PHYSICAL REVIEW B **91**, 140504(R) (2015)

Spontaneous breakdown of time-reversal symmetry induced by thermal fluctuations

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(Received 1 December 2014; revised manuscript received 21 January 2015; published 16 April 2015)

In systems with broken $U(1)$ symmetry, such as superfluids, superconductors, or magnets, the symmetry restoration is driven by the proliferation of topological defects in the form of vortex loops (unless the phase transition is strongly first order). Here we discuss that the proliferation of topological defects can, by contrast, lead to the breakdown of an additional symmetry. We demonstrate that this effect should take place in $s+is$ superconductors, which are widely discussed in connection with iron-based materials (although the mechanism is much more general). In these systems a vortex excitation can create a "bubble" of fluctuating Z_2 order parameter. The thermal excitation of vortices then leads to the breakdown of Z_2 time-reversal symmetry when the temperature is *increased*.

DOI: 10.1103/PhysRevB.91.140504 PACS number(s): 67.10.−j, 64.60.De

Usually states which break symmetries and exhibit long- or quasi-long-range order (such as superconductors, superfluids, and ordered magnetic states) form at low temperatures. For example, three-dimensional conventional superconductors and superfluids break $U(1)$ local and global symmetries, respectively [1]. At elevated temperatures, fluctuations destroy the order and symmetry is restored. The rather generic mechanism that drives this phase transition in superfluids is the proliferation of vortex loops that destroy long-range order in the corresponding order parameter field $|\psi(\mathbf{r})|e^{i\varphi(\mathbf{r})}$ [2–4] (unless the system has a strong first-order phase transition such as in type-I superconductors [5,6]).

Similarly, in two-dimensional superfluids, the transition to the normal state is driven by the proliferation of topological defects in the form of unbinding of vortex-antivortex pairs [7]. Likewise, in systems with different symmetries, phase transitions to more symmetric states are driven by the proliferation of corresponding topological defects. Examples of this include domain walls in systems that break Z_2 symmetry, or bound states of topological defects in systems with multiple broken symmetries [8–12].

In this Rapid Communication we demonstrate that topological defects can play a radically different role in certain systems, and instead lead to the spontaneous breakdown of a symmetry which is *not* broken in the ground state. We specifically focus on frustrated three-band superconductors, but the scenario is by no means limited to this case.

This effect arises when fluctuations are included in the multicomponent Ginsburg-Landau (GL) free energy density that describes the $s+is$ superconducting state,

$$H=\sum_{a=1}^{3}\left\{\frac{1}{2}|\mathbf{D}\psi_a|^2+\alpha_a|\psi_a|^2+\frac{\beta_a}{2}|\psi_a|^4\right\}+\frac{1}{2}(\nabla\times\mathbf{A})^2+\sum_{a\neq b}\eta_{ab}|\psi_a||\psi_b|\cos(\varphi_a-\varphi_b), \quad (1)$$

where $\mathbf{D}=\nabla+ie\mathbf{A}$ is the covariant derivative and $\psi_a=|\psi_a|e^{i\varphi_a}$ are complex fields representing, for example, the superconducting components in different bands. The last terms in (1) represent Josephson-Leggett interband coupling. The magnetic field is given by $\mathbf{B}=\nabla\times\mathbf{A}$. The $s+is$ state is realized due to frustration with respect to the phase differences between superconducting components. This, for instance, occurs if all η_{ab} are positive since the last terms in Eq. (1) then are minimized by all phase differences being $\varphi_a-\varphi_b=\pi$, which cannot be simultaneously satisfied. Likewise, the case with one positive and two negative couplings is also frustrated. Such a situation also occurs in systems with more than three components [13]. The $s+is$ state is currently attracting substantial interest in connection with iron-based [14–16] as well as other kinds of superconductors [17]. Intercomponent interactions of this type can also be realized in cold atoms experiments.

An example of the ground state of a frustrated system is given in Fig. 1. Here $\eta_{13}=\eta_{23}<0$ is varied on the x axis while $\eta_{12}>0$ is kept constant. The resulting phases are shown in Fig. 1(b) and reveal a transition point at ~-0.0578 that separates two regions with different phase-locking patterns. The state on the left spontaneously breaks $U(1)$ symmetry, but on the right side, time-reversal symmetry is also broken since the resulting state is not invariant under $\varphi_i\rightarrow-\varphi_i$. Broken time-reversal symmetry implies an additional twofold degeneracy of the ground state, and thus the transition is between the broken symmetries $U(1)$ and $U(1)\times Z_2$, respectively. Increasing $\eta_{13}=\eta_{23}$ further, Z_2 symmetry is restored at ~-0.0542 [see Fig. 1(b)].

