller than the lattice constant [3, 4].
\[ E_n = \frac{\mathcal{E}}{2} n(n - 1), \]  

(1)

for the energy of such configurations, each of multiplicity

\[ m_n = \binom{z}{n}, \]  

(2)

where \( \binom{z}{n} \) is the binomial coefficient. The reader might have already spotted an imperfection in our treatment. Equation (1) fails to describe non-symmetric interactions in the vertex, which are typical for instance of the square geometry. We discuss this point later, and for the moment we ask the reader to bear with us.

The first thing to notice is that while our system is analogous to a spin ice material with spins directed along the links and pointing toward the colloid (figure 1), the energetics of (1) differ completely from the frustrated energetics of spin ice. In fact, it is not frustrated at all: very simply, objects repel each other, and the lowest, and unfrustrated, vertex configuration corresponds to all the colloids (or all but one) being happily pushed away, and dumped on neighbors. However, such configuration of minimum energy obviously cannot be achieved by all vertices (nor most vertices) of the lattice. Therefore for colloids, unlike spin ice materials, the pairwise interaction is not frustrated; rather it is the allocation of all vertices in their lowest energy state that is frustrated.

The frustration is thus of the emergent kind. In spin ice, because of the protection afforded by time reversal symmetry, this kind of emergent frustration that pertains to the allocation of the vertex topology can only happen in dedicated and non-trivial geometries, such as those introduced by the author and collaborators [30, 31], and recently realized experimentally [38]. Instead, in trivial geometries, degeneracy in spin ice follows from a pairwise frustrated energetics that is already degenerate at the vertex level: so much so that Pauling’s famous estimate of the residual entropy of ice [42], which applies just as well to the 2D ice [43, 44] and hexagonal ice [45, 46], was based solely on vertex degeneracy, and disregarded completely the mutual arrangement of vertices. And indeed in artificial spin ice the ice rule is accessed even by disjointed vertices and clusters, as shown experimentally [13], something that would not happen for colloids on finite and disjointed clusters of traps.

We will start with a mean field approximation that disregards any correlation between vertices and thus neglects the geometric constraints implicit in the analyzes of Libal et al but describes well the experiment of Latimer.

We introduce \( \rho_n \), the probability of any node to be in the \( n \)-configuration, corresponding to \( n \) close colloids. The ‘free energy’ of an uncorrelated gas of nodes is thus [15, 16, 18]

\[ f = \sum_{n=0}^{\infty} \left( E_n \rho_n + T \rho_n \ln \frac{\rho_n}{m_n} \right) - \kappa \left( \sum_{n=0}^{\infty} \rho_n - 1 \right), \]  

(3)

where the entropy is chosen as the number of ways in which the distribution of vertex types can be realized, via any process that returns a consistent and unbiased statistical ensemble: the Lagrange multiplier \( T \) can thus represent an effective [15–19] or real [21, 22] temperature; \( \kappa \) simply enforces normalization of the probability.

Unlike in spin ice, to derive predictions directly from (3) we need to enforce the scalar constraint. Clearly, the inclusion of the geometric hard constraints implied by Libal’s systems is a rather serious matter, with which we will deal later. However vertex-frustration follows in fact
already from the simpler scalar constraint present in Latimer’s experiment: the conservation of colloids/vortices in the graph, which describes the inability to collectively dump them on neighbors. To establish the similarity with spin ice materials, it is useful to introduce the topological charge associated to the configuration \( n \). This is given by

\[
q_n = 2n - z, \tag{4}
\]

which is zero for the ice-rule \( n = z/2 \): for spin ice \( q_n \) is in fact the magnetic charge of the vertex. Then, the scalar constraint dictates that any distribution \( \rho_n \) must neutralize the average charge, or \( Q = \sum_{n=0}^{z} q_n \rho_n = 0 \), which in turn implies \( \bar{\rho} = \sum_{n=0}^{z} n \rho_n = z/2 \).\(^3\) In fact we can request \( Q + Q^e = 0 \) if an excess charge \( Q^e \) is doped extensively into the system by adding or subtracting colloids to the links, or by changing the magnetic field for vortices.\(^4\)

To include the scalar constraint, we minimize

\[
f_{\text{tot}} = f + \phi \left( \sum_{n=0}^{z} q_n \rho_n + Q^e \right), \tag{5}\]

where \( \phi \) is at this point simply a Lagrange multiplier ensuring charge neutralization/conservation. For fixed \( \phi \), minimization with respect to \( \rho_n \) and \( k \) returns the usual Boltzmann distribution

\[
\rho_n = \begin{pmatrix} z \end{pmatrix}_{n} \exp \left( \frac{-E_n^\phi}{T} \right) / Z(T, \phi), \tag{6}\]

\(^3\) This simply means that the ice rule is obeyed on average. It is not obvious that it should be obeyed at each vertex.

