Topological charge order and binding in a frustrated XY model and related systems

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Abstract. We prove the existence of a finite temperature $Z_2$ phase transition for the topological charge ordering within the fully frustrated XY model. Our method enables a proof of the topological charge confinement within the conventional XY models from a rather general vista. One of the complications that we face is the non-exact equivalence of the continuous (angular) XY model and its discrete topological charge dual. In reality, the energy spectra of the various topological sectors are highly nested, much unlike that suggested by the discrete dual models. We surmount these difficulties by exploiting the reflection positivity symmetry that this periodic flux phase model possesses. The techniques introduced here may prove binding of topological charges in numerous models and might be applied to examine transitions associated with various topological defects, e.g., the confinement of disclinations in the isotropic to nematic transition.

Keywords: rigorous results in statistical mechanics, classical phase transitions (theory)
1. Introduction

In this work, we examine the topological charge ordering of XY models in the presence of various external magnetic fields and prove, by reflection positivity, that these charges order at finite temperature in the ‘fully frustrated XY model’ (wherein, as we will explain, half a fluxon threads each elementary plaquette in an XY model). Beyond the particular quite specific result related to transitions in the fully frustrated XY (and other spin) models [1]–[11], the principal ideas that we advance and the reflection positivity techniques that we employ [12] might be used to prove topological charge order in a host of systems, including those with continuous symmetries for which discrete Coulomb-type and other representations of these charges are highly illuminating yet approximate and may lead
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to incorrect results. Offshoots of the methods that we invoke demonstrate a relatively universal attraction between opposite charges in these and many other symmetric (or, more precisely, ‘reflection positive’ [13]) systems. Extensions of the techniques employed here have ramifications in other fields, such as the sign of Casimir effects, e.g. [14]. Questions concerning the existence of topological charge order in frustrated systems have, in recent years, gained impetus from the study of topological quantum orders [15]–[18]. The study of uniformly frustrated systems has also been of interest in the study of glassy dynamics and ageing [19]–[22].

The outline of this work as follows. In section 2 we define the two-dimensional frustrated XY model. In section 3, a simple set of general trigonometric difference equations and approximate solutions for ground state configurations will be given. Much of this section is not new but is merely our perspective on the matter. We illustrate how in the low-energy sector the continuous XY model and its discrete topological charge dual are almost one and the same. In section 4, several simple exact ground state solutions are given. We then compute energy gaps between different topological charge configurations, which will serve as a springboard in our proof of finite temperature phase transitions.

In the sections thereafter, we largely focus on new non-trivial results. In section 5, we investigate the fully frustrated XY model. Employing the results of section 4, in section 5.1, we establish the existence of energy gaps between the different topological charge sectors. We then show, in section 5.2, that the system is reflection positive and, consequently, prove a finite temperature topological charge ordering transition. In section 6 we provide an alternative proof to the ordering transition. We demonstrate, in section 7, that by a minor variation, our proof immediately relates to the usual finite temperature annihilation of vortex–antivortex pairs occurring in the Kosterlitz–Thouless transition. In section 8 we discuss systems with kaleidoscope pattern frustrations. In section 9, we discuss the extension of the chiral $Z_2$ symmetry of the fully frustrated XY model to a $Z_k$ symmetry present for other rational frustration $f$, which tends to an $O(2)$ symmetry for irrational $f$. Numerically, with the fully frustrated XY model, both symmetries (i.e., (i) the $Z_2$ symmetry which as we prove in this work is broken at low temperatures and (ii) the continuous $O(2)$ symmetry) are lifted at very close temperatures ($T \simeq 1.286 J$ (with $J$ the exchange constant)) [1, 23]. We suggest an analogy to the magnetic groups appearing in the Quantum Hall problem. We end, in section 10, in an application of these ideas to other topological defects—e.g. disclinations in liquid crystals.

2. Definition of the model

An excellent review of the fully frustrated XY model is provided in [1]. We proceed with a particular common rendition of this model, e.g. [24, 25], which we will henceforth analyze. We consider a classical XY model on an $L \times L$ square lattice with periodic or open boundary conditions (with $2L^2$ or $2L^2+2L$ bonds respectively). The two component spins $\{\vec{S}_i\}$ at each lattice site $i$ are labeled by their orientation $\{\theta_i\}$ relative to a chosen axis. The Hamiltonian

$$H = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j - A_{ij})$$

(1)
where \(i,j\) are nearest neighbor sites on the lattice. Throughout this work, unless stated otherwise, we set both the exchange constant \(J\), and (as seen above) the lattice constant to one. Two symmetries of this Hamiltonian are evident:

- A global \(O(2)\) symmetry. The transformation \(\theta_i \rightarrow \theta_i + \phi\) for all sites \(i\) with a uniform shift \(\phi\) leaves the Hamiltonian \(H\) trivially invariant. By the Mermin–Wagner–Coleman [26, 27] theorem, continuous symmetries are never broken in two dimensions: at any finite temperature the local order parameter \(\langle \theta_i \rangle = 0\) for all twice differentiable, rotationally symmetric, momentum space interaction kernels [20]. In this two-dimensional system, the superfluid phase stiffness exhibits a first-order jump at a Kosterlitz–Thouless temperature \(T_{KT}\) below which rotational symmetry is (marginally) ‘broken’ to produce a state with algebraic long-range order [28]–[31].

- For the special cases in which the flux \(\Phi_R \equiv \sum_{ij} A_{ij}\) is the same for all plaquettes \(R\), translational invariance is also a symmetry of the Hamiltonian. We shall primarily focus (for the fully frustrated XY model (FFXY)) on the breaking of translational invariance under a shift by one lattice constant, \(\theta_i \rightarrow \theta_{i+\hat{e}_1}\) for all \(i\), as seen by the arrangement of vortices. A critical temperature \(T_{\text{vortex}}\) may be associated with the breaking of this symmetry. Numerically, as the temperature is lowered within the FFXY, it is found that \(|T_{\text{vortex}} - T_{KT}| \ll T_{KT}\). Whether the two temperatures might be exactly one and the same has been a puzzle surrounded by some controversy, in spite of very promising recent work [32].

Equation (1) describes an array of Josephson junctions immersed in an external magnetic field, e.g., [1]. It may model an extreme type II superconductor built of discrete superconducting elements (‘grains’) at the various lattice sites, where it is assumed that the modulus of the superconducting wavefunction on each grain is pinned and that only its phase may vary\(^1\). The evolution of the phases is easily gleaned within a path integral formulation: an external electromagnetic vector potential \(A_\mu(\vec{x})\) gives rise to the differential action \(dS_{em} = -(e^*/c)A_\mu dx^\mu\) for a displacement \(dx^\mu\), with \(e^*\) the effective charge and \(c\) the speed of light. This leads to a phase shift \(\exp[i S_{em}/\hbar] \rightarrow \exp[i A_{ij}]\) along the link \((ij)\), where

\[
A_{ij} = -\frac{e^*}{\hbar c} \int_i^j A(x) \cdot \overrightarrow{dx}.
\]

(2)

It follows that in going around a plaquette the electromagnetic field incurs an additional phase

\[
-\frac{e^*}{\hbar c} \oint_R A(x) \cdot \overrightarrow{dx} = \sum_{ij} A_{ij},
\]

(3)

the elegant Aharonov–Bohm effect [33]. The above directed loop sum may be replaced (by a simple application of Stokes theorem) by the magnetic flux threading the plaquette

\(^1\) In a continuous quantum system, the amplitude of the wavefunction \(|\psi(\vec{x})|\) vanishes at all singular points (e.g. vortices) to effectively excise these points so that a wavefunction may be globally defined. For the most part, we will consider an effective underlying lattice on which the modulus of the wavefunction is constant; the plaquette ‘vortices’ fall in between the lattice sites. There are no true singularities for such lattice systems.
The spectrum equation (1) is a continuous function of these degrees of freedom. The latter quantity can be interpreted as the total number of spins minus one global rotation. In a system with open boundary conditions there are (2

the total number of constraints (of net circulation about each plaquette),

with integer \( \{m_R\} \). The content of the ‘vorticity’ \( m_R \) is clear. Let us slowly trace its origin and justify the latter name. The vorticity of a plaquette \( R \): \( m_R = \sum_{(ij) \in R} m_{ij} \), where \( \phi_{ij} = \theta_i - \theta_j - A_{ij} + 2\pi m_{ij} \). The vorticity \( m_R \) represents the multiple of \((2\pi)\) that needs to be added to the bare gauge invariant angular differences \((\theta_i - \theta_j - A_{ij})\) such that \(-\pi < \phi_{ij} \leq \pi\). As such, it counts the number of times that the XY rotor circulates as we go counterclockwise round the plaquette \( R \). We can immediately make two statements regarding the effect of a spatially uniform frustration \( f \):

(i) The ground state energies are trivially continuous in \( f \). The proof is very simple: By equation (1), we note that for each given angular configuration \( \{\theta_i\} \), the energy \( E(\{A_{ij}\}; \{\theta_i\}) \) is a continuous function of \( \{A_{ij}\} \); each individual gauge link variable \( A_{ij} \) appears as an argument of a single continuous cosine function. Thus the ground state energy (i.e. the minimum amongst all of these continuous energy curves, each corresponding to a different angular configuration \( \{\theta_i\} \)), \( E_{\text{ground}} = \inf_{\theta} E(\{A_{ij}\}; \{\theta_i\}) \) is also a continuous function of \( \{A_{ij}\} \) or, in a gauge invariant formulation, the ground state energy per link is a continuous function of the frustration \( f \). (In varying \( f \to f + \Delta f \), an extensive number \( O(L^2) \) of link variables \( \{A_{ij}\} \) are altered. More formally, for each of the \( N \) link variables \( A_{ij} \), the continuity of \( E_{\text{ground}}(\{A_{ij}\}) \) implies that for a given individual bond \( \langle ij \rangle \) (for which \( A_{ij} \) appears in the argument of a single cosine function out of the extensive sum of equation (1))

\[
\forall |A_{ij} - A'_{ij}| < \delta_{ij} \\
\exists |E_{\text{ground}}(\{A_{ij}\}) - E_{\text{ground}}(\{A'_{ij}\})| < \epsilon_{ij}.
\]

Note that there are \( 2N \) link gauges \( \{A_{ij}\} \)s (in a system with periodic boundary conditions). As noted earlier, in a system with open boundary conditions there are \( (2L^2 + 2L) \) bond angles \( \{\phi_{ij}\} \). Subtracting from this quantity the total number of constraints (of net circulation about each plaquette), \( N = L^2 \), we are left with \( [(L + 1)^2 - 1] \) degrees of freedom. The latter quantity can be interpreted as the total number of spins minus one global rotation. The spectrum equation (1) is a continuous function of these.
We may now tackle the multi-bond problem by employing \( \sum |a_\alpha| \geq |\sum a_\alpha| \). This implies that
\[
\forall |A_{ij} - A'_{ij}| < \delta_{ij} = O(\delta)
\]
\[
\exists \frac{1}{N}|\Delta E_{\text{ground}}(f)| < \frac{1}{N} \sum ij \epsilon_{ij} = O(\epsilon)
\]
(7)
where the sum now spans all bonds \( \langle ij \rangle \). This continuity argument is shorter than that spanned by an entire earlier letter [34].