A phase diagram of this type has been studied as a function of doping in connection with the iron-based superconductor $Ba_{1-x}K_xFe_2As_2$. At the level of mean-field theory it features a $U(1)\times Z_2$ phase at low temperature (i.e., an $s+is$ state) [14–16]. The corresponding London model has been studied beyond the mean-field approximation, and it was then shown that fluctuations produce an additional phase where Z_2 symmetry is broken but $U(1)$ is restored [18,19]. The effect which we discuss below revises these phase diagrams. This effect appears if density fluctuations are taken into account besides phase fluctuations.

An important point here is that the interband terms take the form

$$\eta_{ab}|\psi_a||\psi_b|\cos(\varphi_a-\varphi_b), \quad (2)$$

i.e., they are modulated by the amplitudes. Since the phase-locking pattern is potentially altered by changing the parameters η_{ij}, it follows that perturbations to the amplitudes also have this capacity. This gives vortices a very particular role in

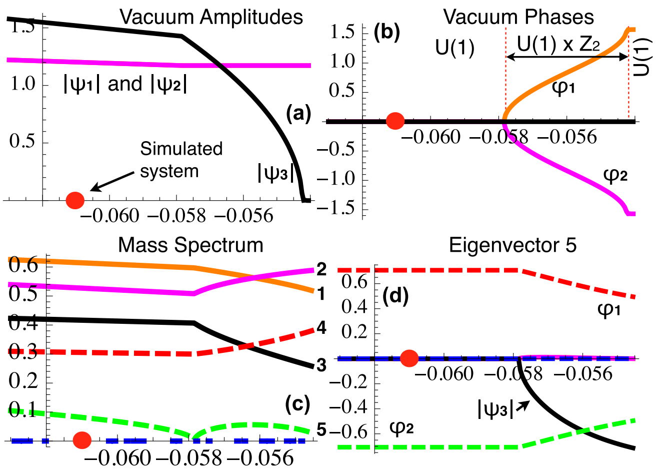

FIG. 1. (Color online) Ground state and mass spectrum of frustrated three-band GL model. Two of the model parameters, $\eta_{13} = \eta_{23}$, are scaled on the x axis. The others are given by $\alpha_1 = \alpha_2 = -3/64$, $\alpha_3 = 2.673/64$, $\beta_1 = \beta_2 = 3/64$, $\beta_3 = 0.18/64$, $\eta_{12} = 2.25/64$, and $e = 1.8/8$. (In this example the parameters were chosen such that the relevant length scales of the theory are larger than numerical lattice spacing and substantially smaller than the system size.) (a) gives the ground-state amplitudes of the fields while (b) gives the phases (φ_3 is fixed to 0). A critical point at $\eta_{13} = \eta_{23} \approx -0.0578$ separates a region with broken $U(1)$ symmetry (left) from a region that also breaks time-reversal symmetry (right). At a second critical point $\eta_{13} = \eta_{23} \approx -0.0542$, time-reversal symmetry is restored. The broken symmetries are indicated in (b). (c) gives the mass spectrum and thus the inverse of the coherence lengths (in units of lattice spacings) associated with the three fields. For detailed discussion of definition of coherence lengths/mass spectrum in this kind of models see Ref. [20]. One mass (5) becomes zero at the critical point, implying a diverging coherence length. The mode that corresponds to this coherence length is shown in (d). On the left side it describes a perturbation to the phases φ_1,φ_2, i.e., a Leggett mode, which becomes massless at the critical point. In the region to the right of the critical point the character of the mode changes, as it now describes a perturbation to both phase and amplitude (mainly $|\psi_3|$). The red dot indicates the parameters simulated below.

this model, since vortex cores suppress densities in a nontrivial way.

The parameter set on which we focus here (marked by the red dot in Fig. 1) features broken $U(1)$ symmetry in the ground state. It is clear from Fig. 1(b), that the system undergoes a symmetry change when the magnitude of $\eta_{13} = \eta_{23}$ is diminished. However, according to Eq. (2), this effect can likewise be obtained by depleting the amplitude $|\psi_3|$.