\(^4\) We need to open a brief parenthesis on the excess charge. It will be used in the following sections, yet needs to be included in the formalism since the beginning (the reader can skip this paragraph at the first reading). In these colloids/vortices systems charge can be added or subtracted with relative ease. This is, by contrast, much harder to implement in lithographically nano-patterned artificial spin ice, whereas interestingly itinerant or localized defects can be present in natural pyrochlore magnets (see [47] and references therein) as well as in water ice [48]. In the case of hard constraints, if an extra colloid is added (or subtracted) to a link, the link contains two (or zero) colloids rather than one, and is thus saturated (or empty). The situation does not appear as completely symmetric, since the two colloids in a link repel each other. If colloids are absolutely prevented to hop from link to link, the extra energy does not act on any of our degrees of freedom. However, one can imagine that extra colloids can in fact hop—at least to a degree. When the extra energy from the inter-link interaction inside a saturated link is comparable to the energy barrier to escape the link-trap, a colloid might then hop out of the saturated link into a nearby link. At the same time one can tune the traps such that a colloid in a half occupied link can hop into an empty link, while it cannot hop into another half occupied link because of the resulting repulsion from the colloid already present. One sees how the system can be engineered to have either mobile, positive excess charges or mobile positive and negative excess charges, something inherently impossible in spin ice materials. For pinned vortices in superconductors patterned with holes the situation is much easier: excess charge simply corresponds to tweaking the magnetic field around the half matching value. In particular in experimental realizations [6, 7] there are no hard constraints and all the charge (not only excess charge) is always mobile. As we will see in following sections, extensive doping of charge can break the ice manifold; non-extensive doping simply leads to local screening effects. In this section however we will consider \( Q^e = 0 \).
in the new, effective energies \( E_n^{\phi} \) given by
\[
E_n^{\phi} = E_n + q_n \phi. \tag{7}
\]
Note that in (7) the value of the energy is offset by what appears as an ‘electrostatic’ contribution from \( \phi \), which now looks suspiciously like an emergent field (albeit spatially uniform, as there is no space variable yet) coupled to the topological charge \( q_n \). When dealing with the hard geometric constraint and its effect on spatially modulated probabilities, we shall see that \( \phi \) indeed deserves the title: if allowed to fluctuate in space, we will see that, it mediates entropic interactions.

The partition function in (6) is given as usual by
\[
Z(T, \phi) = \sum_{n=0}^{z} \exp \left( -\frac{E_n^{\phi}}{T} \right), \tag{8}
\]
and \( \phi \) is found via \( \partial \phi_{\text{tot}} = 0 \), which can then be written as
\[
Q + Q^e = -T \partial \phi \ln Z(T, \phi) = 0. \tag{9}
\]
Solving (9) determines \( \phi \) and therefore, through (7), also \( \rho_n \) in (6), thus closing the problem. From (9), in general \( \phi \) depends on \( T \)—which is indeed always the case for graphs of mixed coordination, or when \( Q^e \neq 0 \) as we will see below. However, for a lattice of single coordination and \( Q^e = 0 \) (no extensive doping), it is immediate to realize that the following temperature-independent choice
\[
\tilde{\phi} = \frac{(1 - z)}{4} \mathcal{E}, \tag{10}
\]
solves the problem of ensuring charge neutralization at any temperature. Indeed, from (10) and (7) we find
\[
E_n^{\tilde{\phi}} = \frac{E_n + E_{\mathcal{E} - n}}{2} = \frac{\mathcal{E}}{8} \left[ q_n^2 + z(z - 2) \right]. \tag{11}
\]
The last equality in (11) establishes an ice-like energetics in the absolute value of the topological charge, essentially identical to that of spin ice materials, which ensures \( Q = 0 \) at any temperature. Thus the collective effect of the lattice is subsumed into a vertex description, courtesy of an emergent ‘field’ that offsets the purely interactive energy by taking into account the constraint of charge conservation.