(ii) The system is invariant under the transformations
\[
f \rightarrow n \mp f
\]
for all integers \( n \). Once again, the proof is trivial: the inversion of the external magnetic field \( f \rightarrow -f \) along with \( \theta_i \rightarrow -\theta_i \) leaves the partition function \( Z = \prod_i f \, d\theta_i \, \exp[-\beta H] \) identically the same as the cosine interaction term is an even function. The periodicity of the cosine secures an additional invariance: \( f \rightarrow f + f \). Compounding the last two operations together proves the symmetries of equation (8). These imply that, as a function of external magnetic flux, the ground state energy \( E_{\text{ground}}(f) \) has local extrema at the symmetry points \( f = 0, \pm 1/2, \pm 1, \ldots \). The points \( f \equiv 0 \, (\text{mod} \, 1) \) are global minima of \( E_{\text{ground}}(f) \)—all bonds are saturated at their minimal value \( (-1) \) within the ground state.

The symmetries of equation (8) have led the \( f = 1/2 \) variant to be regarded as the ‘fully frustrated’ one. After all, any larger value of \( f \) may be folded back to another value of \( f \) lying in the interval \([0, 1/2]\); the model with \( f = 1/2 \) is as frustrated as it can possibly get. However, in some sense, the ‘fully frustrated XY model’ is the least frustrated of all. The time reversal symmetry (or, more formally, a reflection positivity invariance) that this model possesses will allow us to prove that it displays a \( Z_2 \) phase transition.

3. Approximate ground states and the low-energy dual (topological charge) model

The current section, unlike others to follow, is not rigorous. Much of its content is not new (albeit often derived by new routes). Its intent is to provide the reader with a better intuitive grip on the physics of the frustrated XY model. Experts may choose to directly study sections 4 or 5. Enforcing the constraints of given vorticities, equation (5), the Hamiltonian to be minimized reads
\[
\mathcal{H} = -\sum_{\langle ij \rangle} \cos \phi_{ij} + \sum \alpha \lambda_{\alpha} \sum_{\Box R_{ij}} \phi_{ij},
\]
(9)
For a system with periodic boundary conditions, there are \( N = L^2 \) circulation constraints of the form in equation (4) and 2\( L^2 \) gauge variables \( \{A_{ij}\} \). This leaves \( N \) independent gauge variables \( \{A_{ij}\} \). Now imagine fixing \( N \) arbitrary \( \{A_{ij}\} \) such that no three variables are common to the same plaquette. After such a gauge fixing procedure, the remaining \( N \) dependent gauge link variables are fixed by the circulation sums of equation (4). Now consider shifting the flux threading each plaquette \( \Phi \rightarrow \Phi + n\Phi_0 \), or, equivalently, the frustration \( f \rightarrow f + 2\pi n \), with an integer \( n \). This amounts, in a given gauge, to changing the \( N \) dependent gauge link variables by an integer multiple of \( 2\pi \). By the periodicity of the cosine interaction, the spectrum will remain trivially invariant.
where \( \{ \lambda_\alpha \} \) are Lagrange multipliers. Unless some of the angles lie on the boundaries \((\phi = \pm \pi)\), at the extrema

\[
\sin \phi_{ij} + \lambda_{ij\in \alpha} - \lambda_{ij\in \alpha'} = 0
\]  

(10)

where the two adjacent plaquettes \( R_\alpha, R_{\alpha'} \) share the bond \( \langle ij \rangle \). The Lagrange multipliers \( \lambda_{ij\in \alpha} \) and \( \lambda'_{ij\in \alpha} \) refer to the plaquettes \( \alpha \) and \( \alpha' \) which share the same bond \( \langle ij \rangle \) (one having it appear in a counterclockwise circulation of \( \alpha \) and the other having it in a clockwise reading of \( \alpha' \)). Examining figure 1 we see that

\[
\sin \phi_{01} = \lambda_I - \lambda_{II}, \quad \sin \phi_{04} = \lambda_{II} - \lambda_{III} \\
\sin \phi_{03} = \lambda_{III} - \lambda_{IV}, \quad \sin \phi_{02} = \lambda_{IV} - \lambda_I.
\]

(11)

Summing it all up,

\[
\sum_{\{0j\}} \sin \phi_{i=0,j} = 0,
\]

(12)

the sum of all Josephson currents entering any node must vanish. We also arrive at equation (12) when minimizing equation (1) within a given gauge to find the global ground state. Equations (9) and (12) show that current conservation holds at extrema of each of the individual topological sectors \((m_1, m_2, \ldots, m_N)\) (unless the minima lie on the boundaries of the topological sectors: i.e. \( \phi_{ij} = \pm \pi \)).

If \( f = 0 \) and \( m_R = 0 \) in the region outside a given set of vortices then we may work in a gauge in which \( \phi_{ij} = \theta_i - \theta_j \equiv \theta_{ij} \). In this gauge, equation (12) reads

\[
\nabla_\mu (\sin[\nabla^\mu \theta]) = 0,
\]

(13)

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with $\nabla^\mu$ denoting the discrete lattice difference along the $\mu$ direction. This is equivalent to the difference equations

$$\nabla^\mu \theta = \sin^{-1} \left( [\vec{\nabla} \times \vec{A}(\vec{x})]^{\mu} \right).$$  \hspace{1cm} (14)

The function $\vec{A}(\vec{x})$ must satisfy

$$\sum_{\text{bonds} \in \Gamma} \theta_{ij} = \sum_{\langle ij \rangle \in \Gamma} \sin^{-1} \left( [\vec{\nabla} \times \vec{A}(\vec{x})]^{\mu_{ij}} \right)$$  \hspace{1cm} (15)

for all contours $\Gamma$. Here $\mu_{ij}$ are chosen to lie along each of the individual bond directions $\langle ij \rangle$ in the contour product. In the continuum limit equation (13) becomes

$$\cos^{2} \frac{\theta}{2} \frac{\partial^\mu}{\partial x^\mu} \theta(\vec{x}) \equiv D^2 \theta(\vec{x}) = 0.$$  \hspace{1cm} (16)

Effectively, the phase $\theta(\vec{x})$ isotropically dilates the metric. Apart from the special case $\theta = \pm \pi$, we obtain the Laplace equation. Thus, in the vortex-free $(m = 0)$, frustration-free $(f = 0)$, region $\theta(\vec{x})$ is a harmonic function. Let us now return to the discrete lattice equation (13) and examine its behavior in the linear regime far away from the vortices. When the angular differences are small we can replace equation (13) by

$$\nabla^\mu \nabla^\mu \theta = 0.$$  \hspace{1cm} (17)

where $m_{\text{net}}$ and $f_{\text{net}}$ are respectively the net topological charge and external magnetic flux/(2$\pi$) in the region bounded by the contour $C$. Choosing a gauge for the pseudo magnetic field $\vec{B} = \vec{\nabla} \theta$ (with $\vec{\nabla}$ the discrete lattice gradient), the condition for a minimum becomes $\vec{\nabla} \cdot \vec{B} = 0$ at all lattice sites. On the other hand, the boundary conditions (recall that we focused on a region in which $m_{R} = f_{R} = 0$ such that a decomposition $\phi_{ij} = \theta_{i} - \theta_{j}$ is possible) imply that

$$\sum_{C} \vec{B} \cdot \delta\vec{l} = 2\pi [m_{\text{net}} - f_{\text{net}}].$$

Employing the Biot–Savart law and the magnetic analogy, boundary effects may be included by extending the integral to include images of the singularities. The ground state energy given a certain distribution of $\{m_{\vec{x}}\}$ and $\{f_{\vec{x}}\}$ outside our domain is

$$E_{\text{ground}} = \frac{1}{2} \sum_{\vec{x}, \vec{x}'} [m_{\vec{x}} - f_{\vec{x}}] G(\vec{x}, \vec{x}') [m_{\vec{x}'} - f_{\vec{x}'}].$$

where $m_{\vec{x}}$ and $f_{\vec{x}}$ are the local vorticity and frustration in the plaquette $\vec{x}$. The sum over $\vec{x}'$ spans the entire lattice. (In higher dimensions the denominator readily generalizes to $2 \sum_{i=1}^{d} (1 - \cos k_{i})$.)
The ‘Coulomb gas’-type character of the XY model suggested by equation (19) is well known and has been derived by various methods both approximate [1], [35]–[38] and explicitly related to more exact dualities [39, 40]. The Coulomb gas representation has played a commanding role in the understanding of the frustrated (and non-frustrated) XY model. A principal complication that we will face in our endeavor of establishing low-temperature transitions is that the typical dual Coulomb gas representation is not exact and thus may give rise to incorrect results. The techniques that we use in the current work allow us surmount these difficulties and will enable us prove the existence of low-temperature topological charge order associated with the vorticities $m\vec{x}$.

In the small-$k$ (continuum) limit, the kernel $G(\vec{x} - \vec{x}')$ above becomes logarithmic, as befits the two-dimensional Coulomb charges. The resulting expression becomes identical, for all practical purposes, to the Villain model [35]. In this limit, the energy of interaction between two vortices is

$$E = 2\pi q_1 q_2 \ln(a/r_{12}) \quad (20)$$

where $q_i \equiv (m_i - f_i)$. For the time being, we have inserted a length $a$ in order to make the argument of the logarithm dimensionless. When supercurrent screening is introduced, $a$ naturally becomes the screening length in the short-distance limit. Thus, in this unscreened case, $a$ may be regarded as the system size: $a = O(L)$. (The following is standard. The kinetic energy

$$E_{\text{kin}} = \frac{1}{2} \int \rho(\vec{x}) v^2(\vec{x}) \, d^2x = \frac{1}{8\pi} \int \frac{mc^2}{4\pi ne^2} (\nabla \times H)^2 \, d^2x, \quad (21)$$

where we invoked Ampere’s law $\nabla \times H = (4\pi/c)\vec{j}$. The energy (kinetic + field) of a vortex line of length $L$

$$E = \frac{L}{8\pi} \int d^2x \left[ H^2(\vec{x}) + \lambda_L^2 (\nabla \times H)^2 \right] \quad (22)$$

where $\lambda_L^2 = mc^2/(4\pi ne^2)$ marks the ratio between the kinetic energy and the magnetic energy. The resulting variational (London) equation for the field configuration reads

$$\vec{H} + \lambda_L^2 \nabla \times (\nabla \times \vec{H}) = 0. \quad (23)$$

A vortex may be described by a source term,

$$\vec{H} + \lambda_L^2 \nabla \times \nabla \times H = q_0 \hat{z} \delta^2(\vec{x}) \quad (24)$$

with $q_0$ the flux. In cylindrical coordinates

$$H_z - \frac{\lambda_L^2}{r} \frac{d}{dr} \left( r \frac{dH_z}{dr} \right) = q_0 \delta^2(\vec{x}). \quad (25)$$

