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Spontaneous Breakdown of Time-Reversal Symmetry Induced by Thermal Fluctuations

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In systems with broken $U(1)$ symmetry, such as superfluids, superconductors or magnets, the symmetry restoration is driven by proliferation of topological defects in the form of vortex loops. Here we discuss that in certain systems the proliferation of topological defects can, by contrast, lead to the breakdown of an additional symmetry. As a particular example we demonstrate that this effect should take place in $s + is$ superconductors, which are widely discussed in connection with the Iron-based materials. In these systems a vortex excitation can create a "bubble" of fluctuating Z_2 order parameter. Thermal excitation of vortices then leads to breakdown of Z_2 time-reversal symmetry when the temperature is *increased*.

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 respectively¹. At elevated temperatures, fluctuations destroy the order and symmetry is restored. The generic mechanism that drives this phase transition in superfluids is proliferation of vortex loops that disorder the phase $\varphi(\mathbf{r})$ so that the order parameter $\langle |\int d\mathbf{r} |\psi| e^{i\varphi} \rangle$ vanishes²⁻⁴ (unless the system has a strong first order phase transition like type-I superconductors^{5,6}). Similarly in two dimensional superfluids, the transition to the normal state is driven by proliferation of topological defects in the form of vortex-antivortex pairs⁷. Likewise, in systems with different symmetries, phase transitions to more symmetric states are driven by corresponding topological defects: a standard example being the proliferation of domain walls in systems that break Z_2 -symmetry. Multicomponent superconductors and superfluids can break higher symmetries than $U(1)$. In that case symmetry restoration can occur in several stages via proliferation of bound states of topological defects⁸⁻¹³.

In this work we show that proliferation of topological defects can instead lead to 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.

To model a frustrated three-band superconductor we use the following multi-component Ginsburg-Landau free energy density:

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

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 $\mathbf{B} = \nabla \times \mathbf{A}$. In principle additional terms are allowed on symmetry grounds in the functional (1). This minimal model is however sufficient to demonstrate the effects we are interested in. For microscopic derivation of

such a functional see e.g.^{14,15}

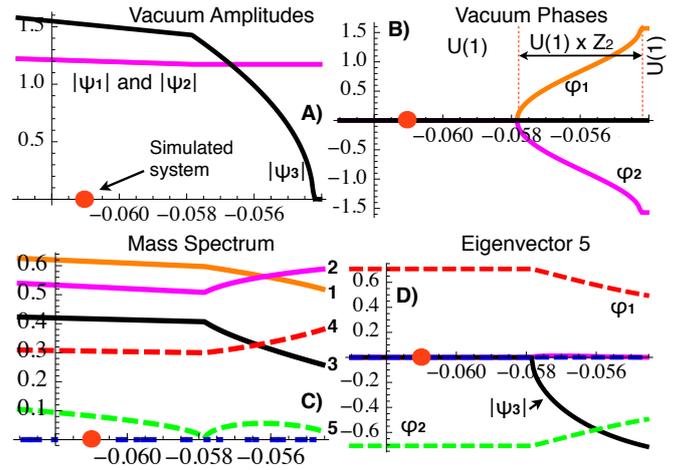


Figure 1. Ground state and mass spectrum of frustrated three-band GL model. Two of the model parameters, $\eta_{13} = \eta_{23}$ are scaled on the x-axis. The others are given by $\alpha_1 = \alpha_2 = -0.0469$, $\alpha_3 = 0.0418$, $\beta_1 = \beta_2 = 0.0469$, $\beta_3 = 0.00281$, $\eta_{12} = 0.0352$ and $e = 0.225$. (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 the inverse of the length scales associated with the three fields. One mass (5) becomes zero at the critical point, implying a diverging length scale. The mode that corresponds to this mass 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.

The case of interest for us is where there is 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 minimised 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 is rather generic in systems with more than three components¹⁶.

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 (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 (B) in Fig. 1.

A phase diagram of this type has been studied 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 (also termed s+is state)^{14,17,18}. 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^{19,20}. The effect which we discuss below revises these phase diagrams. It has not been observed in the previous studies because it appears only beyond the mean-field approximation when fluctuations of phase and density are taken into account.

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 this model, since vortex cores suppress densities in a non-trivial way.

The parameter set which is considered here (marked by the red dot in Fig. 1) features broken $U(1)$ symmetry in the ground state. It is clear from (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^{15,21}). For the parameters considered here, the third component has the largest vortex cores. The consequence of this is that vortices deplete the three inter-band interaction terms to 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 non-trivial phase difference between the superconducting components, 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. Here, numerical minimisation of the model (1) was carried out on a two-dimensional grid. The system was prepared with a group

of 12 numerically pinned vortices, and the energy was minimised subject to the constraint that the vortex-core positions remained unchanged. This problem has two solutions that share the same distribution of magnetic flux (A). The plots (B,C) correspond to different solutions and reveal an induced phase difference between the components ψ_1 and ψ_2 , which can be either positive (B) or negative (C). See also remark²²