It is now useful to relabel nodes in terms of charge \( q \) from (4) rather than colloids \( n \). From (11) and (6) we have \( \rho_q = \rho_{-q} \); from this energetics, at low temperature the system crosses over to a manifold containing only the vertices of lowest charges. For even \( z \), for which vertices of \( q = 0 \) are allowed when \( n = z/2 \), the system enters a low temperature, genuine ice manifold (figure 2). For odd \( z \) the lowest effective vertex-energy pertains to charges \( q = \pm 1 \), corresponding to \( n = (z \pm 1)/2 \). Then at low temperature the system enters a quasi-ice manifold: as the odd coordination prevents charge cancellation at the vertex level, the quasi-ice manifold is a plasma of embedded charges \( q = \pm 1 \), represented in equal proportion [4, 8].
2.3. Fits of numerical results

Although our results were obtained simply by imposing the scalar constraint of topological charge cancellation, interestingly they can be used to fit the strongly constrained model of Libal et al. The authors of these works considered two cases, the hexagonal and square lattice.

Applications involving 2D hexagonal lattices \( z = 3, d = 2 \) fall directly into our framework. In figure 2, right panel, we plot data obtained from simulated Brownian dynamics of a superconductive vortex system (figure 4(b) in [4]) versus the predictions of (6). The data pertains to different lattice constant measured in multiples of the London penetration depth \( \lambda \).

As the effective \( \mathcal{E}/T \) for the repulsive interaction of vortices scales with the modified Bessel function \( K_1(a/\lambda) \), where \( a \) is the lattice constant, we plot the frequencies obtained numerically by Libal et al versus \( aK_1(a/\lambda) \), where \( a \) is a fitting parameter. We found very good agreements with our predictions for \( a = 950 \). Black squares (circles) represent frequencies of vertices with charge \( q = +1 \) (black, solid), \( q = +3 \) (red, dotted) are plotted against numerical data for the square colloidal lattice obtained by Libal et al [3], for vertex populations corresponding to \( n = 2, q = 0 (\bullet), n = 1, q = 2 (\triangledown), n = 0, q = 4 (\bullet), n = 4, q = 0 (\blacksquare) \).

Insets: the screening length as a function of \( E/T \) showing the exponential divergence (left) corresponding to the ice manifold.

\[ \text{Figure 2.} \text{ Left: for } z = 4, \text{ relative vertex frequencies } \rho_q \text{ as a function of } E/T \text{ as in (6) for } q = 0 (\text{black, solid}), q = \pm 2 (\text{red, dotted}), q = \pm 4 (\text{blue, dashed}), \text{ are plotted against numerical data for the square colloidal lattice obtained by Libal et al [3], for vertex populations corresponding to } n = 2, q = 0 (\bullet), n = 1, q = 2 (\triangledown), n = 0, q = 4 (\bullet), n = 4, q = 0 (\blacksquare). \]

\[ \text{Right: for } z = 3 \text{ relative vertex frequencies } \rho_q \text{ as a function of } E/T \text{ as in (6) for } q = \pm 1 (\text{black, solid}), q = \pm 3 (\text{red, dotted}) \text{ are plotted against numerical data for the hexagonal superconductive vortex system of Libal et al [4], for vertex populations corresponding to } n = 1 (\bullet), n = 2 (\blacksquare), n = 3 (\triangledown), n = 0 (\bullet). \]

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Applications involving 2D hexagonal lattices \( z = 3, d = 2 \) fall directly into our framework. In figure 2, right panel, we plot data obtained from simulated Brownian dynamics of a superconductive vortex system (figure 4(b) in [4]) versus the predictions of (6). The data pertains to different lattice constant measured in multiples of the London penetration depth \( \lambda \).

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energetics in (1). However, considering the scope of our current analysis, to proceed here along that route would not be particularly illuminating. Indeed the interesting physics of this ordering pertains to the formation of domain walls in the ordered phases—which can have two different ‘orientations’ [3, 17]—as well as the out-of-equilibrium issues related to their motion, which has been used to address more general and quite interesting issues of grain boundary dynamics. However, these predictions on local behavior would escape our mean field approach anyway. Moreover our scope is to analyze similarities between ice systems, and therefore we concentrate on a model that can access degenerate and thus genuine ice manifolds rather than ordered phases. Relevantly, there are many ways in which the degeneracy of the ice manifold can be maintained even in a square lattice, for instance the proposal of Möller [34].