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The solution with the required singular behavior near the origin is

\[ H_z = \frac{q_0}{2\pi \lambda_L^2} K_0 \left( \frac{r}{\lambda_L} \right), \tag{26} \]

with \( K_0 \) a Bessel function. If there are two vortices, then on the right-hand side of the London equation we should insert two source terms: \( \hat{z}[q_1 \delta^2(\vec{x} - \vec{x}_1) + q_2 \delta^2(\vec{x} - \vec{x}_2)] \). The corresponding solution is a simple superposition,

\[ H_z = \frac{1}{2\pi \lambda_L^2} \left[ q_1 K_0 \left( \frac{|\vec{x} - \vec{x}_1|}{\lambda_L} \right) + q_2 K_0 \left( \frac{|\vec{x} - \vec{x}_2|}{\lambda_L} \right) \right]. \tag{27} \]

Inserting this in the equation for the energy of a vortex line, the interaction energy is seen to be

\[ \frac{E_{12}^L}{L} = 2 \left( \frac{q_1 q_2}{4\pi \lambda_L^2} \right) K_0 \left( \frac{|\vec{x}_1 - \vec{x}_2|}{\lambda_L} \right). \tag{28} \]

Asymptotically,

\[ K_0(x) \sim \begin{cases} \ln \left( \frac{1}{x} \right) & (x \ll 1), \\ \sqrt{\frac{\pi}{2x}} \exp[-x] & (x \gg 1). \end{cases} \tag{29} \]

\( K_0(x) \) is monotonically decreasing with \( x \) leading, at all distances, to an attractive/repulsive forces between opposite/identical poles. The top (small-\( x \)) form of last equation is the one encountered in this work. We identify the length scale appearing in the argument of the logarithm of our continuum limit treatment with the screening length \( \lambda_L \)—tending to the system size in the absence of screening.)

In the continuum limit, lines connecting opposite sign vortices become cuts in the complex plane with branch points at the positions of the vertices. A solution to the Laplace equation (equation (16)) jumping by \( 2\pi q_i \) across the branch cut while traversing each pole (vortex) \( z_i = x_i + i x_{i,2} \) (where \( (x_{i,1}, x_{i,2}) \) are the vortex coordinates within the plane) is the well-known [41]

\[ \theta(z) = \sum_i q_i \text{Im}\{\ln(z - z_i)\}. \tag{30} \]

In the previous (magnetic) analogy the singular branch cut takes on the role of a Dirac-like string. If we have a pair of equal and opposite vortices \( q_1 = -q_2 \), then \( \theta/q_1 \) simply becomes the ‘angle of site’ of the segment connecting \( z_1 \) and \( z_2 \) as viewed from the point \( z \). \( \theta \) may be written as the phase of the wavefunction (which may be superficially viewed as a Laughlin-like wavefunction [42] as a function of only one of the ‘electronic’ coordinates)
with the odd integer power replaced by $q$:

$$\psi(z) = \prod_i (z - z_i)^q.$$  \hspace{1cm} \text{(31)}$$

The phase of this wavefunction $\theta = \text{Im}\{\ln \psi(z)\}$.

The continuum limit unfrustrated XY Hamiltonian,

$$H = \frac{1}{2} \int d^2 x (\nabla \theta)^2$$

$$= \frac{1}{2} \int d^2 x \nabla \text{Im}\{\ln \psi(z)\} \cdot \nabla \text{Im}\{\ln \psi(z)\}$$

$$= \frac{1}{2} \sum_{i,j} q_i q_j \int d^2 x \nabla \text{Re}\{\ln(z - z_i)\} \cdot \nabla \text{Re}\{\ln(z - z_j)\},$$

where we employ the Cauchy–Riemann relations

$$\partial_{\alpha} u = \epsilon_{\alpha \beta} \partial_{\beta} v \implies (\nabla u)^2 = (\nabla v)^2$$  \hspace{1cm} \text{(32)}$$

(with $\epsilon_{12} = -\epsilon_{21} = 1$) for the complex function $F(z) = \ln \psi(z) = u + iv$ (where the squared gradients are $1/r^2$). Integrating by parts,

$$H = -\frac{1}{2} \sum_{i,j} q_i q_j \int d^2 x \ln |z - z_i| \nabla^2 \ln |z - z_j|.$$ \hspace{1cm} \text{(33)}$$

By the $2\pi$ discontinuity around a logarithmic pole, $\nabla^2 \ln |z - z_j| = 2\pi \delta(z - z_j)$. Thus,

$$H = -\pi \sum_{i,j} q_i q_j \ln |z_i - z_j|$$

$$= \pi \sum_{i,j} q_i q_j \ln(a/r_{ij}) + \text{const}$$ \hspace{1cm} \text{(34)}$$

with an arbitrary $a$ and inter-vortex separation $r_{ij} = |z_i - z_j|$. This swift independent derivation is merely a slight twist on the treatment of Itzykson and Drouffe [43]. Note that the final result is identical to equation (20) derived by a seemingly alternate route. Such a plasma-like interaction is also present in the Boltzmann weights of Quantum Hall Laughlin states. Along this route, the standard Villain model duality [35] acquires a new meaning—an interchange between the real and imaginary parts of a complex function $F(z)$. Here the nature of the duality is manifest: the imaginary part of $F(z)$ leads to a description in terms

4 We also note that at a complete extreme—if the requirement the electronic quantum mechanical wavefunction has a fixed amplitude $|\psi(\vec{x})| = 1$ were relaxed, then instead of a phase-only model, we would arrive, in the continuum limit (replacing the cosine by a covariant gradient $D_\mu = \partial_\mu - i(\epsilon^\sigma/c)A_\sigma$), at the Quantum Hall problem. The Laughlin-like wavefunction that we found in equation (31) is to be expected. $\psi(z)$ was a function of a single spinless electronic coordinate in the background of topological charges incurred by the other (formally ‘frozen’) electrons. (This is, of course, merely formal and not a valid physical procedure for the system of identical particles.) The charge $q$ plays the role of the inverse filling fraction $\nu^{-1}$. If the amplitude of the wavefunction is allowed to vary (or, equivalently, if the phase $\phi_{ij}$ is allowed to become complex, subject only to a spherical (large $n$) constraint $\langle |\phi_{ij}|^2 \rangle = 1$) then the problem becomes Gaussian. Alexander [60] has shown that in this approximation the system is described by the Harper equation [52, 61].
of the angular configuration of the XY rotors. The real part of $F(z)$ leads to a description in terms of the topological charges of the defects (when the frustration $f = 0$). Formally, we linked the two dual pictures by employing the Cauchy–Riemann relations. We note that, for $f = 1/2$, the $Z_2$ transition temperature $T_{\text{vortex}}$ corresponds to the ordering of charges in the dual model, whereas $T_{\text{KT}}$ corresponds to the critical temperature in the original angular variables. Number (charge) and phase variables appear in many instances (e.g. in the triangular XXZ models displaying both $Z_2$ and XY transitions with nearly equivalent temperatures [44]).

We now provide a new geometrical interpretation of the frustrations. Forgetting about boundary conditions, let us arrange the lattice sites on a sphere of radius $R$ (or many fractured portions of such spheres pasted together). The sum of the angles of a spherical quadrilateral $= 2 \pi + \text{Area}/R^2$. It follows that in this naive mapping, we can identify a uniform frustration $f = (\text{area of the plaquette})/R^2$. The frustrated XY Hamiltonian is now

$$H = - \sum_{\langle ij \rangle} \vec{S}_i \circ \vec{S}_j$$

(35)

where $\circ$ denotes the scalar product between the vector resulting from parallel transporting the spin $\vec{S}_i$ to site $j$ and the spin $\vec{S}_j$ already situated at site $j$. This Hamiltonian is translationally invariant when $f = \text{const}$ and may be diagonalized in Fourier space [20]. (As mentioned earlier, one way of describing a uniformly frustrated spin model is in terms of parallel transport on a sphere. Consider a three-spin $\vec{S}(\vec{x})$ with the

$$H = - \sum_{\langle \vec{x},\vec{y} \rangle} \vec{S}(\vec{x}) \circ \vec{S}(\vec{y})$$

(36)

where the $\circ$ operation denotes the scalar product between a spin $\vec{S}(\vec{x})$ rolled on a sphere of radius $R = \theta^{-1} \sim f^{-1/2}$ to a neighboring site $\vec{y}$ and the spin $\vec{S}(\vec{y})$ situated at $\vec{y}$. If the frustration is uniform then, in momentum space, a viable representation is

$$H = \frac{1}{2N} \sum_{\vec{k}} S_i(\vec{k}) v_{ij}(\vec{k}) S_j(-\vec{k})$$

(37)

where

$$v_{ij}(\vec{k}) = - \begin{pmatrix} A & 0 & -D \\ 0 & B & -E \\ D & E & C \end{pmatrix}$$

(38)

with

$$A = \cos \theta \cos k_1 + \cos k_2, \quad B = \cos k_1 + \cos k_2 \cos \theta$$

$$C = \cos \theta \sum_{l=1}^{2} \cos k_l, \quad D = i \sin \theta \sin k_1,$$

$$E = i \sin \theta \sin k_2.$$  

(39)
Locally, within the tangential spin coordinate system of the sphere, the spin has two components. By this crude analysis, we would expect the ground state modulation length (for a constant value of $f$) to scale roughly as the radius $R \sim f^{-1/2}$ for small fractions $f$ such that one fluxon pierces the surface of the sphere (giving rise to a trivial Aharonov–Bohm phase). This conforms with numerical observations for $f = 1/q$ with an integer $q \gg 1$: each fluxon (or vortex) occupies an area of size $1/f$.

More conventionally, requiring overall charge neutrality in the Villain model (or for our pseudo-currents $\{q_a\}$ that interact Coulombically) yields the same result. By net charge neutrality, the background charge $-\sum_a f_a$ should cancel against $\sum_a m_a$ originating from the vorticities. Once again, from this ‘angle’ as well, the density of vortices should scale as $f^{1/2}$ for a small uniform frustration $f$. In any system having periodic boundary conditions, the net topological charge must vanish. It follows that any system having ferromagnetic boundary conditions cannot enclose a net nonzero vorticity. All vortices must appear in vortex–antivortex pairs. On a less precise level, within the approximate dual model, this follows from a divergent Coulomb penalty for any lone unpaired vortex.

Let us define a radius $r$ vortex in the unfrustrated problem as one in which

$$\sum_{(ij)\in\Gamma} \phi_{ij} = 2\pi m_R, \quad (40)$$

with $m_R = 1$ is satisfied for all contours $\Gamma$ which encircle the plaquette $R$ up to a maximal distance $r$ away from it. Employing the Euler–Maclaurin summation formula, we find that, for large $r$, the energy of a radius $r$ vortex is bounded from below by that of a vortex in the continuum limit where an integration may be performed. In the large-$r$ limit the energy may bounded from below by $K_1 \ln(r/r_1)$, where, in this unfrustrated case, the constants $0 < K_1 < \pi$ and $r_1 > 1$. ‘Phase space’ volume calculations may also be enacted for these systems.