Vortex excitations in this three-band model are composite (i.e., can be viewed as a bound state of vortices with 2π winding in each of the phases φ_a) and have three cores which, in general, have different sizes (for a detailed study of the different characteristic length scales in vortex cores in such models, see Refs. [20,21]). For the parameters considered here, the third component has the largest vortex cores. The consequence of this is that vortices deplete the three interband interaction terms to a different extent, affecting interactions that involve the third component more. For a sufficiently dense group of vortices, this results in the formation of a bubble of induced nontrivial phase difference between the superconducting components, which is on average different from 0 or π, that is, a region of fluctuating Z_2 order parameter.

An example of this is given in Fig. 2. The data in this figure was obtained by, numerical minimization of the model (1), which was carried out on a two-dimensional grid. The system was prepared with a group of 12 numerically pinned vortices, and the energy was minimized subject to the constraint that the vortex-core positions remained unchanged. This problem has two solutions that share the same distribution and direction of magnetic flux [Fig. 2(a)]. Figures 2(b) and 2(c) correspond to different solutions and reveal an induced phase difference between the components ψ_1 and ψ_2, which can be either positive [Fig. 2(b)] or negative [Fig. 2(c)]. See also Ref. [22].

We now turn to the main question of this Rapid Communication: whether topological excitations with this property drive a transition to a state with spontaneously broken Z_2 symmetry upon heating. Unless the systems is strongly type 1, thermal fluctuations in the $U(1)$ sector result in the excitation of vortex loops. These tend to disorder the $U(1)$ sector, but at the same time, as shown above, they create bubbles of fluctuating Z_2 order parameter. Indeed, as long as the vortex loops are finite and well separated this cannot lead to a breakdown of Z_2 symmetry. However, a conjecture which we investigate below is that once the density of vortex loops in the system grows to some characteristic value, the bubbles with "locally broken" Z_2 symmetry form a connected network that spans the entire system. This in turn can lead to spontaneously broken time-reversal symmetry in the system that results from heating. Restoration of the symmetry requires further heating to higher temperature. The phase with broken Z_2 symmetry thus exists between two characteristic temperatures.

To test this hypothesis we have conducted large scale Monte Carlo simulations of the model (1) using the Metropolis algorithm. In the discretized version of the Hamiltonian the covariant derivative and magnetic flux take the form

$$|\mathbf{D}_x\psi_{a,ijk}|^2 = |\psi_{a,ijk} - \psi_{a,(i+1)jk}e^{ie\mathbf{A}_{xijk}}|^2, \tag{3}$$

$$\mathbf{B}_{zijk} = \mathbf{A}_x(i,j,k) + \mathbf{A}_y(i+1,j,k) \tag{4}$$

$$-\mathbf{A}_x(i,j+1,k) - \mathbf{A}_y(i,j,k), \tag{5}$$

where the subscript $xijk$ means the vector component x on the lattice point ijk and so forth. The discrete Hamiltonian is then given by

$$H = \sum_{i,j,k}\left\{\sum_{a=1}^{3}\frac{1}{2}|\mathbf{D}\psi_{a,ijk}|^2 + \frac{1}{2}\mathbf{B}_{ijk}^2 + U_{ijk}\right\}, \tag{6}$$

where the last term is the potential which does not depend on the gradients. The corresponding partition function is given by $Z = \int\mathcal{D}\mathbf{A}(\mathbf{r})\mathcal{D}\psi_1(\mathbf{r})\mathcal{D}\psi_2(\mathbf{r})\mathcal{D}\psi_3(\mathbf{r})e^{-\beta H}$, with the inverse temperature β. The model (1) is expressed in dimensionless units, with a length scale that is equal to the lattice spacing. The parameters used in the simulations are given in Fig. 1 with $\eta_{13} = \eta_{23} = 0.0611$. At zero temperature this system breaks $U(1)$ symmetry only. The figure also gives the masses of normal modes which, by definition, are inverse coherence lengths. In this model they are associated with linear combinations of