Even disregarding the possible symmetry breaking within the ice-manifold, our treatment still predicts correctly the average frequency of ice-rule vertices. Figure 2, left panel, demonstrates this by plotting data points for Brownian dynamics of colloids (figure 2(a) in [3]), grouped by topological charge, versus $E/T$. Black circles denote ice-rule vertices, of charge $q = 0$ and thus $n = 2$. Red triangles pointing down (up) represent frequencies of vertices with charge $q = +2, (q = -2)$ or $n = 3 (n = 1)$. Blue squares (diamonds) represent frequencies of vertices with charge $q = +4, (q = -4)$ or $n = 4 (n = 0)$. Solid lines are predictions obtained from (6) for $q = 0$ (black), $q = \pm 2$ (red) $q = \pm 4$ (blue).

We have shown that although the frustration in pinned vortices is of the emergent kind and thus differs essentially from that of spin ice materials, their behavior can be seen as controlled, at least in a mean field treatment, by a similar, effective energetics, which adds to the actual energetics the contribution of an emergent ‘field’ $\phi$ associated to the topological charge. This (quasi) ice rule is a consequence of the scalar constraint on charge conservation (and thus average half filling) of which $\phi$ is simply the Lagrange multiplier. Indeed we will show in section 4 that the ice manifold is lifted by charge transfers. In the next section we will show that in the case of hard geometric constraint provided by links, the analogy can be pushed to the low energy dynamics of the ice manifold.

3. Geometric constraint: emergent interactions

Lest the reader grows rightfully annoyed at the author for calling an ‘emergent field’ what is simply a uniform Lagrange multiplier, we show how $\phi$, when allowed to fluctuate in space, can provide information on the low-energy dynamics and local perturbations, as a field should.

Below we extend the formalism to a linked lattice such as the ones employed by Libal and coauthors in their simulations. There, unlike in Latimer’s experiment, a vertex can only give or take colloids/vertices to its nearest neighbors with which it is linked in a pairwise fashion. Clearly this geometric hard constraint introduces a spatial modulation within the ice manifold that cannot be described by the spatially averaged $\rho_n$ introduced so far.

3.1. Spatial modulation

We have seen how the vertex energies in (7) are modified by a uniform ‘electrostatic’ contribution $q_n \phi$: this suggests that entropic interactions might be mediated by a spatially modulated field $\phi(x) = \bar{\phi} + \psi(x)$, where $\bar{\phi}$ from (10) enforces the ice rule while its fluctuating part $\psi(x)$ perturbs the local effective energetics. For a spatially varying probability $\rho_n(x)$ (the probability of a node in position $x$ to be in configuration $n$), the intuitive generalization of (6)
should then allow for a non-uniform field $\phi$ in (7), and thus non-uniform probabilities $\rho_n(x)$, in the form

$$
\rho_n(x) = \left( \frac{z}{n} \right) \exp \left\{ - \left[ E_n^\phi + q_n \psi(x) \right] / T \right\} / Z(T, \phi).
$$

(12)

Then a field equation is needed for $\psi(x)$.

Let us see how that can come across formally.

If $\rho_n(x)$ is the probability of a node $x$ to be in configuration $n$, then the free energy $f$ in (3) generalizes to the functional

$$
F[\rho] = \sum_n f(\rho(x)) + \Delta F[q],
$$

(13)

which adds to the uncorrelated local free energy (3) the non-local term $\Delta F[q]$, which accounts for the effect of the underlying spin structure, including charge conservation and correlation effects. The reader will have noted that we have already introduced a low temperature approximation in (13), since $\Delta F$ depends on $\rho_n(x)$ through the density of charge $q(x) = \sum_n q_n \rho_n(x)$. To fathom the form of $\Delta F[q]$ we (re)introduce $\phi$ as the conjugate field

$$
\phi(x) = \frac{\delta \Delta F}{\delta q(x)}
$$

(14)

which leads to the Legendre transform

$$
\mathcal{L}[\phi] = (\Delta F - q \cdot \phi)_{q=q[\phi]},
$$

(15)

(where $q \cdot \phi = \sum_x q(x) \phi(x)$), which in turn implies

$$
q(x) = -\frac{\delta \mathcal{L}}{\delta \phi(x)}.
$$

(16)

Finally, the free energy functional in (13) can be rewritten as

$$
F[\rho, \phi] = \sum_n f(\rho(x)) + q \cdot \phi + \mathcal{L}[\phi].
$$

(17)

The local part of the functional in (17) (first two terms on the right) looks now more like the uniform average free energy in (5) and the non-local functional $\mathcal{L}[\phi]$ (third term) pertains to the emergent field, which mediates the entropic interaction.

We can now construct $\mathcal{L}$ by perturbing over our previous spatially averaged treatment. We saw in the previous section that the uniform formalism based solely on the scalar constraint could predict well the numerical results for the average vertex constraint. Therefore $\rho_n$ in (6), the probability of any vertex to have $n$ close colloids, must be given by $\rho_n = N_v^{-1} \sum_x \rho_n(x)$ ($N_v$ is the number of nodes).