4. Exact flux patterns

All that follows in this section and hereafter is new and exact and is not based on any of the approximations of section section 3. The periodicity (if any) of the ground state phase pattern $\{\theta_i\}$ depends upon the gauge. Even in the unfrustrated ($f = 0$) case a gauge with irrational $\{A_{ij}\}$ may be chosen such that the phases are never periodic. As throughout most of this paper, we will attempt to focus on the gauge invariant bond angles $\{\phi_{ij}\}$. A periodicity in $\{\phi_{ij}\}$ implies a periodicity in the physically measurable Josephson currents ($\sin \phi_{ij}$). It is easy to determine, analytically, the ground state of small fragments of the lattice. As before, we enforce the constraints via Lagrange multipliers; now we leave the extrema equations in their plain form and resort to solving a few trigonometric equations and, in the aftermath, compare contenders amongst the resulting constrained extrema (along with various states that lie on the boundaries of $\{\Pi_{\text{bonds}} \otimes \phi_{ij}\}$ of the different topological charge sectors: scenarios in which a few of the bond angles are $\phi_{ij} = \pm \pi$).

5 For infinitesimal $\Delta E$, a simple calculation reveals that the fraction of unfrustrated ($f = 0$) XY states having energies between the ground state energy $E_{\text{ground}}$ and $E_{\text{ground}} + \Delta E$ relative to the net ‘phase space’ volume $(2\pi)^N$ is trivially $\frac{\Delta E/(2\pi J)^{N/2}}{\Gamma(N/2 + 1)}$, when dimensions are fully restored.
Let us start by considering a single plaquette with open boundary conditions. If this plaquette is unfrustrated, the ground state is trivially a ferromagnet: all $\phi_{ij} = 0$ (this state lies in the $m = 0$ sector). If this plaquette is threaded by half a fluxon ($f = 1/2$) then within the ground state the gauge invariant angles are all the same: $\phi_{12} = \phi_{23} = \phi_{34} = \phi_{41} = \pm \pi/4$ where $i = 1, 2, 3, 4$ are the vertices of the plaquette. (Note that the directions in these bond angles are important $\phi_{ij} = -\phi_{ji}$.) If all angles are $\pi/4$ then the plaquette has topological charge $q = 1/2$ or a vorticity $m = 1$; if all bond angles are $-\pi/4$ then the plaquette charge is $q = -1/2$ and the plaquette lies in the $m = 0$ sector. Other topological charge sectors are elevated relative to the ground state by a finite gap. For instance, the minimum energy for the unfrustrated plaquette ($f = 0$) subject to the constraint $m = 1$ is $\epsilon_{\text{min}}^{m=1} = -1/2$ (with a configuration having $\phi_{ij} = \pi/3$ for three bonds and with the remaining bond on the boundary of the angular zone ($\phi_{ij} = \pi$) lies above the ground state $\epsilon_{\text{min}}^{m=0} = -4$. Thus, each state in the $m = 1$ sector is elevated by at least $7/2$ ($J$—if units are restored) relative to the ground state. Similar bounds may be generated in frustrated plaquettes. These finite energy gaps will allow us, later on, to argue for finite temperature vortex ordering for certain values of $f$ and to prove the existence of a $Z_2$ phase transition for the fully frustrated XY model observed numerically in [46]. Note that here the ground states computed with open boundary conditions can trivially tile the plane. One of the complications of the continuous XY spectrum—\textit{unlike that of the approximate Coulomb charge dual}—is that the various topological charge configurations partially overlap and are \textit{nested}. The energies of the single unfrustrated plaquette span the region $-4 \leq \epsilon(m = 0) \leq 4$ when $m = 0$ and $-1/2 \leq \epsilon(|m| = 1) \leq 4$ when a vortex/antivortex is present. The energy of a vortex-free plaquette may be higher than that of a vortex-full plaquette! The \textit{nesting} of the energy spectrum just found hints that the XY model cannot be probed by merely replacing its plaquettes by topological charges. This subtle non-equivalence between the continuous model and its discrete counterpart is not heavily emphasized in the literature. The dual model (derived by various approximations for the \textit{low-energy sector} in equations (19) and (34)) is a useful tool, but it is merely an approximation, albeit an amazingly beautiful and powerful one. The complication arising from the non-equivalence of these models will be one of major obstacles that we will need to surmount.

As noted, the only ground states for a uniform $f = 1/2$ are the two checkerboard patterns where $\phi_{ij \in R} = \pm \pi/4$ for all plaquettes $R$. The proof is quite simple: the energy

$$E = \frac{1}{2} \sum_{\alpha} \epsilon_{\alpha} \geq \frac{1}{2} \sum_{\alpha} \min \{ \epsilon_{\alpha} \} ,$$

where $\epsilon_{\alpha}$ is the energy of each individual plaquette. Thus if a configuration in which for each plaquette $\epsilon_{\alpha} = \epsilon_{\text{min}}$ exists, then that configuration is a minimum energy configuration. For each individual plaquette $R_{\alpha}$, if $\epsilon_{\alpha} = \epsilon_{\text{min}}$ then all $\phi_{ij \in R_{\alpha}} = \pm \pi/4$. Now, a bond $\langle ij \rangle$ is common to two adjacent plaquettes. If its value, as read counterclockwise from the center of one plaquette is $\pi/4$, then its value as read counterclockwise from the center of the

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6 Note that if this plaquette was immersed in a lattice in which all other spins $i$ apart from those belonging to our plaquette point in the same direction ($\theta_i = \text{const}$) then an antivortex of strength $m = -1$ would appear immediately adjacent to it. Vortex neutrality is strictly enforced in any system with periodic boundary conditions (of which the condition $\theta_i = \text{const}$ is one extreme example allowing a $3 \times 3$ plaquette system to be wrapped around a two-torus).
adjacent plaquette is $-\pi/4$. If we start from one plaquette in which all bond angles are $\pi/4$ and then add an adjacent plaquette and require that in the new additional plaquette all bond angles will be of equal value, which is set to either $\pi/4$ or $-\pi/4$, then we will trivially see the bond common to both plaquettes will force all bonds in the new plaquette to be equal to $-\pi/4$. We can then add a new additional plaquette to the last one and repeat the argument. Thus if within the ‘seed plaquette’ (the plaquette situated at the origin of the dual lattice) all gauge invariant bond angles $\phi_{ij} = \pi/4$ then any other plaquette lying at a point $\vec{x} = (x_1, x_2)$ will also saturate the minimum energy bound with all bond angles set to $[(−1)^{(x_1+x_2)}]\pi/4$. We could have similarly started with a plaquette at the origin in which all bond angles were $-\pi/4$. These are the only two possible ‘seeds’ and the resultant configurations are the only two global ground states. Within these two ground states we find a checkerboard pattern of topological charges: if, in a given plaquette $R$, all the gauge invariant bond angles $\phi_{ij} = \pi/4$ then the vorticity $m_R = 1$; when all $\phi_{ij} = -\pi/4$ there is no vorticity ($m_R = 0$). The one and zero values of the local vorticities form a checkerboard matrix $m_{\vec{x}} = \pm \frac{1}{2}(1 + (−1)^{(x_1+x_2)})$. This phase is a specific example of a staggered flux phase investigated in the high-temperature superconductivity literature [47]. An explicit ground state configuration is shown in figure 2.

To distinguish between the two viable ground states and to highlight their $Z_2$ symmetry and pinpoint the breaking of this symmetry a staggered magnetization

$$M \equiv \left| \sum_{\vec{x}} (-1)^{x_1+x_2} m_{\vec{x}} \right|$$

is defined [46]. The current patterns within the two different chiral ground states are rotated by $\pi/2$ relative to each other. Domain walls separate the two checkerboard ground states—these cannot be transformed into each other by a continuous rotation. The walls consist of links which separate two plaquettes with the same sign of the chirality. In some numerical studies the onset of XY symmetry ‘breaking’ is extracted from an analysis of the helicity modulus. As mentioned earlier, the helicity modulus exhibits a universal jump at the Kosterlitz–Thouless transition [48]. The helicity modulus may be measured by applying strains on the Josephson currents [45]. Let us next consider a $2 \times 2$ block with $f = 1/2$ everywhere. Such a small fragment is depicted in figure 3, where, in the chosen gauge, $A_{25} = A_{58} = \pi$ with all other $A_{ij} = 0$.

Within the open boundary condition minimum of this small $2 \times 2$ block: $\phi_{21} = \phi_{14} = \phi_{74} = \phi_{87} = \phi_{80} = \phi_{96} = \phi_{36} = \phi_{23} = \cos^{-1}(\frac{2}{\sqrt{5}})$ and $\phi_{45} = \phi_{52} = \phi_{65} = \phi_{58} = \cos^{-1}(\frac{1}{\sqrt{5}})$. This state lies in the topological sector ($m_1 = 0, m_{II} = 1, m_{III} = 1, m_{IV} = 0$). A similar state appears in the sector $(1, 0, 1, 0)$. The energy of these states is $\epsilon_{0,1,0,1}^{\text{min}} = \epsilon_{1,0,1,0}^{\text{min}} = -4\sqrt{5}$. The energy per bond in this state is lower than that of the global (entire lattice) ground state minimum. This is hardly surprising: open boundary conditions were placed on this small $2 \times 2$ block. At worst the energy of this block would have coincided with the global ground state energy.

Let us denote the amount by which the open boundary condition state improves on the global ground state configuration (as placed on this small $2 \times 2$ block) by

$$\Delta_- = 4\sqrt{5} - 6\sqrt{2} = 0.458991 \ldots$$

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The minimum of all $(1, 1, 0, 0)$ or $(0, 0, 1, 1)$ states is $\epsilon_{1,1,0,0}^{\text{min}} = \epsilon_{0,0,1,1}^{\text{min}} = -8$ (corresponding to $\phi_{25} = \phi_{58} = \pi$ with all other gauge invariant bond angles $\phi_{\langle ij \rangle} = 0$). The lowest energies of all other non-checkerboard topological sectors are even more elevated than those of the $(1, 1, 0, 0)$ or $(0, 0, 1, 1)$ sectors. Thus the energy of all non-checkerboard configurations are elevated by at least

$$\Delta_+ = 6\sqrt{2} - 8 = 0.485281\ldots$$

relative to the global ground state configuration.

5. $\mathbb{Z}_2$ symmetry breaking in the fully frustrated model

We described the ground states of the fully frustrated XY model on the square lattice. The topological charges behaved as they should—repelling each other and in the process generating a checkerboard pattern. We now prove that the uniformly frustrated XY model
Figure 3. A $2 \times 2$ block with $f = 1/2$: $A_{25} = A_{58} = \pi$. 

has a $Z_2$ phase transition: a claim that, till now, has only been verified numerically and suggested by approximate schemes [46]. We show that the existence of a finite temperature phase transition is a consequence of finite energy domain walls between the two ground state domains. Very interesting earlier works examining topological excitations (including domain walls) are found in [49, 50].

