Topological order in XY models in $D = 3$

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Abstract

A simple picture is developed to show how XY models in $D = 2 + 1$ dimensions can acquire phases with $\mathbb{Z}_2$ topological order.

I. THE CLASSICAL XY MODELS

This section recalls some well-established results on the classical statistical mechanics of the XY model at non-zero temperature in dimensions $D = 2$ and $D = 3$. Later, we will extend these models to studies of topological order in quantum models at zero temperature.

The degrees of freedom of the XY model are angles $0 \leq \theta_i < 2\pi$ on the sites i of a square or cubic lattice. The partition function is

$$\begin{aligned}
\mathcal{Z}_{XY} &= \prod_i \int_0^{2\pi} \frac{d\theta_i}{2\pi} \exp\left(-\mathcal{H}_{XY}/T\right) \\
\mathcal{H}_{XY} &= -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j)\,,
\end{aligned} \tag{1}$$

where the coupling $J > 0$ is ferromagnetic and so the θ_i prefer to align at low temperature. A key property of the model is that the $\mathcal{H}_{XY}$ is invariant under $\theta_i \to \theta_i + 2\pi n_i$, where the n_i are arbitrary integers.

A. Symmetry breaking in $D = 3$

There is a well-studied phase transition in $D = 3$, associated with the breaking of the symmetry $\theta_i \to \theta_i + c$, where c is any i-independent real number. As shown in Fig. 1, below a critical temperature T_c, the symmetry is broken and there are long-range correlations in the complex order parameter

$$\Psi_j \equiv e^{i\theta_j} \tag{2}$$

with

$$\lim_{|r_i - r_j| \to \infty} \left\langle \Psi_i \Psi_j^* \right\rangle = |\Psi_0|^2 \neq 0\,. \tag{3}$$

For $T > T_c$, the symmetry is restored and there are exponentially decaying correlations, along with a power-law prefactor, as indicated in Fig. 1. This prefactor is the Ornstein-Zernike form [1], and arises from the three-dimensional Fourier transform of $(\vec{p}^2 + \xi^{-2})^{-1}$, where $\vec{p}$ is a three-dimensional momentum. The critical theory at $T = T_c$ is described by the XY Wilson-Fisher CFT [2].

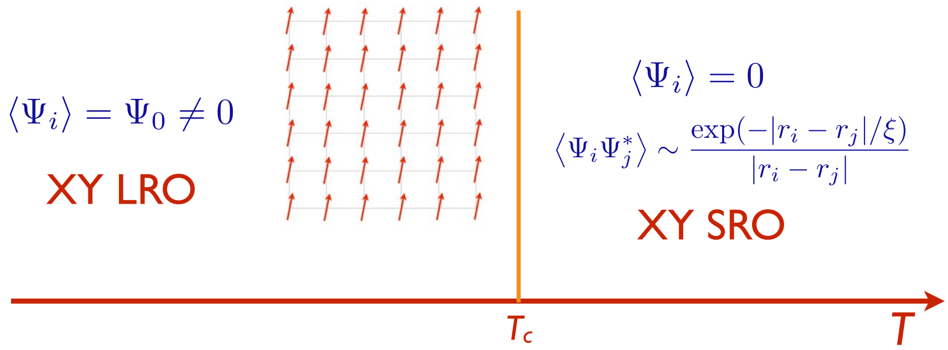

FIG. 1. Phase diagram of the classical XY model in Eq. (1) in $D = 3$ dimensions. The low T phase has long-range order (LRO) in Ψ, while the high T has only short-range order (SRO).

B. Topological phase transition in $D = 2$

In dimension $D = 2$, the symmetry $\theta_i \to \theta_i + c$ is preserved at all non-zero T. There is no LRO, and

$$\langle \Psi_i \rangle = 0 \text{ for all } T > 0.$$

Nevertheless, as illustrated in Fig. 2, there is a Kosterlitz-Thouless (KT) phase transition at $T = T_{KT}$ [3–6], where the nature of the correlations changes from a power-law decay at $T < T_{KT}$, to an exponential decay (with an Ornstein-Zernike prefactor) for $T > T_{KT}$. At low T, long-wavelength spin-wave fluctuations in the θ_i are sufficient to destroy the LRO and turn it into quasi-LRO (QLRO) with a power-law decay of fluctuations. At high T, there is SRO with exponential decay of correlations. KT showed that the transition between these phases occurs as a consequences of the proliferations of point-like vortex and anti-vortex defects, illustrated in Fig. 2. Each defect is associated with a winding in the phase gradient far from the core of the defect:

$$\oint dx_i \, \partial_i \theta = 2\pi n_v \,, \tag{4}$$

where the integer n_v is a topological invariant characterizing the vorticity. In the QLRO phase, the vortices occur only in tightly bound pairs of $n_v = \pm 1$ so that there is no net vorticity at large scales; and in the SRO phase, these pairs undergo a deconfinement transition to a free plasma. So the QLRO phase is characterized by the suppression of the topological vortex defects. By analogy with the suppression of $\mathbb{Z}_2$ flux defects in the topological-ordered phase of the $\mathbb{Z}_2$ gauge theory, we conclude that the low T phase of the $D = 2$ XY model has *topological order*, and the KT transition

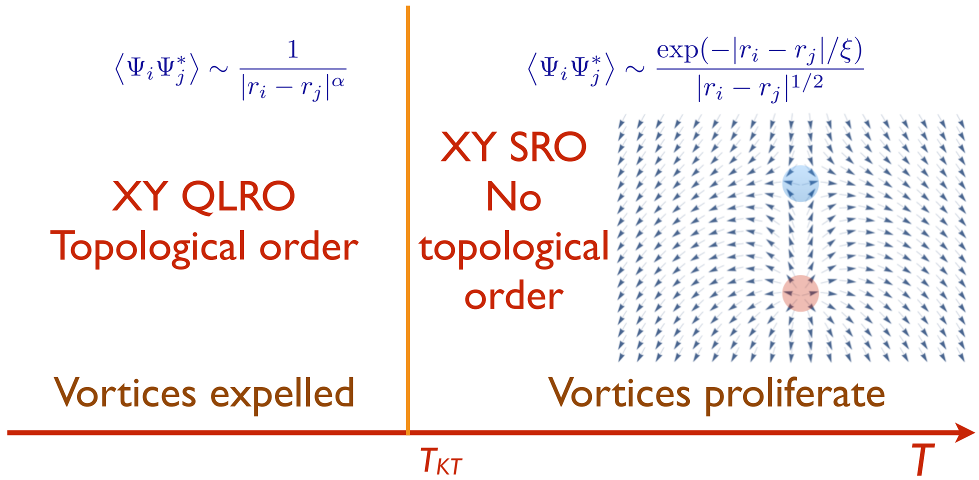

FIG. 2. Phase diagram of the classical XY model in Eq. (1) in $D = 3$ dimensions. There is no LRO at any T. The low T phase has quasi long-range order (QLRO) in Ψ, while the high T has SRO. The KT transition is associated with the proliferation of vortices, and also a change in the form of the correlations of the XY order parameter from power-law to exponential.

is a topological phase transition [5]. Of course, in the present case, the phase transition can also be identified by the two-point correlator of Ψ_i changing from the QLRO to the SRO form, but KT showed that the underlying mechanism is the proliferation of vortices and so it is appropriate to identify the KT transition as a topological phase transition.

II. TOPOLOGICAL ORDER IN XY MODELS IN $D = 2 + 1$

In the study of classical XY models in Section I, we found only a symmetry breaking phase transition in $D = 3$ dimensions. In contrast, the $D = 2$ case exhibited a topological phase transition without a symmetry breaking order parameter. This section shows that modified XY models can also exhibit a topological phase transition in $D = 3$ dimensions.