It follows that our functionals, restricted to uniform fields, should reduce to the previous forms of (5). From (14), when $\rho_n(x)$ are uniform, so is $\phi(x)$. Then, in order to recover (5) from (17), $\mathcal{L}$, restricted to uniform fields, must be

$$
\mathcal{L}[\phi] = \sum_x q^\phi(x) \phi = N_v Q^\phi \phi
$$

(18)
\( q^e(x) \) is the excess charge in the node \( x \) and \( Q^e = N_v^{-1} \sum x q^e(x) \) is the average excess charge per node.

Perturbing over the uniform, average manifold we expand in the derivatives of \( \phi \). We assume that the lattice is regular and allows coarse graining of \( x \) into a continuum variable, and thus \( \sum x \to a^{-d} \int_{L^d} d^d x \), where \( a^d = L^d/N_v \) is the volume of the unit cell. At second order the only admissible form is

\[
\mathcal{L}[\phi] = \int_{L^d} \left[q^e \phi - \frac{1}{2} e \partial_i \phi \partial^i \phi \right] \frac{d^d x}{a^d}.
\]  

(19)

Indeed, to reduce to (18) for uniform fields, (19) must contain only terms at second order in the derivatives of \( \phi \), thus excluding terms such as \( \phi^2 \) or \( \partial^i \phi \partial_i \phi \). Here \( e \) is the generalized permittivity of the emergent field (in general one has \( \epsilon_{ij} \), a suitable tensor).

3.2. Entropic Debye screening

The solution can now be obtained by optimizing the functional (17) in the fields \( \rho_\phi(x) \) and \( \phi(x) \). In taking the functional derivative with respect to \( \phi \) we cannot dump its derivatives at the boundaries since we already know that \( \phi \) is not zero at infinity: indeed its spatial average must be \( \bar{\phi} \). It is convenient to replace \( \phi(x) \to \bar{\phi} + \psi(x) \), with \( \psi \to \infty \), and minimize in both. Minimization in \( \psi \) then returns

\[-\Delta \psi = (q + q^e)/\epsilon, \]  

(20)

which from (20), (19), and (17), also gives

\[
\mathcal{F} = \int_{L^d} \left[f + \frac{1}{2} e \partial_i \psi \partial^i \psi \right] \frac{d^d x}{a^d}.
\]  

(21)

and thus \( \epsilon > 0 \).

Then optimization of (17) with respect to \( \rho(x) \) returns the Boltzmann law (12), whereas optimization with respect to \( \bar{\phi} \) leads again to the charge constraint \( Q + Q^e = 0 \) for the spatially modulated \( \rho_\phi(x) \) of (12). We have obtained a Debye–Hückel model for an electrolyte solution (not uncommon in spin ice materials [49]) where charges are topological while the interaction \( \phi \) is emergent from the underlying network of links: the excess charges are screened by the charges of the manifold.

Consider \( Q^e = 0 \) but \( q^e(x) \neq 0 \). Expanding (12) in \( \phi(x) \) around \( \bar{\phi} = E(1 - z)/4 \), one finds

\[
\rho_\phi(x) = \rho_h + \eta_h(x), \]  

where \( \rho_h \) given by (6) and \( \eta_h \) given by

\[
\eta_h(x) = -\rho_h q^e \psi(x)/T \]  

(22)

which correctly implies \( \sum_n \eta_n = 0 \). Then from (22) and (20) and the fact that the excess charge is sub-extensive \( (Q^e = 0) \), we can verify that \( \rho_h = N_v^{-1} \int_{L^d} \rho_h(x) d^d x/a^d \): \( \rho_h \) is the probability of any vertex to be in topology \( n \), as expected.

\footnote{This perturbative approach to weak correlation, viable on a disordered manifold, would be impossible in an ordered phase.}

\footnote{Note that \( Q^e = 0 \) neither implies absence of excess charge \( q^e(x) \), nor that the net excess charge \( Q^e = \int_{L^d} q^e(x) d^d x/a^d \) is zero, or even finite, but only that it is sub-extensive. Then the average excess charge per node \( Q^e = Q^e/N_v \) is zero.}
Since $\sum_n \rho_n q_n = 0$, we have $q(x) = \sum_n \eta_n(x)q_n$ and from (22)
\[q(x) = -Q^2 \psi(x)/T,\] (23)
where $Q^2 = \sum_n \rho_n q_n^2$ is the average charge fluctuation of the manifold. Finally from (20) and (23) $\psi$ satisfies
\[(\lambda^{-2} - \Delta)\psi = q^e/\epsilon,\] (24)
a screened Poisson equation whose screening length
\[\lambda = \sqrt{\epsilon T/Q^2},\] (25)
precisely corresponds to the Debye formula where the embedded screening charge comes from the charge fluctuation within the manifold.