5.1. Energy gaps on the square lattice

The topological charge sectors’ minima are separated from each other by finite energy gaps. For the $2 \times 2$ block in figure 3 the lowest energy configuration which does not belong to the ‘good’ sectors \( \{m_I = 1, m_{II} = 0, m_{III} = 1, m_{IV} = 0\} \) or \( \{m_I = 0, m_{II} = 1, m_{III} = 0, m_{IV} = 1\} \) topological charge sectors is given by \( \phi_{14} = \phi_{47} = \phi_{78} = \phi_{89} = \phi_{96} = \phi_{32} = 0 \) and \( \phi_{25} = \phi_{58} = \pi \) and it lies in \( \{m_I = 0, m_{II} = 0, m_{III} = 1, m_{IV} = 1\} \). The energy of this state is \( E_{0,0,1,1} = -8 \). Similarly if \( \phi_{25} = \phi_{58} = \epsilon - \pi \) (with \( \epsilon = 0^+ \)) a state of a similar energy lies in \( \{m_I = 1, m_{II} = 1, m_{III} = 0, m_{IV} = 0\} \). The energy of this state on a $2 \times 2$ block is \( E_{1,0,1,0} = -8 \). Thus the infimum of the energy in all other ‘bad’ topological charge sectors is \( E_{\text{inf}} = -8 \). The \( \{\phi_{ij} = \pm \pi/4\} \) states, although they are the global minima configurations, are not the lowest energy configuration on this fragment of the lattice with open boundary conditions. Nonetheless, these reference states lie in the ‘good sectors’ \( \{m_I = 0, m_{II} = 1, m_{III} = 0, m_{IV} = 1\} \) and \( \{m_I = 1, m_{II} = 0, m_{III} = 1, m_{IV} = 0\} \). The energy of this state is \( E_{\text{ref}} = -6\sqrt{2} \). In a system with periodic boundary conditions

\[
E = \frac{1}{L_c(L_c + 1)} \sum_{\text{Blocks}} \epsilon_{\lambda} \tag{45}
\]

where \( \epsilon_{\lambda} \) is the net energy of all bonds lying in an $L_c \times L_c$ block $\lambda$. The sum is performed over all overlapping $L_c \times L_c$ blocks. The multiplicative factor in front stems from the fact
that each bond will be included in the sum $L_c(L_c + 1)$ times if one were to cover a square lattice, with periodic boundary conditions, with all overlapping $L_c \times L_c$ blocks. We focus on the simplest case: $L_c = 2$. In equation (44), $\Delta_\pm \equiv \epsilon_{\text{bad}}^\text{inf} - \epsilon_{1,0,1,0}^\text{ref}$, with $\epsilon_{\text{ref}}$ the energy of a reference global ground state configuration (i.e. $\{\phi_{ij} = \pm \pi/4\}$) when evaluated on a finite $L_c \times L_c$ plaquette block. Within each small block $\lambda$, for states of the ‘bad’ incorrect topological charge registry:

$$\Delta_+ \leq \epsilon^\Lambda[{\{m_{x_1x_2}\}}] \neq \frac{1}{2}(1 + (-1)^{x_1 + x_2}) \text{ or } \frac{1}{2}(1 + ((-1)^{x_1 + x_2 + 1})) - \epsilon_{\text{ref}}$$

(46)

where, as before, $(x_1, x_2)$ label the plaquette coordinates in the plane. Averaging the last set of inequalities over the entire lattice ($\Lambda$):

$$E^\Lambda[{\{m_{x_1x_2}\}}] \geq E^{\Lambda_0} + \frac{\Delta_+}{L_c(L_c + 1)} N_b - \frac{\Delta_-}{L_c(L_c + 1)} N_{\text{good}}$$

(47)

where $E^{\Lambda_0}$ is the global ground state energy (of the lattice with periodic boundary conditions), $N_b$ denotes the number of blocks with incorrect $\{m_{x_1x_2}\}$ registry, while $N_{\text{good}}$ denotes the number of $2 \times 2$ blocks with the correct checkerboard registry. Henceforth, we denote

$$\Delta \equiv \Delta_+ - \Delta_- > 0.$$ 

(48)

Similarly, for the unfrustrated ($f = 0$) system, an $|m| = 1$ plaquette ($L_c = 1$) with open boundary conditions is elevated by, at least, $\Delta = \frac{7}{2}$ relative to the $m = 0$ ground state configuration. Here we employ the last relation to obtain a lower bound on the energy gap given the number of blocks (plaquettes in the $f = 0$ case) which do not have the correct topological charge registry (i.e. have nonzero vorticity $m \neq 0$). The reader can see how these bounds may be generalized to higher-order commensurate values of $f$, where the block size $L_c$ will be larger. These simple inequalities can be seen as a generalization of the Peierls bound [51].

We are now ready to apply the machinery of reflection positivity. Let us quickly outline the underlying logic: we assume that at infinity we have ‘good’ $g_2$ boundary conditions, by which we mean that one of the two types of topological charge checkerboard configurations will be found. We consequently bound the size of the region that is occupied by the other ‘good’ checkerboard ground state $g_1$. In essence, we bound the size of the region separating the two checkerboard configurations; in this region the topological charge configurations are ‘bad’ and costly in energy. The number $N_b$ of the blocks which have ‘bad’ topological charge configurations is, at least, linear in the perimeter of the regions (domain walls) surrounding the $g_1$ droplets. The correspondence to the Peierls proof of a phase transition in an Ising ferromagnet becomes transparent towards the end of the proof. We avoid Peierls’ contour inversion [51], opting instead for a direct computation of the ratio of partition functions in order to find the probabilities of various contours. We prove, trivially, that at sufficiently low temperatures the energy bounds on the cost of ‘bad’ regions (domain walls) translate into bounds on their probabilities.

5.2. Reflection positivity

We employ reflection positivity [13] as applied to a system invariant under a reflection about an axis $P$ passing through lattice sites. The uninitiated reader is referred to
appendix A for a brief exposure to this technique. We partition the plane into two sides which flank the axis $P$ (which itself lies along a line of bonds): $P\pm$. Let us define $P\pm$ as the union of $P\pm$ with $P$. Under reflection about $P$:

\[ R_p F(\vec{S}(\vec{x}_1), \ldots, \vec{S}(\vec{x}_n)) = F(R_p \vec{S}(\vec{x}_1), \ldots, R_p \vec{S}(\vec{x}_n)) \]  

with $\vec{x}_i$ planar locations. Thus, under reflection

\[ R_p A_{ij} = A_{R_i R_j}, \quad R_p \theta_i = \theta_{R_i} \]

if $\langle ij \rangle$ is vertical: $R_p \phi_{ij} = \phi_{ij}$

if $\langle ij \rangle$ is horizontal: $R_p \phi_{ij} = -\phi_{ij}$.  

(50)

For both horizontal and vertical bonds, $\cos \phi_{ij}$ is invariant under $R_p$. Defining

\[ B \equiv -\left[ \sum_{\langle ij \rangle \in P_{\pm}} -\frac{1}{2} \sum_{\langle ij \rangle \in P_{\pm}} \right] \cos \phi_{ij}, \]

(51)  

the Hamiltonian $H = B + R_p B$ is manifestly invariant under $R_p$ (yet the reflected plaquettes correspond to the same frustration $0 \leq f \leq 1/2$ only when $f = 0, 1/2$). As the sense of the circulation in the sum $\sum_{\langle ij \rangle \in P_{\pm}} \phi_{ij}$ is fixed over the entire lattice, under $R_p$: $(m_x - f) \rightarrow -(m_x - f)$. For $f = \frac{1}{2}$, the vorticities transform as

\[ m = -1, 0, 1, 2 \rightarrow 2, 1, 0, -1 \]  

(52)

under reflections. The correct (ground state pattern) set of topological charges \{\$m_x\$\} at the various planar locations $\vec{x}$ is invariant under $R_p$. This is to be expected, as the energies are unchanged by $R_p$—there is no energy increase along the reflection axis $P$. When $f = 0$, the vorticities transform as

\[ m = -1, 0, 1 \rightarrow 1, 0, -1 \]  

(53)

under $R_p$. For $0 < f < 1/2$, the quantity $2\pi [-(m - f)]$ is not an allowed value for the circulation sum. Let us define $b_k$ as the $L_c \times L_c$ topological charge pattern about the central plaquette at $\vec{x}_k$, and introduce a function $\omega_{b_k}(\vec{x})$ which is equal to one if $b_k$ is found within the $2 \times 2$ block centered about $\vec{x}$, and is equal to zero otherwise. Let us next reflect $b_k$ to cover the entire lattice $\Lambda$ and generate a vortex pattern $C_k$. One may define a partition function ($Z_{C_k}$) that is the sum of all of the Boltzmann weights corresponding to these configurations. There are two correct (checkerboard) topological charge configurations within the $L_c \times L_c$ block; we shall denote these topological charge configurations by $g_1$ and $g_2$. For all faulty (non-$g_1$ or non-$g_2$) blocks $b_k$ reflections generate $N_b > t'N$ faulty $L_c \times L_c$ blocks within the lattice with $t' > 0$. As before, let \{\$\lambda_i\$\} denote vortex patterns in the $L_c \times L_c$ blocks centered about the sites $i$, and let $\{g_1, g_2\}$ denote the two correct (checkerboard) vortex configuration within an $L_c \times L_c$ block. Note that the set \{\$\lambda_i\$\} consists of all maximally overlapping $L_c \times L_c$ blocks.
5.3. The kaleidoscope patterns: energy gaps on the reflected blocks

By repeatedly reflecting any $L_c \times L_c$ block $\lambda$ to cover the entire lattice we generate a periodic pattern of repetitive $2L_c \times 2L_c$ super-blocks. The planes $P$ may be either vertical or horizontal and for each orientation $R^2_{\text{horizontal}} = R^2_{\text{vertical}} = 1$. After two reflections by any two parallel planes the original pattern must emerge. Taking note of all possible ‘bad’ (non-checkerboard) $L_c \times L_c$ blocks one sees that in all cases the global pattern $C_k$ generated by consecutive reflections contains more bad $L_c \times L_c$ overlapping blocks than those of the checkerboard type: in equation (47) $N_b > N_{\text{good}}$. Consequently, the energies of the all-repetitive patterns satisfy

$$E_{C_k} > E_0 + \frac{\Delta}{L_c(L_c + 1)} N_b$$

$$> E_0^A + \frac{\Delta}{L_c(L_c + 1)} t'N,$$  \hspace{1cm} (54)

with $L_c = 2$, and, as denoted earlier, with the number of bad blocks in each repetitive pattern $N_b > t'N$.