Classical XY models also have an interpretation as quantum XY models at zero temperature in spatial dimensionality $d = D - 1$, where one of the classical dimensions is interpreted as the imaginary time of the quantum model. And the quantum XY models have the same phases and phase transitions as models of lattice bosons with short-range interactions. Specifically, the classical $D = 3$ XY models we study below map onto previously studied models of bosons on the square lattice at an average boson number density, $\langle \hat{N}_b \rangle$, which is an integer [7–10]. These boson models are illustrated in Fig. 3. As indicated in Fig. 3, it is possible for such boson models to have

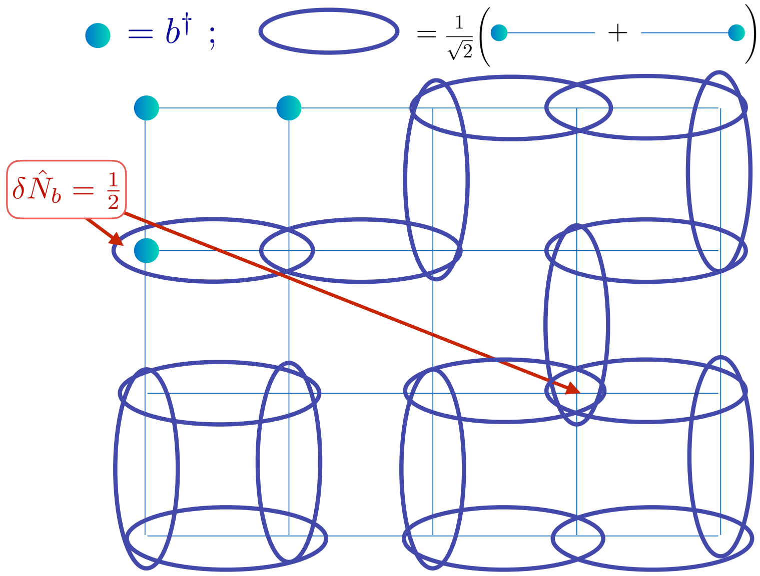

FIG. 3. Schematic representation of a topologically ordered, 'resonating valence bond' state in the boson models of. The boson $b^\dagger$ can reside either on sites (indicated by the filled circles) or in a bonding orbital, or 'valence bond', between sites (indicated by the ellipses). The average boson density of the ground state is 1. A single additional boson has been added above, and it has fractionalized into 2 excitations carrying boson number $\delta\hat{N}_b = 1/2$ (this becomes clear when we consider each bonding orbital as contributing a density of 1/2 to each of the two sites it connects).

topologically ordered phases which have excitations with a fractional boson number $\delta\hat{N}_b = 1/2$.

We now return to the discussion of classical XY models in $D = 3$ because they offer a transparent and intuitive route to describing the nature of topological order in $D = 2 + 1$ dimensions. The quantum extension of the discussion below will appear in Section III. We consider an XY model which augments the Hamiltonian in Eq. (1) by longer-range couplings between the θ_i, *e.g.*:

$$\widetilde{\mathcal{H}}_{XY} = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) + \sum_{ijk\ell} K_{ijk\ell} \cos(\theta_i + \theta_j - \theta_k - \theta_\ell) + \ldots\ldots \tag{5}$$

The additional couplings $K_{ijk\ell}$ preserve the basic properties of the XY model: invariance under the global U(1) symmetry $\theta_i \to \theta_i + c$, and periodicity in $\theta_i \to \theta_i + 2\pi n_i$. We will not work out the specific forms of the $K_{ijk\ell}$ needed for our purposes, but instead use an alternative form in Eq. (6)

below, in which these couplings are decoupled by an auxiliary Ising variable, and they all depend upon a single additional coupling K. At small K, the model will have the same phase diagram as that in Fig. 1. But at larger K, we will obtain an additional phase with topological order, as shown in Fig. 4. We will design the additional couplings so that the topological phase proliferates only