Since a genuine ice manifold (even $z$) lacks charge fluctuation, from (25) we have $\lambda^{-1} = 0$ and infinite screening length. A non-extensive excess charge does not disturb a genuine ice manifold: indeed from (23) since $Q^2 = 0$ we have $q(x) = 0$ and therefore all the vertices stay in an ice configuration. This can also be seen in (22) which gives, in all cases, $\eta_n(x) = 0$ in the ice manifold, and therefore $\rho_n(x) = \rho$: the ice manifold remains uniform in the presence of excess charge, which must therefore be pushed at the boundaries. Indeed $\lambda$ approaches infinity exponentially fast in $\mathcal{E}/T \to \infty$, as depicted in figure 2, because $Q^2 \propto \exp(-\mathcal{E}/2T)$. Therefore as the system crosses over into an ice manifold it approaches an entropic solenoidal (or Coulomb) phase for $\psi$ in (24). Then standard potential theory in any dimension implies that a mobile excess charge is expelled at the boundaries as the system enters the ice rule. At small or non-zero temperature mobile excess charges will have a density $\lambda^{-d}$ which goes to zero as $T$ approaches zero.

If the charge is not mobile, equation (22) still predicts $\eta_n(x) = 0$. Indeed, consider the ice manifold and add an extra colloid to saturate a link, causing a charge +2 in a vertex. The ice manifold is restored by flipping unsaturated links (spins) to move the charge to the infinitely distant boundaries, thus creating a ‘Dirac string’ from the bulk to the boundaries. Then $q(x)$ remains zero in the bulk, as expected. However if $Q^e \neq 0$ and the excess charge is extensive, this cannot happen (see next section).

In absence of excess charge, excitations at $T > 0$ interact via (20), as the magnetic monopoles [39, 50] of spin ice, yet with a difference: because of the short range energetics hereby assumed [3], the interaction between monopoles is entirely of the emergent kind and dimensionality dependent: for $d = 3$ it is a $1/r$ potential and thus opposite charges are separable, while for $d = 2$ they are logarithmically confined.

Conversely in a quasi-ice manifold (odd $z$) there are always embedded ±1 charges and thus $Q^2 = 1$. This plasma of embedded charges always provides for entropic screening of excess charges, something seen numerically in colloidal systems [4], but also in artificial spin ice of odd coordination [31, 35]. As temperature lowers this screening becomes tighter and can form bound states, or polarons [35], which, when spaced at a distance much larger than $\lambda$, simply fluctuate thermally.

7 Naturally, there is also an entropic interaction among monopoles in natural spin ice materials coming from the underlying spin manifold, and there, since $d = 3$, it also has the form of an emergent $1/r$ potential [49].
As temperature increases, one expects the screening to become less tight. Indeed, consider now $q^e = 0$. When $T/\mathcal{E} \to \infty$ all links flip independently and vertices are allocated by multiplicity. From (12) this implies $\phi(T) \to 0$, which from (20) entails $eT \to \infty$. Since $e$ is inversely proportional to an energy, dimensional considerations fix it at $e = \xi^2 a^2 \mathcal{E}^{-1}$, where $\xi$ is a number, and is limited in $\mathcal{E}/T$. Then (25) implies, correctly, $\lambda^2/a^2 \propto T/E$ (since $Q^2 \leq \overline{Q^2}_{T=\infty} = z$).

In conclusion, while a uniform emergent field enforces the scalar constraint and leads to the ice rule, a modulated emergent field mediates the effect of the geometric constraint via a local entropic interaction between charged excitations and excess charges, explains the attraction of opposite topological charges seen in numerical simulations [4], and extends the similarity with magnetic spin ice materials to the low-energy dynamics above the ice manifold.

4. Charge transfer: breaking the ice

Where do the similarities between repulsive colloids/vortices and spin ice break down? We have seen that the ice rule follows from the scalar constraint of charge cancellation. On a lattice of single coordination this constraint can be violated by extensively doping excess charge. However, in a lattice of mixed coordination, even without excess charge, a charge transfer between sub lattices of different coordination can lift the ice manifold.