5.4. Checkerboard estimates

Let us next define an angular volume $\Omega_\lambda$ within a $L_c \times L_c$ block such that $\sup_{\theta \in \Omega_\lambda} |\theta_i - \theta_i^{\text{ground}}| = \delta$ for all sites $i$ (where $\theta_i^{\text{ground}}$ denotes the angular configuration of a global ground state minimum on the entire lattice—the pinned down reference angular configuration with broken global $Z_2$ and $U(1)$ symmetries) and, correspondingly,

$$\max_{L_c \times L_c \text{ block partitions } \lambda} \sup \{\epsilon_\lambda\} = \epsilon_{\text{ref}} + \epsilon_0.$$  \hspace{1cm} (55)

The size of $\Omega_\lambda$ is $|\Omega_\lambda| = (2\delta)^9$. The volume $\Omega_\lambda$ is strictly contained in a single checkerboard sector. On the fringes ($\partial\Omega_\lambda$) of this volume:

$$\epsilon|_{\partial\Omega_\lambda} \leq \epsilon_{\text{ref}} + \epsilon_0,$$  \hspace{1cm} (56)

with $\epsilon_{\text{ref}}$ the energy of a global ground state configuration when evaluated on a finite $L_c \times L_c$ plaquette block, and $\epsilon_0 < \Delta$. Next, we define a global angular volume $\Omega$ such that $\sup_{\theta \in \Omega} |\theta_i - \theta_i^{\text{ground}}| = \delta$ for all lattice sites $i$. The energy of any global lattice configuration within this volume has an energy which is bounded from above by

$$E_{\partial\Omega} \leq E_0^A + \frac{N\epsilon_0}{L_c(L_c + 1)}.$$  \hspace{1cm} (57)

The definition of $\Omega$ and $\Omega_\lambda$ is made possible by the continuity in $\{\theta_i\}$ of the Hamiltonian in equation (1). Now $[Z_{C_k}/Z_{\text{tot}}]$ may be easily bounded at low temperatures

$$\frac{Z_{C_k}}{Z_{\text{tot}}} < \frac{Z_{C_k}}{Z_\Omega} < \frac{(2\pi)^N}{(2\delta)^N} \exp \left[ -\beta t'N \frac{\Delta - \epsilon_0}{L_c(L_c + 1)} \right]$$  \hspace{1cm} (58)

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where \((2\pi)^N\) is the net angular volume of the entire system and \((2\delta)^N\) is the volume of \(\Omega\). Here we noted the angular volume of \(C_k\) is bounded by \((2\pi)^N\). Let us define a ‘logical’ test function on a block \(\lambda_i\) centered about site \(i\) by 

\[ F(\lambda_i) = g_1, g_2 \] 

and 

\[ F(\lambda_i \neq g_1, g_2) = 0 \] 

(\(g_1, g_2\) is merely a variant of \(\omega_{b_k}(\bar{x}) : F = \omega_{g_1} + \omega_{g_2}\)). Let us furthermore define

\[ V(\bar{x}) \equiv \prod_{x \in \lambda_i} F(\lambda_i). \] 

The region where \(V(\bar{x})\) vanishes defines a domain \(D\). In the spirit of providing very generous upper bounds, let \(\ell\) denote the outer perimeter of \(D\), and let us pick merely 

\[ \ell' \equiv \max \left\{ \text{Int} \left[ \frac{\sqrt{\ell}}{8L_c} \right], 1 \right\}, \] 

non-overlapping faulty \(b_k\) (where \(\text{Int}[\ ]\) denotes the integer part). The probability of a domain \(D\),

\[ \text{Prob}(D) \leq \max \langle \omega_{b_1}(\bar{x}_1) \ldots \omega_{b_\ell}(\bar{x}_\ell) \rangle \leq \prod_{k=1}^{\ell'} \left[ \frac{Z_{C_k}}{Z_{\text{tot}}} \right]^{W/N} < \exp[-\beta W t \ell'] \] 

with

\[ t \equiv [t' (\Delta - \epsilon_0) - \beta^{-1} \ln(\pi/\delta)]/(L_c(L_c + 1)). \]

In the last inequality, the blocks \(\{\lambda_i\}\) are chosen to be non-overlapping: no spins are shared by two blocks (including the boundaries of the blocks). The second inequality in equation (61) followed from reflection positivity. (The reader is referred to equation (A.16) in appendix A for details.) Let \(G^i\) \((i = 1, 2)\) denote the support of the correct vortex configuration \((g_i)\) in a region of any size. Let us assume that at infinity, we have \(G^2\) boundary conditions. The probability of having a domain \(D\) incurred by \(N_{G^1}\) units (in a partitioning of the lattice to non-overlapping blocks) of the opposite checkerboard state is bounded by equation (61). The bounds on the area covered by the opposite checkerboard state may proceed as in the usual Peierls argument (see appendix B and equation (B.4) for details), to yield

\[ r \equiv \left\langle \frac{N_{G^1}}{N} \right\rangle < \sum_{\ell=4L_c, \ldots} \ell^2 3^\ell \exp \left[ -\beta W t \max \left\{ \text{Int} \left[ \frac{\sqrt{\ell}}{8L_c} \right], 1 \right\} \right]. \] 

The right-hand side can made as small as desired for \(\beta > \beta_c(r)\). Stronger bounds hold for all other ‘bad’ topological charge configurations. Thus, at sufficiently low temperatures, a spontaneous symmetry breaking is sparked by applying boundary conditions at infinity.

Analogously, for \(f = 0\), the fraction of \(|m| = 1\) vortices (which, for \(L_c = 1\), are elevated by at least \(\Delta = 7/2\) relative to the lowest lying \(m = 0\) configuration) is bounded from

7 Though not imperative here, more sophisticated bounds may be enacted via spin-wave calculations. See, e.g., [62], lemma 6.8 in particular.
above by arbitrary, exponentially small, numbers at sufficiently low temperatures: ‘pair
annihilation’.

Here we avoid the contour flipping algorithm of the standard Peierls argument by use
of reflection positivity to bound \( \text{Prob}(D) \) in equation (61). We kept \( L_c \) general (and have
not explicitly set \( L_c = 2 \)) in order to suggest other plausible extensions (not hinging on
reflection positivity) to other values of \( f \) for which \( L_c \) will be larger). To emphasize—in
this proof a necessary (but not sufficient requisite) is to establish a gap between the
minimum energy per site of ‘bad’ topological configurations on the \( L_c \times L_c \) block with
open boundary conditions and thermodynamic limit ground state tiling the entire plane
belonging to the ‘good’ topological sector (which we dubbed the ‘reference’ state). In
general, the open boundary condition minimum on \( \lambda \) cannot tile the entire plane and will
produce a slightly lower ground state energy per site than the ground state of the entire
lattice.

6. An alternative proof

The reader might be a bit dismayed that our proof seems to rest on the relatively fortuitous
event that for the small \( L_c = 2 \) the gap \( \Delta \equiv \Delta_+ - \Delta_- > 0 \). Had this not been the case we
might have been required to compute energies on much larger \( L_c \times L_c \) blocks. Moreover,
in the previous proof, in section 5.3, an explicit check that the number of bad blocks \( N_b \)
is greater than the number of good blocks was necessary for the configurations generated
by consecutive reflections of \( \{b_k\} \) to cover the entire lattice. Here we show that this is
not the case when attacking the problem along a slightly disparate path. In the spirit of
equations (51) and (A.1) let us define

\[
\epsilon_{\lambda'} \equiv \sum_{\langle ij \rangle \in R} \cos \phi_{ij} - \frac{1}{2} \sum_{\langle ij \rangle \in \partial \lambda'} \cos \phi_{ij}
\]  

(64)

for each \( s \times s \) block \( \lambda' \) (with an arbitrary integer \( s > 1 \)) such that

\[
E = \sum_{\lambda'} \epsilon_{\lambda'}
\]  

(65)

in a partition of the lattice with ‘marginally’ non-overlapping blocks \( \lambda' \) (nearest neighbor
blocks share only a common boundary \( \partial \lambda' \)). The form equation (64) is particularly suited
for reflection positivity treatments. Note that the open boundary condition ground state
\( \{\theta_i\} \) of \( \epsilon_{\lambda'} \) on the block \( \lambda' \) (the previous ‘reference state’) may be repeatedly reflected (as
\( f = 1/2 \) is congruent to \( (-f) \)) along the boundaries \( \partial \lambda' \) to tile the entire plane. Thus the
open boundary condition minimum on the small block is, in this case, a portion of the
global ground state.

Now, a finite energy gap \( \Delta > 0 \) (necessitated by our definition of ‘bad’ and ‘good’
topological sectors) separates the various ‘bad’ topological charge configurations (which
do not contain a ground state of \( \epsilon_{\lambda'} \) on the finite \( s \times s \) slab with open boundary conditions)
and the ground state value of \( \epsilon_{\lambda'} \). The reader might recognize \( \Delta \) as none other than \( \Delta_+ \)
for the particular case \( s = L_c \) as defined for the energy in equation (64). In computing
the probability of a domain $D$ we note that net domain size $N_b'$ depends on how we partition the plane into marginally non-overlapping blocks $\lambda'$. If, in a partitioning of a lattice into maximally overlapping blocks $\{\lambda\}$, we find $N_b$ faulty blocks of the incorrect topological charge registry then in the optimal partitioning of the lattice into marginally non-overlapping blocks $\{\lambda'\}$ we will find, at least,

$$N_b' = \text{Int} \left[ \frac{N_b + s^2 - 1}{s^2} \right]$$  \hspace{1cm} (66)

faulty blocks $\{\lambda_b'\}$. Consequently, in equation (62), we may substitute

$$\Delta \to \frac{\Delta}{s^2}$$  \hspace{1cm} (67)

and repeat the previous arguments of section 5.

Although, in the above, we focused attention on $s \times s$ square blocks, we could have chosen $\lambda'$ to be a domino: the minimal $(2 \times 1)$ plaquette configuration. There are two checkerboard $g_1, g_2$ states (the sectors $(m_1, m_2) = (1, 0)$ or $(0, 1)$) within the domino and all of our arguments may be reproduced with the factor $s^2$ of equations (66) and (67) replaced by the area of the domino (two plaquettes).

Thus, putting all of the pieces together, we have rigorously demonstrated, using various approaches, that at sufficiently low positive temperatures, the topological charges in the fully frustrated XY model form arrangements which lift the $Z_2$ symmetry associated with the two-fold degeneracy associated with the two ground state vortex patterns. This rigorous result reaffirms earlier tour de force numerical and extremely insightful, yet more approximate analytical treatments [1].

7. The standard XY model—vortex confinement

We may similarly bound the number of radius $r$ vortices ($r \gg 1$), which were defined previously, within the unfrustrated system. When $r \gg 1$ the energy penalty is no longer a mere $7J/2$, as it was for a vortex of size $r = 1$ (which was immediately adjacent to an antivortex), but rather a forbidding logarithmic function of $r$. Employing the reflection positivity inequality equation (A.11) with the energy penalty associated with the large radius vortex of equation (40), the probability of a vortex of size equation (40), the probability of a vortex of size $r$

$$\text{Prob}(r - \text{vortex}) < \left( \frac{r_1}{r} \right)^{\beta WK_1},$$  \hspace{1cm} (68)

where we once again employed the fact that the volume of the state generated by repeated reflections of the radius $r$ vortex to cover the entire plane has an angular volume which is trivially bounded by $(2\pi)^N$. This probability can be made as small as desired at sufficiently low temperatures (large $\beta$). The probability of a radius $r$ vortex drops algebraically with $r$.