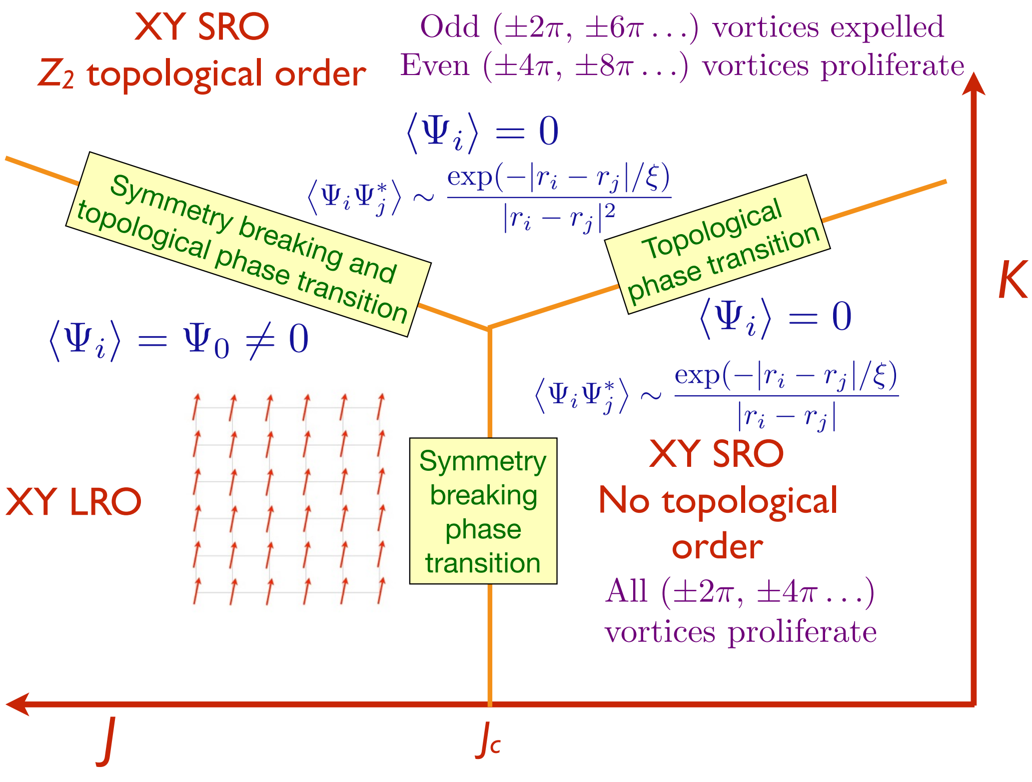

FIG. 4. Schematic phase diagram of the classical $D = 3$ XY model at non-zero temperature in Eq. (6), or the quantum $D = 2 + 1$ XY model at zero temperature in Eq. (9) along with the constraint in Eq. (11). The XY order parameter is Ψ (Eq. (2). These models correspond to the case of bosons on the square lattice with short-range interactions, and at integer filling. The two SRO phases differ in the prefactor of exponential decay of correlations of the order parameter. But more importantly, the large K phase has topological order associated with the expulsion of odd vortices: this topological order is the same as that in the $\mathbb{Z}_2$ gauge theory of Lec7 at small g. The transition between the SRO phases is also in the same university class as the confinement-deconfinement transition of the $\mathbb{Z}_2$ gauge theory of Lec7. A numerical simulation of a model with the same phase diagram is in Ref. [9].

even line vortex defects *i.e.* vortex lines for which the integer n_v in Eq. (4) is even. So the transition to topological order from the non-topological SRO phase occurs via the expulsion of odd vortex defects, including the elementary vortices with $n_v = \pm 1$. The additional K-dependent couplings in the XY model will be designed to suppress vortices with $n_v = \pm 1$. This transition should be compared to the KT transition in $D = 2$, where both even and odd vortices are suppressed as the temperature is lowered into the topological phase. Note that the new topological phase only has SRO with exponentially decaying correlations of the order parameter, unlike the QLRO phase of the $D = 2$ XY model. But, there is a subtle difference between the two-point correlators of Ψ_i in the two SRO phases in Fig. 4: the power-law prefactors of the exponential are different between the topological and non-topological phases.

We now present the partition function of the XY model of Fig. 4, related to models in several previous studies [7–19]:

$$
\begin{aligned}
\widetilde{\mathcal{Z}}_{XY} &= \sum_{\{\sigma_{ij}\}=\pm 1} \prod_i \int_0^{2\pi} \frac{d\theta_i}{2\pi} \exp\left(-\widetilde{\mathcal{H}}_{XY}/T\right) \\
\widetilde{\mathcal{H}}_{XY} &= -J \sum_{\langle ij \rangle} \sigma_{ij} \cos\left[(\theta_i - \theta_j)/2\right] - K \sum_{\square} \prod_{(ij)\in\square} \sigma_{ij} \,,
\end{aligned}
\tag{6}
$$

where sites i reside on the $D = 3$ cubic lattice. This partition function is the basis for the schematic phase diagram in Fig. 4, and numerical results for such a phase diagram appear in Ref. [9].