4.1. Extensive doping

As explained above, unlike in spin ice materials, excess charge (colloids) can here be added to or subtracted from the systems under consideration. If the doping is non-extensive ($Q^e = 0$) effects are only local, leaving the previous picture unchanged. Conversely, adding extensively a (possibly negative) average number $n^e$ of colloids induces an average topological charge per unit vertex $Q^e = -2n^e$. This charge breaks the ice—but not the quasi-ice—manifold.

If $n^e \ll 1$ (only a small fraction of all the vertices are defected) we can apply the previous approach with $Q^e \neq 0$ in (9). Now $\phi$ can depend on $T$. However, from (6) and (7), $\rho_\beta$ are determined by the expansion

$$\phi(T) = \phi_0 + \alpha T + O(T^2), \quad (26)$$

of $\phi$ at the first ordering $T$: $\phi_0$ determines the energetics in (7), and can be chosen to make either one or two states degenerate; $\alpha$ simply adds a factor to the multiplicities, $m_n \to m_n \exp(-q_\alpha\alpha)$, and thus controls the ratio of degenerate states at low $T$.

In lattices of odd $z$, which at low temperature enter a quasi-ice phase of embedded charges $q = \pm 1$ in equal proportion, the excess charge can be neutralized within the manifold. Then $\phi_0 = -(z - 1)\mathcal{E}/4$ as in (10) and $\alpha$ fixes the multiplicities of the $q = \pm 1$ charges, such that

$$\rho_{q=1} \xrightarrow{T \to 0} \frac{1 - Q^e}{2}, \quad \rho_{q=-1} \xrightarrow{T \to 0} \frac{1 + Q^e}{2}. \quad (27)$$

---

8 To avoid confusion, we remark on the difference between doping colloids to a system, which creates positive or negative excess topological charge by adding (or removing) colloids to the links, and the topological charge transfer between sub-lattices of a mixed coordination geometry, where no colloid is added or removed from any link, and links remain half-occupied.
We see therefore that the presence of embedded charges in the quasi-ice manifold allows for neutralization of a small density of external charge without leaving the manifold but simply by changing the relative proportion between positive and negative charges. To make sense of (27): consider a quasi-ice manifold, for instance $z = 3$. Each vertex is in the $n = 2$, $q = +1$ or $n = 1$, $q = -1$ configuration. If we add a charge $Q^e$, half of the excess colloids (or $|Q^e|/4$ colloids) go on $n = 1$, $q = -1$ vertices turning them in $n = 2$, $q = +1$. Half fall on $q = +1$, $n = 2$ vertices creating $n = 3$ excitations over the manifold. These will dump the excess charge via a different, unsaturated link, on a neighboring vertex in the $n = 1$, $q = -1$ topology (or else non-neighboring, through a cascade effect), thus eliminating the excitation and regaining the $n = 2$ status.

The situation is rather different for a genuine ice manifold, which contains no charge of its own: then extensive excitations are needed to absorb the excess charge. Assume $Q^e$ positive. We can always choose $\phi_0$ so that the $q = -2$ charges (corresponding to $n = z/2 - 1$) are degenerate with the $q = 0$ charges (corresponding to $n = z/2$) in the effective energetics of (7). Then $\alpha$ in (26) gauges the relative admixture of the two giving

$$\rho_{q=0} \xrightarrow{T \to 0} 1 - Q^e/2, \quad \rho_{q=-2} \xrightarrow{T \to 0} Q^e/2$$

or the screening of the excess charge by means of a suitable density of $q = -2$ excitations. Dropping colloids (or subtracting them) on an ice-rule manifold in an extensive, diluted way creates excitations in the very vertex in which the colloid falls, excitations that cannot be suppressed by flipping unsaturated links (as explained in the previous section).

This difference in behavior between odd and even coordination number is relevant to lattices of mixed coordination, where a transfer of net topological charge eliminates the ice manifold.

4.2. Mixed coordination

Consider lattices of mixed coordination number, an intriguing scenario that opens a window on more complex geometries [30, 31, 35] and in general on dynamics in complex networks, which we will develop elsewhere. Then the free energy is the sum of terms given by (3), each corresponding to sub-lattices of different coordination, and weighted by the relative abundance of vertices of that coordination. However, the emergent field must be the same for all sub-lattices. Indeed it is the total charge, not the sub-lattice charges, that must be conserved.