There are no ‘real’ macroscopic vortices at sufficiently low temperatures. In [40], rigorous results on the related low-temperature Kosterlitz–Thouless phase in $k > 4$ state clock models (which, as we will further discuss in section 9, become the XY model in the $k \to \infty$ limit) were arrived at by a combination of contour arguments, exact dualities, and Griffiths’-type inequalities.
8. Kaleidoscope field patterns

Although in many instances (e.g. uniform non-commensurate $f$) the determination of the exact ground state is nontrivial there are several exceptions to the rule.

If the frustrations $\{f_{\lambda}\}$ form a kaleidoscope pattern—i.e. if they may be generated, starting from an arbitrary sequence of frustrations in a small region, by consecutive reflections in different planes to cover the entire lattice, then a ground state may also be formed by the same sequence of reflections. Let us now ‘elaborate’ and prove this statement. Let $\lambda'$ be a block spanning one or more plaquettes on which the frustrations at the different plaquettes are arbitrary. If the block is of finite size then the determination of the exact open boundary condition minimum of the energy functional $\epsilon_{\lambda'}$ defined in equation (64) will yield an angular configuration(s) $\{\theta_i\}$ on $\lambda'$. Now let us invert the frustrations and set $f_{\lambda''} = -f_{\lambda'}$ for the block $\lambda''$ which is the mirror image of $\lambda'$ about a plane $P_1$ which passes through one of the edges of $\lambda' : \lambda'' = R_{P_1} \lambda'$. We now note that the open boundary condition minimum of $\epsilon_{\lambda'}$ on the fused super-block $\lambda' \cup \lambda''$ must satisfy $\min\{\epsilon_{\lambda' \cup \lambda''}\} = \min\{\epsilon_{\lambda'} + \min\{\epsilon_{\lambda''}\}\}$, yet just such a configuration saturating the lower bound with an energy $\min\{\epsilon_{\lambda'} + \min\{\epsilon_{\lambda''}\}\}$ may be constructed. To do so we may simply leave the original angular configuration $\{\theta_i\}$ for all sites $i$ within the block $\lambda'$ untouched and set $\theta_i = \theta_{R_{P_1} i}$ for all sites $i$ in the reflected block $\lambda''$. We may now choose a different plane $P_2$ and keep repeating the process until $\lambda' \cup \lambda'' \cup \cdots$ spans the entire lattice. Perhaps the simplest realizations of such ground states are the staggered flux phases (of which the $f = 1/2$ ground state hitherto considered is a special example). As other realizations we may consider systems in which the frustration

$$f_{\bar{x}} = f \sin \left( \frac{\pi x_1}{n} \right) \sin \left( \frac{\pi x_2}{n} \right)$$

for all plaquettes $\bar{x}$ within the dual lattice with an arbitrary $f$ and a finite integer $n$. Here $\lambda'$ is the elementary $n \times n$ block. Any reflection of the frustrations $f_{\bar{x} \in \lambda'}$ inverts their sign on the sites $R_{P_2} \bar{x}$ which lie in $\lambda'_{i+1}$. Many systems, such as that of equation (69), are reflection positive and a proof of a finite temperature ordering similar to that for $f = 1/2$ follows.

9. Generalized $Z_k$ symmetry and magnetic groups

For a uniform frustration $f = p/q$ with relatively prime $p, q \geq 3$, the topological charge ground state consists of repetitive units extending $k_1, k_2$ units along the $x_1, x_2$ axis respectively. By translating the origin in the covering of the lattice by non-overlapping blocks, we may generate $k = k_1 k_2$ ground state configurations within the repetitive blocks. To describe this viable translational $Z_{k_1} \otimes Z_{k_2}$ symmetry, we may extend the definition of the $Z_2$ order parameter previously defined:

$$M_k \equiv \sum_{\lambda} \sum_{g} \omega_g(\lambda) \exp[2\pi i g/k]$$

(70)
where the sum is now over non-overlapping blocks $\lambda$ and possible ground state topological charge sectors $g$. As before, $\omega_g(\lambda) = 1$ if the pattern $b_g$ appears in $\lambda$ and is zero otherwise. We may similarly define the two block correlator $\langle \omega_i(\lambda)\omega_j(\lambda') \rangle$ for two blocks $\lambda$ and $\lambda'$ appearing in a partitioning of the lattice into non-overlapping blocks. In the limit $q \to \infty$ (irrational $f$) the discrete translational symmetry transforms into a continuous symmetry

$$Z_{k_i} \to_{k \to \infty} O(2),$$

(71)

and the translational symmetry group becomes the symmetry group of the two-torus.

Classical two-dimensional $Z_{k>4}$ clock models exhibit two transitions at self-dual temperatures values [40]. In the temperature regime between the higher and lower transition temperatures the system exhibits algebraic long-range order with algebraically decaying correlations; below the lowest transition temperature, the system exhibit long-range order while it is disordered at temperatures above the higher of the two transition temperatures. In the large-$k$ limit of the clock model, the lower transition temperature veers to zero and the algebraic Kosterlitz–Thouless phase appears all of the way down to zero temperature.

The $Z_2$ and $O(2)$ symmetries present in the $f = 1/2$ XY model become two $O(2)$ symmetries in the limit of large $q$ (continuous $f$). Physically, all possible translations of a given ground state configuration amount to a rotation of the spins by all possible angles. One might speculate that perhaps for irrational $f$, there is no finite temperature vortex ordering (no explicit $Z_{k_i} \to O(2)$ symmetry breaking) but rather a finite temperature Kosterlitz–Thouless-like transition. Such a viable link between the degeneracy amongst states generated by displacements and those created by global rotations is also found elsewhere. In the Quantum Hall problem, the degenerate states may be labeled in terms of their angular momentum quantum numbers or, alternatively, by their magnetic translation operator eigenvalues. On a lattice (the Hofstader problem [52]) the correct degeneracy is easily read off in terms of the magnetic translation operators; the flux piercing the fundamental cell is an integer multiple of the elementary fluxon. An irrational flux $f$ might lead to an effective loss of commensurability effects (the size of the elementary cell becomes of the order of the system size) and the equivalence between those degeneracies spawned by translations and those created by rotations may be restored. The sole (albeit important) distinction between the Quantum Hall problem and the frustrated XY model is that in the latter the magnitude of the ‘wavefunction’ is pinned ($|\psi(\vec{x})| = 1$) and only the (XY) phase varies whereas in the Quantum Hall problem both phase and amplitude vary.

In addition to the trivial $Z_{k_i}$ groups generated by displacements, one finds in certain instances a greatly enhanced symmetry group. The ground states of the frustrations $f = 1/3$ and $f = 1/4$ are a case in point [1]. Here a multitude of ‘zero-energy domain walls’ appear. Phrased in our language this implies that nontrivial coverings of the lattice are possible such that within all overlapping blocks $\lambda$ we find the reference global ground state minimum configuration. At low temperatures the infinite degeneracy is lifted by the free energy of spin waves.

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8 Further, as the magnetic flux $f$ piercing a type II superconductor increases, the superconducting $T_c$ (associated with phase ordering) monotonically decreases. By a naive analogy one might expect the phase ‘ordering’ temperature $T_{XY}(f)$ to drop monotonically for small $f$. 

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10. Isotropic to nematic transitions

Just as we were able to bound, at low temperatures, the number of free vortices within the unfrustrated XY model we may also prove that free disclinations in a liquid crystal system must condense at sufficiently low temperature; such a confinement of disclinations occurs in the transition between the isotropic and nematic (or ‘topologically’ ordered [55]) phases. Similar arguments apply for other systems having other order parameter symmetries. Within the (unfrustrated) XY model, the $O(2)$ vortices are elevated by a finite amount relative to the ground state. Similarly within lattice models of liquid crystals the $RP^2$ topological defects (disclinations) of the headless director fields $\mathbf{n}$ must incur an energy cost relative to the defect-free ground state. This fused with a reflection positivity symmetry which is present in many of these models (for some lattice and continuum models, including those for which reflection positivity and other considerations were employed for proofs of intermediate phases, as evinced by angular correlation functions, see [53]–[57]), allows us to set bounds via checkerboard estimates on the frequency of disclinations (the topological charges in nematic systems) at sufficiently low temperatures. Analogously, one may examine an analogue of the fully frustrated XY model: a nematic model on a lattice (as in [55]) having half an $RP^2$ fluxon thread each of its plaquettes. Similar arguments may be used to bound the frequency and size of topological defects associated with different systems.

11. Conclusions

We presented a theoretical study of the XY model with specific emphasis on the fully frustrated case. A main result is a proof of the existence of a $Z_2$ symmetry breaking transition within the fully frustrated XY model consistent with previous numerical results and approximate analytical treatments available in the literature [1]. More generally, we discussed extensions of the methods that we introduced here to other arenas and models where similar binding and orders of topological charges appear (confinement of disclinations in the isotropic to nematic transition, topological charge orders in various XY models and bounds on vortices within the unfrustrated XY model). A key complication that our treatment overcomes is the non-exact equivalence between the energies of the continuous angular system that we investigate and the energies of the system in different sectors of discrete topological charges; unlike the spectral character of the discrete dual topological charge system with Coulomb-type interactions, the energies of angular configurations that lie in different topological charge sectors partially overlap with each other and are nested.

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Appendix A. What is reflection positivity?

Reflection positivity has long been a tool reserved for the cabinets and drawers of mathematical physicists. Our simple minded nuts and bolts approach presented below [12] is geared toward our very specific limited set of problems and is quite superficial. It does the field no justice. For a more detailed and rigorous exposition the reader is referred to [13, 58]. We remark that in a more recent interesting work, reflection positivity has been employed to study quantum topological orders [18].

To simply understand reflection positivity with a relative minimum formalism, let us imagine that we partition our model into two sides which flank an orthogonal bisecting plane $P$ (which itself lies along a line of bonds): $P_\pm$. Let us define $P_\pm$ as the union of $P_+$ with $P$. In a reflection positive system, there exists an operator $B$ such that the Hamiltonian may be expressed as

$$H = B + R_P B.$$  \hfill (A.1)

As noted earlier in the text, the reflection operator $R_P$ about the plane $P$ is defined by

$$R_P F(\vec{S}(\vec{x}_1), \ldots, \vec{S}(\vec{x}_n)) = F(R_P \vec{x}_1, \ldots, R_P \vec{x}_n),$$  \hfill (A.2)

where $\vec{x}_i$ denotes the planar location of site $i$.\footnote{If any Hamiltonian is initially defined only on a finite size fragment of the lattice (where it is $B$) then by applying equation (A.1) repeatedly with different bounding planes $P_\alpha$, we may generate a reflection positive Hamiltonian (with respect to the planes $\{P_\alpha\}$) which spans the entire lattice.}

The basic inequality that we will need is given by the following statement: the thermal average

$$\langle OR_P O \rangle \geq 0$$  \hfill (A.3)

for all functions $\{O\}$. (In other words, such thermal averages behave like inner products in a ‘positive’ sense.)