As written, the partition function has an additional degree of freedom $\sigma_{ij} = \pm 1$ on the links $\ell \equiv (ij)$ of the cubic lattice: these are Ising gauge fields. It is not difficult to sum over the σ_{ij} explicitly order-by-order in K, and then the resulting effective action for θ_i has all the properties required of a XY model: periodicity in $\theta \to \theta + 2\pi$ and global U(1) symmetry. We can view the σ_{ij} as a discrete Hubbard-Stratanovich variable which has been used to decouple the $K_{ijk\ell}$ term in Eq. (5). So we are justified in describing $\widetilde{\mathcal{Z}}_{XY}$ as a modified XY model. However, for our purposes, it will be useful to keep the σ_{ij} explicit.

In the form in Eq. (6), a crucial property of $\widetilde{\mathcal{Z}}_{XY}$ is its invariance under $\mathbb{Z}_2$ gauge transformations generated by $\varrho_i = \pm 1$:

$$
\theta_i \to \theta_i + \pi(1 - \varrho_i) \quad , \quad \sigma_{ij} \to \varrho_i \sigma_{ij} \varrho_j \,. \tag{7}
$$

Note that the XY order parameter, Ψ_i, is gauge-invariant.

The rationale for our choice of $\widetilde{\mathcal{H}}_{XY}$ becomes evident upon considering the structure of a 2π vortex in θ_i, sketched in Fig. 5. Let us choose the values of θ_i around the central plaquette of this vortex as (say) $\theta_i = \pi/4, 3\pi/4, 5\pi/4, 7\pi/4$. Then we find that the values of $\cos\left[(\theta_i - \theta_j)/2\right] > 0$ on all links except for that across the branch cut between $\pi/4$ and $7\pi/4$. For $J > 0$, such a vortex will

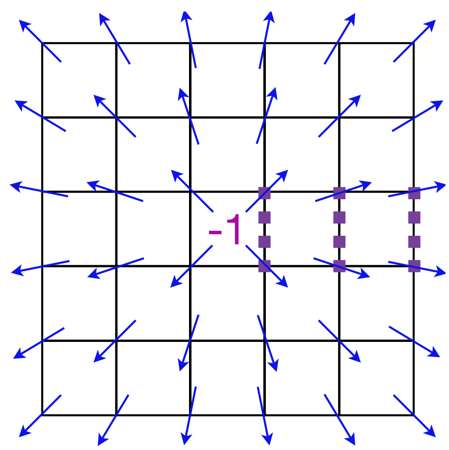

FIG. 5. A 2π vortex in θ_i. The $\mathbb{Z}_2$ gauge field $\sigma_{ij} = -1$ on links (indicated by thick dashed lines) across which θ_i has a branch cut, and $\sigma_{ij} = 1$ otherwise. The $\mathbb{Z}_2$ flux of -1 is present only in the central plaquette, and so a vison is present at the vortex core. If the contour of $\sigma_{ij} = -1$ deviates from the branch cut in θ_i, there is an energy cost proportional to the length of the deviation. Consequently, the vison is confined to the vortex core.

have $\sigma_{ij} = -1$ only for the link across the branch cut. So a 2π vortex will prefer $\prod_{(ij)\in\square} \sigma_{ij} = -1$, *i.e.* a 2π vortex has $\mathbb{Z}_2$ flux $= -1$ in its core, and then a large $K > 0$ will suppress (odd) 2π vortices. Note that there is no analogous suppression of (even) 4π vortices. This explains why it is possible for $\widetilde{\mathcal{H}}_{XY}$ to have large K phase with odd vortices suppressed, as indicated in Fig. 4.

The existence of a phase transition between the two SRO phases of Fig. 4 can be established by explicitly performing the integral over the θ_i in $\widetilde{\mathcal{Z}}_{XY}$ order-by-order in J. Such a procedure should be valid because correlations in θ_i decay exponentially. Then, it is easy to see that the resulting effective action for the σ_{ij} is just the $\mathbb{Z}_2$ gauge theory of Lec7, in Wegner's classical cubic lattice formulation; this is evident from the requirements imposed by the gauge invariance in Eq. (7). To leading order, the main effect of the θ_i integral is a renormalization in the coupling K. The $\mathbb{Z}_2$ gauge theory has a confinement-to-deconfinement transition with increasing K, and this is just the transition for the onset of topological order in the SRO regime.