Consider for simplicity the treatment of section 2, which neglects the geometric hard constraints. One finds that in each sub-lattice the probability of a node of coordination $z$ to be in topology $n$ follows a Boltzmann distribution as in (6); however the field $\phi$ must be the same for all $z$. This implies that there must be charge transfer between sub-lattices of different coordination, since (10) cannot be satisfied for all $z$ simultaneously by the same field. Therefore at most one sub-lattice can reach the ice (or quasi-ice) manifold at low $T$, whereas the others are no longer equivalent to a spin ice system. This situation is distinctively different from the case of artificial spin ice of mixed coordination, which instead always enters an ice manifold [30, 31]: there, charge conservation is implied by an energetics that is genuinely degenerate in the sign of the charge.

For definiteness, consider the case of mixed coordination 4 and 3, in figure 3. Our previous discussion on doping and (26) can be employed. If we choose $\phi_0/E = -1/2$ in (26), then the $z = 3$ sub-lattice enters the quasi-ice manifold at low $T$. Yet in the $z = 4$ sector we have from (7)
that $q = -2$ and $q = 0$ become degenerate and of lowest effective energy. This means that the $z = 4$ vertices dump positive topological charge on the $z = 3$ ones by ‘exciting’ negative charges ($q = -q^2$).

The reason is straightforward. In truth, the $q = -2$ configurations are excitations only in the effective energetics of (7) for a lattice of single coordination number. For mixed coordination they are in fact a way to lower the real energy in (1), by pushing away colloids wherever geometry permits. Then the $z = 3$ sub-lattice can screen the excess charge without abandoning the quasi-ice manifold, in a way reminiscent of what happens to the shakti artificial spin ice [30, 31, 38] and pentagonal [35] artificial spin ice above their ice manifold.

4.3. Extensions to social settings

This framework, suggested by physics, invites intriguing extensions to sociological and economical problems. Frustration being, after all, a typical aspect of our lives, one sees how the treatment above can be generalized naturally to sociological networks of actors sharing burdens, undesirable tasks or costs, and how it can be employed to predict optimal distributions of connectivity in a social setting. If $\mathcal{E}$ is negative, however, the model describes instead a network
of shared benefits, or desirable wealth. In both cases net wealth (or cost) only amounts to half the available slots—which we can call opportunities in the case of wealth ($\mathcal{E} < 0$), or availabilities in the case of burdens ($\mathcal{E} > 0$). Then the treatment of section 2 describes a completely fluid situation, in which costs or benefits can go freely from a node to another.

We will show in future work that this lack of hard geometric constraints leads trivially to extreme polarization of wealth: actors with more opportunities have all their opportunities satisfied whereas actors below a certain opportunity threshold simply get nothing. The case of shared costs is intrinsically more fair: above a certain availability threshold everybody performs the same number of tasks, regardless of their availabilities. Below that threshold, performance equals availability. In both cases the ice rule is broken.

One can clearly see how this facile picture is then severely modified by the introduction of hard constraints. These correspond to joining in a pairwise way the opportunities/availabilities of different actors through links of shared ‘colloids’, thus obtaining a network generalization of the lattices described above. For instance, by coordinating among themselves actors with large opportunity, and thus forcing them to share wealth, one breaks down the wealth disparity. Conversely we can cement disparity by assuring that highly coordinated actors have enough links with lower coordinated ones, allowing the former to draw wealth from the latter.

To maintain the physical focus on the current work, we will offer a treatment of these sociologically relevant models in a future report. There we will also show ways to account for the hard constraint in a mean field fashion and we will test them on exact solutions for peculiar graphs, generalizations of the Bethe lattice.

5. Conclusion

We have studied the equivalence between systems of trapped colloids or pinned vortices, and spin ice. We have seen that although their energetics differs essentially from that of the spin ice systems, a constraint on topological charge cancellation introduces an ice-like effective energetics. The energetics is altered by a uniform emergent scalar field associated with the topological charge. Because of that, lattices of even coordination number can access an ice manifold. Lattices of odd coordination access a quasi-ice manifold. In the case of strong geometrical constraints, the analogy extends to the low energy dynamics. Then a spatially modulated emergent field translates the geometric constraint into an entropic interaction. In a genuine ice manifold such interaction is solenoidal, leading to a Coulomb phase. In lattices of odd coordination, which access a quasi-ice-rule characterized by embedded charges, the charge fluctuations of the manifold can screen the excess charge, as also seen in artificial spin ice, in which polaron can form. Finally the equivalence breaks down in lattices of mixed coordination, whose behavior is essentially different from mixed coordination spin ices. In the case of colloids charge transfer must occur between vertices of different coordination, thus lifting the ice rule.

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