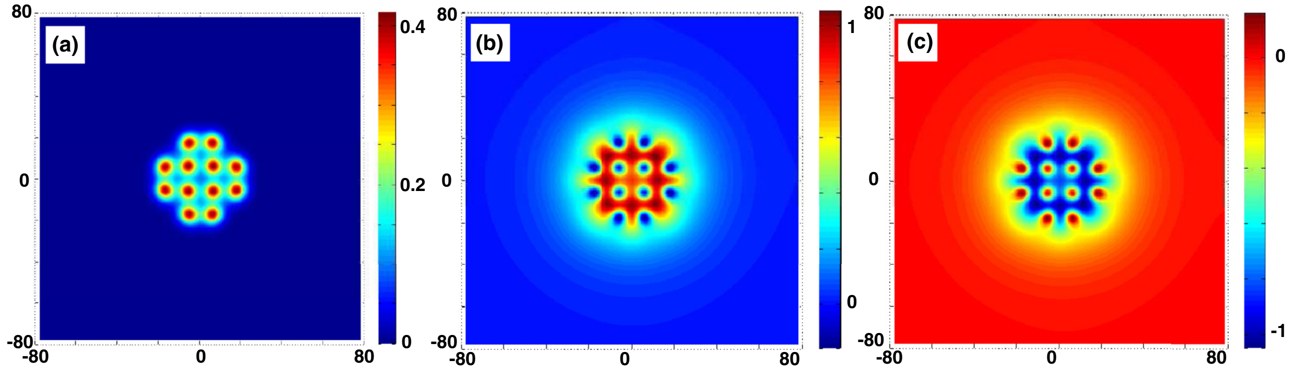

FIG. 2. (Color online) Vortex group solutions resulting from energy minimization of the model (1) on a two-dimensional grid. An initial configuration of 12 vortices was prepared and the energy minimization was carried out with the constraint that the positions of the centers of the vortex cores remain fixed. This problem has two solutions that share the same magnetic field $\nabla \times \mathbf{A}$, shown in (a). However, the solutions do not exhibit the same phase difference between the components. (b) and (c) display $|\psi_1||\psi_2|\sin(\varphi_1 - \varphi_2)$ for these two cases. The GL parameter set is given by the red dot in Fig. 1 and features a ground state that breaks $U(1)$ symmetry only, implying that in the ground state, $\sin(\varphi_1 - \varphi_2) = 0$. The presence of vortices, however, induces a phase difference between the components ψ_1 and ψ_2 which is positive in the first solution (b) and negative in the second solution (c). Away from the vortices, the phase differences decay exponentially to zero. The group thus produces a bubble of Z_2 order parameter.

the fields ψ_a [20]. The effects which we discuss do not require fine tuning. Our parameters are selected so that all the length scales are bigger than the lattice spacing but smaller than the system size [23].

To construct the order parameter associated with time-reversal symmetry breaking we introduce a projection of the configuration space $\{\psi_1,\psi_2,\psi_3\} \to \pm 1$ given by $f(\bar{\varphi}) = \mathrm{sgn}(\sin[\varphi_3](-\cos[\varphi_1] + \cos[\varphi_2]) + \sin[\varphi_1](-\cos[\varphi_2] + \cos[\varphi_3]) + \sin[\varphi_2](-\cos[\varphi_3] + \cos[\varphi_1]))$, which is odd under time reversal and changes sign if, and only if, phases are permuted. Ordering in the Z_2 sector can then be determined by an order parameter that takes the same form as that of the Ising model:

$$O_{Z_2} = \left\langle \left| \sum_{k,l,m} f(\bar{\varphi}_{k,l,m}) \right| \right\rangle \frac{1}{L^3}. \quad (7)$$

Restoration of the local $U(1)$ symmetry and thus the onset of the nonsuperconducting state can be identified by the scaling properties of the Fourier components of the magnetic field. We start by introducing

$$c = 2L^{-3} \sum_{ijk} \mathbf{B}_y \cos \frac{2\pi i}{L}, \quad s = 2L^{-3} \sum_{ijk} \mathbf{B}_y \sin \frac{2\pi i}{L}. \quad (8)$$

In the normal state, the gauge field is massless and the expectation value of c,s is given by

$$\langle s^2 \rangle = \langle c^2 \rangle = \frac{\int dc\, c^2 e^{-\beta L^3 c^2/4}}{\int dc\, e^{-\beta L^3 c^2/4}} = \frac{2}{\beta L^3}. \quad (9)$$

We thus define

$$F_A(L,\beta) = L^3 \langle c^2 + s^2 \rangle, \quad (10)$$

which should be scale invariant in the nonsuperconducting state. Plotting $F_A(L,\beta)$ vs β for several system sizes, we expect the curves to collapse onto the same line once $U(1)$ symmetry is restored.