III. QUANTUM XY MODELS AND BOSONS AT INTEGER FILLING

Further discussions on the nature of topological phase are more easily carried out in the language of the corresponding quantum model in $d = 2$ spatial dimensions. The quantum language will also enable us to connect with the discussion on the $\mathbb{Z}_2$ gauge theory in Lec7.

The quantum form of $\widetilde{\mathcal{H}}_{XY}$ in Eq. (6) is obtained by transforming the temporal direction of the partition function into a 'kinetic energy' expressed in terms of canonically conjugate quantum variables. We introduce the half-angle:

$$\vartheta_i \equiv \theta_i/2\,, \tag{8}$$

and a canonically conjugate number variable $\hat{n}_i$ with integer eigenvalues. The σ_{ij} are promoted to the Pauli matrices σ^z_{ij}, and we will also need the Pauli matrix σ^x_{ij}. So we obtain

$$\begin{aligned} \overline{\mathcal{H}}_{XY} &= -J \sum_{\langle ij \rangle} \sigma^z_{ij} \cos(\vartheta_i - \vartheta_j) - K \sum_{\square} \prod_{(ij)\in\square} \sigma^z_{ij} \\ &\quad + U \sum_i (\hat{n}_i)^2 - g \sum_{\langle ij \rangle} \sigma^x_{ij}\,; \\ &[\vartheta_i, \hat{n}_j] = i\delta_{ij}\,. \end{aligned} \tag{9}$$

The set of operators which commute with $\overline{\mathcal{H}}_{XY}$ are

$$G^{XY}_i = e^{i\pi\hat{n}_i} \prod_{\ell \in +} \sigma^x_\ell\,. \tag{10}$$

Each $e^{i\vartheta}$ boson carries unit $\mathbb{Z}_2$ electric charge, and so the Gauss law has been modified by the total electric charge on site i. The Gauss law constraint is

$$G^{XY}_i = 1\,. \tag{11}$$

The properties of the large K topological phase of $\overline{\mathcal{H}}_{XY}$ are closely connected to those of the deconfined phase of the $\mathbb{Z}_2$ gauge theory in Lec7. There is four-fold degeneracy on the torus, and a stable 'vison' excitations carrying magnetic $\mathbb{Z}_2$ flux of -1. In the present context, the 'vison' can also be interpreted as gapped odd vortex in the θ_i; because of the condensation of even vortices, there is only a single independent odd vortex excitation.

A significant new property is the presence of fractionalized bosonic excitations which carry 'electric' charges under the $\mathbb{Z}_2$ gauge field. These are the particles created by the

$$\psi = e^{i\vartheta} \tag{12}$$

operator, and the anti-particles created by $\psi^* = e^{-i\vartheta}$. These are the excitations illustrated in the boson models of Fig. 3, and they carry boson number $\hat{N} = 1/2$. Note that the XY order parameter, Ψ, and correspondingly the XY boson number, $\hat{N}_b$, obey

$$\Psi = \psi^2 \quad , \quad \hat{N}_b = \hat{n}/2. \tag{13}$$

It is clear from Eq. (7) that the ψ particles carry $\mathbb{Z}_2$ charges. Also, parallel transporting an electric charge around a vison leads to a Berry phase of -1, and hence the ψ and the visons are mutual semions. This structure of electric and magnetic excitations, and of the degeneracy on the torus, is that found in the solvable 'toric code' model [20].

The presence of the ψ excitations also helps us understand the nature of the XY order parameter correlations in the topological SRO phase, as indicated in Fig. 4. The ψ are deconfined, gapped, bosonic excitations, and the Hamiltonian has a charge conjugation symmetry under $\psi \to \psi^*$: so the ψ are described at low energies as massive relativistic charge particles, and this implies that the 2-point ψ correlator has a Ornstein-Zernike form, with a $1/r$ prefactor. Then using $\Psi = \psi^2$, we find the exponential decay of the XY order, with the $1/r^2$ prefactor, as shown in Fig. 4.

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