Proof. Let us write the thermal average longhand

$$\langle OR_P O \rangle = Z^{-1} \sum_{\{\vec{S}_i\} \in \mathcal{P}_+} \sum_{\{\vec{S}_i\} \in \mathcal{P}_-} \sum_{\{\vec{S}_i\} \in \mathcal{P}} OR_P O \exp[-\beta (B + R_P B)],$$  \hfill (A.4)

where the partition function $Z > 0$. Thus the sign of the thermal average is the sign of the multiple sum which, by symmetry, may be folded back onto one half plane to become a sum of squares when $\{O\}$ is a local operator defined on $\mathcal{P}_+$ or on $\mathcal{P}_-$. Let $F \equiv O \exp[-\beta B]$ be an operator on $\mathcal{P}_+$. Let us explicitly segregate the spin arguments in $\mathcal{P}_+$ which correspond to spins lying on $P$ (which we shall denote by $\{S(\vec{x})\}$) and those that lie on $P_+$ (labeled by $\{S(\vec{x})\}$). Note that (equation (A.2)) $R_P F$ on $\mathcal{P}_-$ is identical to $F$ on $\mathcal{P}_+$. Thus equation (A.4) reads

$$Z^{-1} \sum_{\{\vec{S}_i\} \in \mathcal{P}_+} \left[ \sum_{\{\vec{S}_i\} \in \mathcal{P}_-} F(\{\vec{S}(\vec{x}_i \in \mathcal{P}_+), \{\vec{S}(\vec{x}_j \in \mathcal{P}_-)\} \right]^2 \geq 0,$$  \hfill (A.5)

which proves the principal equation (A.3). \hfill \blacksquare
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Inserting $O = A - B \langle BR_p A \rangle / \langle BR_p B \rangle$ in equation (A.3), a Schwarz inequality

$$\langle AR_p B \rangle^2 \leq \langle AR_p A \rangle \times \langle BR_p B \rangle$$  (A.6)

results. Setting $O = A - \langle A \rangle$ in equation (A.3) (or $B = 1$)

$$\langle A \rangle^2 \leq \langle AR_p A \rangle.$$  (A.7)

We note [12] that this general inequality allows us immediately to prove that in symmetric (reflection positive) opposite topological charges always attract (the probability of having a vortex–antivortex pair is greater than or equal to having vortices separated by an infinite distance. The proof is trivial: let $A$ denote the event of finding a vortex centered about point $\vec{x}$: $A = 1$ if a vortex is found at $\vec{x}$ and is zero otherwise. In such a case $\langle AR_p A \rangle$ denotes the probability of finding one vortex at $\vec{x}$ and one antivortex at its mirror image $R_p \vec{x}$.

The inequality derived in equation (A.7)

$$\langle AR_p A \rangle \geq \langle A \rangle^2$$  (A.8)

reads, upon letting $A$ be the above function,

$$\text{Prob(vortex at } \vec{x} \text{ and antivortex at } R_p \vec{x}) \geq [\text{Prob(vortex at } \vec{x})]^2.$$  (A.9)

$[-\ln \langle AR_p A \rangle]$ is, diagrammatically, the free energy of the system with two additional external legs at $\vec{x}$ and $R_p \vec{x}$ minus the free energy of the closed system without any external topological charges. The last set of inequalities implies that the free energy of a finite separation vortex–antivortex pair is lower than that at infinite distance. This also applies to situations wherein uniform boundary effects are considered—these may be reflected relative to a plane $P$ orthogonal to the boundary. This applies to all topological charges in reflection positive theories)—a similar yet weaker version of the relations derived in [59]. This provably attractive nature in symmetric systems [12] has ramifications in numerous arenas, including the sign of the Casimir forces [14]. We may repeat the last step $n$ times in a row to get

$$\langle A \rangle^{2^n} \leq \langle A(R_{P_1} A(R_{P_2} A(\ldots R_{P_n} A \ldots)) \rangle.$$  (A.10)

If we set the size of the system to be $N = 2^n$ then the last inequality would imply that

$$\langle \text{local } A \rangle \leq \langle \text{Reflected } A \rangle^{(W/N)}$$  (A.11)

where local $A$ denotes the local function $A$ and Reflected $A$ denotes the function $A$ generated by consecutive reflections of $A$ in different planes, until it covers the entire lattice. We have more cautiously inserted a constant $W$ instead of one. The functions $A$ that were of interest to us were local test functions that were equal to one if a specific local configuration was found and were zero otherwise. In this manner the probability of finding certain necessarily ‘bad’ configurations, lying on the interface between the two
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ground state domains, may be bounded. Here the thermal average $\langle A \rangle$ is the probability that such a ‘bad’ configuration would be found.

$$\langle \text{Reflected } A \rangle = \frac{Z_{\text{Reflected } A}}{Z}$$ \hspace{1cm} (A.12)

where $Z_{\text{Reflected } A}$ is the sum of all Boltzmann weights corresponding the Reflected A configuration which spans the entire lattice, and $Z$ is, as usual, the sum of all Boltzmann weights—the partition function. Equations (A.11) and (A.12) bound the probabilities of certain local configurations.

We will now fortify and extend these relations to reach the more sophisticated inequality (equation (A.16)) employed in our proof. Suppose that $A_1$ denotes the observation of a certain local configuration about point $\vec{x}_1$ while $A_2$ denotes the test function for another configuration being seen at $\vec{x}_2$. By the Schwarz inequality (equation (A.6))

$$\langle A_1 A_2 \rangle^2 = \langle A_1 R_p \bar{A}_2 \rangle^2 \leq \langle A_1 R_p A_1 \rangle \times \langle A_2 R_p A_2 \rangle,$$ \hspace{1cm} (A.13)

where $\bar{A} \equiv R_p A$. We now repeatedly apply equation (A.7) (as in equation (A.10)) to the right-hand side of equation (A.13) to obtain

$$\langle A_1 A_2 \rangle \leq \langle \text{Reflected } A_1 \rangle^{(W/N)} \times \langle \text{Reflected } A_2 \rangle^{(W/N)},$$ \hspace{1cm} (A.14)

which may be followed by an insertion of the identity in equation (A.12). For the correlation function of three local configuration test functions we may note that

$$\langle A_1 A_2 A_3 \rangle^3 = \langle (A_1 A_2) R_p \bar{A}_3 \rangle \times \langle (A_1 A_3) R_p \bar{A}_2 \rangle \times \langle (A_2 A_3) R_p \bar{A}_1 \rangle,$$ \hspace{1cm} (A.15)

i.e., a product of terms of the form $\langle A R_p B \rangle$. We may consequently apply the Schwarz inequality, as was done in equation (A.13), and then invoke equation (A.12) to obtain a simple extension of equation (A.14). Thus, as the reader can see, for the $\ell$th-order correlator we have

$$\left\langle \prod_{i=1}^{\ell} A_i \right\rangle \leq \prod_{i=1}^{\ell} \left[ \frac{Z_{\text{Reflected } A_i}}{Z} \right]^{W/N}.$$ \hspace{1cm} (A.16)

Equations (A.16) are a central result. With these relations (the checkerboard estimates), local correlations (appearing on the left-hand side) may be efficiently bounded in terms of global events (which form the right-hand side).

Appendix B. Contour arguments

In a two-dimensional nearest neighbor Ising system the probability of having a certain specific contour of length $\ell$ separating an island of ‘−’ ($'N'_G\bar{i}$) spins in a sea of ‘+’ spins (or vice versa) is bounded by $\exp[-2\beta J\ell]$ when the exchange constant units are restored. Here we repeat a variant of the standard Peierls argument for the benefit of our readers. Let us assume that there are ‘+’ conditions at infinity. We may evaluate the probability

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that the lattice site \( \vec{x} = 0 \) is occupied by a ‘−’ spin. To have a minus spin at the origin there must be at least one contour \( \Gamma \) encircling the site 0.

\[
\text{Prob}(S(\vec{x} = 0) = -1) \leq \sum_{\Gamma \text{ enc. } 0} \text{Prob}(\Gamma). \tag{B.1}
\]

The probability of a given contour \( \Gamma \) of length \( \ell \):

\[
\text{Prob}(\Gamma) = \frac{Z_{\Gamma}}{Z} < \frac{Z_{\Gamma}}{Z_{\Gamma \text{ flipped}}} = \exp[-2\beta J\ell], \tag{B.2}
\]

where \( Z_{\Gamma \text{ flipped}} \) is the sum of Boltzmann weights over all spin configurations in which the contour \( \Gamma \) is flipped: all of the spins inside \( \Gamma \) are flipped with all other spins in the system being untouched. The energy of each individual configuration summed upon in \( Z_{\Gamma} \) is exactly \( 2J\ell \) higher than that configuration in which \( \Gamma \) is flipped—whence the second equality in equation (B.2) follows. A moment’s reflection reveals that \( Z_{\Gamma \text{ flipped}} \) only contains a subset of all the terms which are present in \( Z \) and consequently \( Z_{\Gamma \text{ flipped}} < Z \), implying the inequality in equation (B.2). Equation (B.1) implies that

\[
\text{Prob}(S(\vec{x} = 0) = -1) < \sum_{\ell=4,6,...} n(\ell) \exp[-2\beta J\ell]. \tag{B.3}
\]

We now bound the number, \( n(\ell) \), of contours of specified length \( \ell \). This number is bounded from above by the number of unrestricted random walks of length \( \ell \). If given a unique starting point, the number of non-backtracking random walks of length \( \ell \) on the square lattice is bounded by \( 4 \times 3^{\ell-1} \). The number of possible starting points for a random walk enclosing the origin \( (\vec{x} = 0) \) is strongly bounded by the area enclosed by the contour. For a given contour length \( \ell \) this maximal area is \( (\ell/4)^2 \), corresponding to a square of side \( \ell/4 \). Bounding this maximal area by \( 3\ell^2/4 \) provides a very generous overestimate.

Fusing all of the bounds together:

\[
\text{Prob}(S(\vec{x} = 0) = -1) = \left( \frac{N_G}{N} \right) < \sum_{\ell=4,6,...} \ell^2 3^\ell \exp[-2\beta J\ell]. \tag{B.4}
\]

The last sum can be made smaller than \( 1/2 \) (indicating symmetry breaking) for sufficiently large \( \beta \) (low temperatures). The proofs presented for the XY models (section 5.2) rest on the same logic with the twist that the contour inversion probability bounds (equation (B.2)) are replaced by the reflection positivity inequality of equation (A.16). In [40], similar bounds were employed to prove a low temperature orders; exact duality arguments were then invoked to establish the existence of an upper Kosterlitz–Thouless-type transition temperature for \( Z_k>4 \) models. As noted earlier, in the \( k \rightarrow \infty \) limit, \( Z_k \rightarrow O(2) \) which cannot be broken in two-dimensions and only the upper (Kosterlitz–Thouless) transition temperature remains.

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