To determine how thermally excited vortex loops affect the O_{Z_2} order parameter we define the total length of all vortex lines ϱ, and introduce the quantity

$$\rho_V = \varrho L^{-3}, \quad (11)$$

which allows us to define the correlator of the amount of thermally induced vortex matter and the order parameter O_{Z_2},

$$C_{V,Z_2} = \frac{\langle \rho_V O_{Z_2} \rangle - \langle \rho_V \rangle \langle O_{Z_2} \rangle}{\sigma(\rho_V)\sigma(O_{Z_2})}, \quad (12)$$

where σ denotes the standard deviation.

The results of the simulations, shown in Fig. 3, confirm the scenario described above. At low temperature the system does not break time-reversal symmetry. Note that in that case O_{Z_2} is only nonzero due to finite size effects: It decreases rapidly with system size. As the temperature increases, we see the onset of a genuine Z_2 order, which reaches a maximum at $\beta \approx 1.35$–1.4. This symmetry change is primarily driven by excitation of vortices (as opposed to nontopological fluctuations). This is clear from the correlator C_{V,Z_2} shown in Fig. 3(d), which reaches ~ 0.72, indicating a very strong correlation between the density of vortices and the order parameter O_{Z_2}. It is also consistent with the fact that the Z_2 order parameter is only nonzero in a temperature region where there is an appreciable density of vortices.

As the temperature increases further, O_{Z_2} starts to decrease, as expected. While thermal fluctuations generally tend to restore broken symmetries, an additional effect is also present. At higher temperatures the correlator C_{V,Z_2} becomes strongly negative, suggesting that further a increase in the density of thermally induced vortices helps to destroy the Z_2 order. Returning to Fig. 1(b), it is clear that in the model we use, the region with broken time-reversal symmetry corresponds to *intermediate* magnitudes of $\eta_{13} = \eta_{23}$. Decreasing the magnitude beyond $|\eta_{i3}| \sim 0.0542$ restores time-reversal symmetry and results in the "$s_\pm$ state," which is characterized by phase "antilocking," i.e., $\varphi_1 - \varphi_2 = \pi$. Likewise, depleting $|\psi_3|$ beyond a certain point contributes to destroying the Z_2

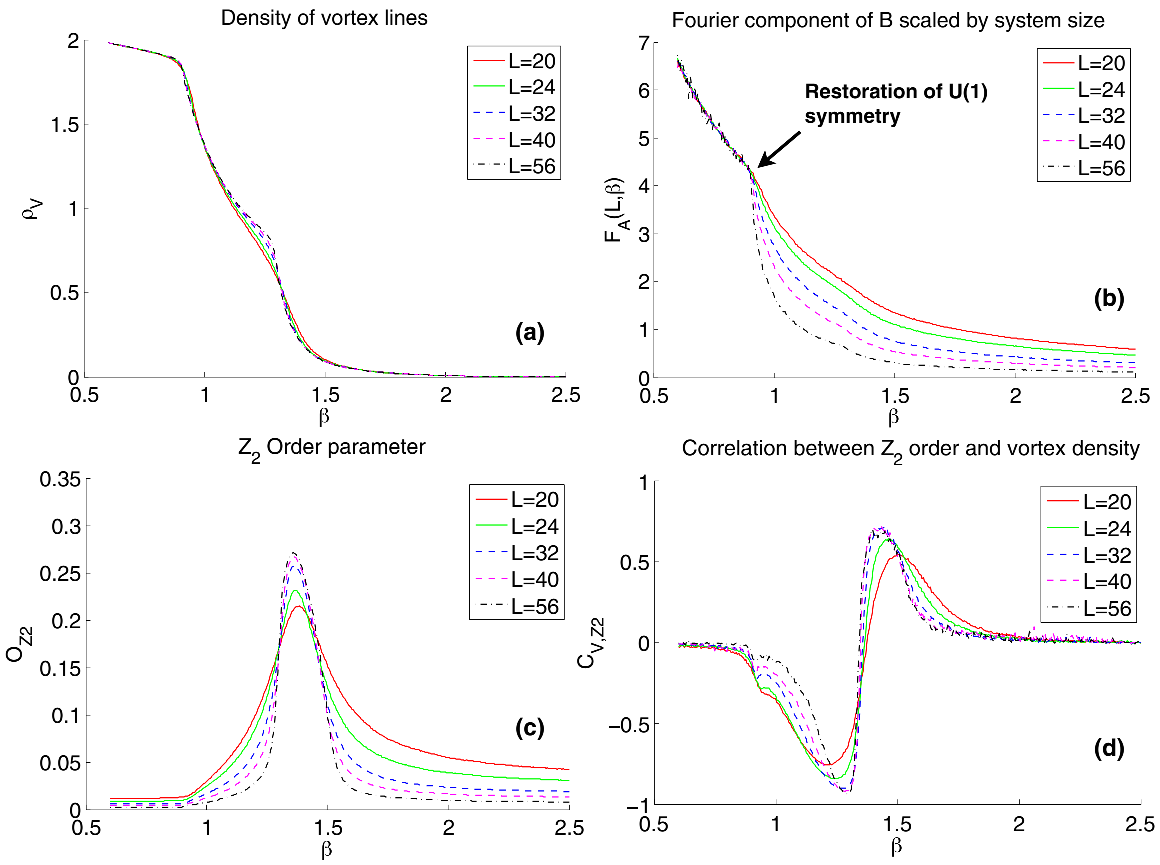

FIG. 3. (Color online) Summary of the simulation results. (a) The density of thermally induced vortices [ρ_V, Eq. (11)]. It approaches zero at low temperature, but starts to increase substantially at $\beta \approx 1.5$. (b) The Fourier components of the magnetic field scaled by system size [$F_A(L,K)$, Eq. (10)] collapse onto the same curve, indicating that the system is nonsuperconducting for $\beta < \beta_c \approx 0.9$. (c) The order parameter of the broken time-reversal symmetry O_{Z_2} [Eq. (7)] is zero at low temperature (except for finite size effects). As the temperature increases, an order emerges and reaches a maximum at $\beta \approx 1.35$–1.4. At higher temperatures this order starts to decay rapidly. (d) The correlation between the density of thermally induced vortices ρ_V and the Ising order parameter O_{Z_2} [Eq. (12)] is positive at low temperature and reaches a maximum of ~ 0.72, implying that breaking of the Z_2 symmetry is driven by vortex proliferation. At higher temperatures the correlation becomes negative, indicating that vortices contribute to restoring the symmetry.

order by the same mechanism. The other process which should, in general, contribute to the anticorrelation at elevated temperatures is the splitting of composite vortices into fractional ones connected by Z_2 domain walls (for a detailed discussion of these objects, see Ref. [24]).

In conclusion, it is well known that broken symmetries can be restored by the entropy-driven proliferation of topological defects. Here we have shown that for a class of systems, the proliferation of topological defects instead leads to a spontaneous breakdown of an additional symmetry. The implication of this is a phase transition where a symmetry is broken as the temperature is increased. We have demonstrated this effect using a three-component GL model with a frustrated interband interaction as an example. These models are currently discussed in connection with $Ba_{1-x}K_xFe_2As_2$ for a certain range of dopings. This transition should be detectable in calorimetry experiments. The mechanism described here is, however, more generic and should also apply to other systems where topological defects induce a bubble of fluctuating order parameter associated with a different symmetry.

This work was supported by the Knut and Alice Wallenberg Foundation through a Royal Swedish Academy of Sciences Fellowship, and by the Swedish Research Council Grants No. 642-2013-7837 and No. 325-2009-7664. Part of the work was done at University of Massachusetts Amherst supported by the NSF CAREER Award No. DMR-0955902. Computations were performed on resources provided by the Swedish National Infrastructure for Computing (SNIC) at the National Supercomputer Center in Linköping, Sweden.

[1] Arguments have been advanced recently that superfluidity does not necessary require broken $U(1)$ symmetry even in three dimensions, but can also arise from $U(1)$-like degeneracies in the free energy [25].

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[22] Note that, in principle, in these kinds of models, the appearance of the bubbles of the fluctuating Z_2 order parameter is not necessarily correlated with vortices. However, we are specifically interested in the situations where there is a strong correlation of this type. For the parameter set which we consider, small perturbations of the phase difference decouple from the density fluctuations. Thus the appearance of a fluctuating Z_2 order parameter requires strong density perturbations, such as the presence of vortex cores, which appear here as a consequence of fluctuations in the $U(1)$ sector of the model.

[23] The simulations were conducted on cubic lattices with system sizes $20 \leqslant L \leqslant 56$, periodic boundary conditions, and a lattice spacing of 1, meaning that at $T = 0$, the shortest coherence length is almost twice the lattice spacing (with a mass of ~ 0.6). For each system size, simulations were conducted at 384 inverse temperatures which were uniformly distributed in the range $0.6 \leqslant \beta \leqslant 2.5$. The large number of inverse temperatures allowed for parallel tempering to be employed. In all simulations, every data point was updated at least 1.5×10^7 times.

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