The question which we address in this paper is; can topological excitations with this property drive a transition to a state with spontaneously broken Z_2 symmetry upon heating? That is, unless the system is strongly Type-1, thermal fluctuations in the $U(1)$ sector results in excitation of vortex loops. These tend to disorder the $U(1)$ sector, but at the same time 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 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 resulting 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 discretised version of the Hamiltonian the covariant derivative and magnetic flux take the form

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

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

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

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

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

where the last term is the potential which does not depend on gradients. The corresponding partition function is given by

$$Z = \int \mathcal{D}\mathbf{A}(\mathbf{r}) \mathcal{D}\psi_1(\mathbf{r}) \mathcal{D}\psi_2(\mathbf{r}) \mathcal{D}\psi_3(\mathbf{r}) e^{-\beta H} \quad (7)$$

with the inverse temperature β . The parameter values 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 the fields ψ_a ²¹.

The simulations were conducted on cubic lattices with system sizes $20 \leq L \leq 56$, 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

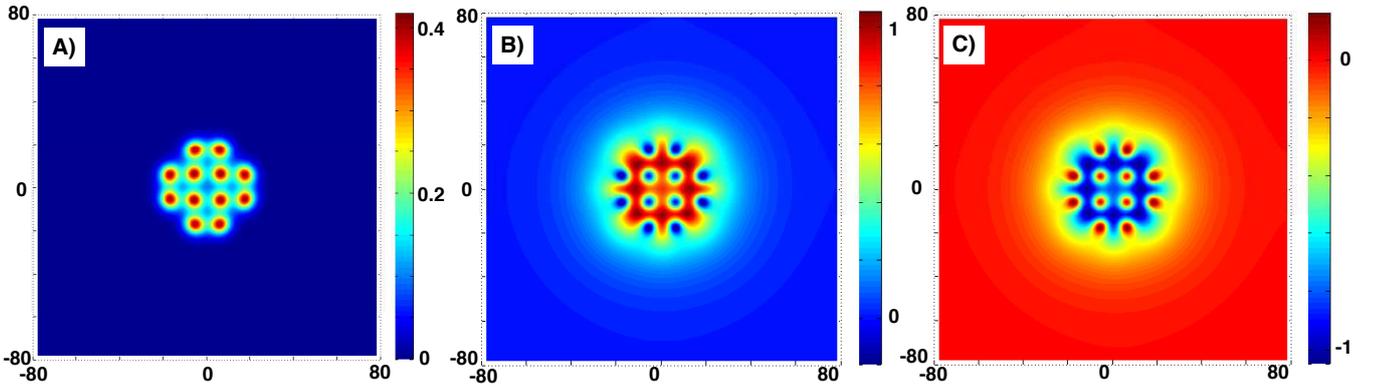


Figure 2. Vortex group solutions resulting from energy minimisation of the model (1) on a two-dimensional grid. An initial configuration of 12 vortices was prepared and the energy minimisation was carried out with the constraint that the positions of vortex cores remain fixed. This problem has two solutions 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. The panels (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 range $0.6 \leq \beta \leq 2.5$. 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.

To construct the order parameter for the time-reversal symmetry breaking we introduce a projection of the configuration space $\{\psi_1, \psi_2, \psi_3\} \rightarrow \pm 1$ given by

$$f(\bar{\varphi}) = \text{sgn} \left(\begin{aligned} &\sin[\varphi_3](-\cos[\varphi_1] + \cos[\varphi_2]) \\ &+ \sin[\varphi_1](-\cos[\varphi_2] + \cos[\varphi_3]) \\ &+ \sin[\varphi_2](-\cos[\varphi_3] + \cos[\varphi_1]) \end{aligned} \right), \quad (8)$$

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:

$$O_{Z_2} = \left\langle \left| \sum_{k,l,m} f(\bar{\varphi}_{k,l,m}) \right| \right\rangle \frac{1}{L^3}. \quad (9)$$

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

$$c = 2L^{-3} \sum_{ijk} \mathbf{B}_y \cos \frac{2\pi i}{L}, \quad (10)$$

$$s = 2L^{-3} \sum_{ijk} \mathbf{B}_y \sin \frac{2\pi i}{L}. \quad (11)$$

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

$$\langle s^2 \rangle = \langle c^2 \rangle = \frac{\int dc c^2 e^{-\beta L^3 c^2/4}}{\int dc e^{-\beta L^3 c^2/4}} = \frac{2}{\beta L^3}. \quad (12)$$

We thus define

$$F_A(L, \beta) = L^3 \langle c^2 + s^2 \rangle \quad (13)$$

which should scale invariant in the non-superconducting state. Plotting $F_A(L, \beta)$ versus 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 first introduce the quantity

$$\rho_V = \frac{\text{Total length of all vortex lines}}{L^3} \quad (14)$$

which allows us to define the correlator

$$C_{V,Z_2} = \frac{\langle \rho_V O_{Z_2} \rangle - \langle \rho_V \rangle \langle O_{Z_2} \rangle}{\sigma(\rho_V) \sigma(O_{Z_2})}, \quad (15)$$

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 non-topological fluctuations). This is clear from the correlator C_{V,Z_2} shown in (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

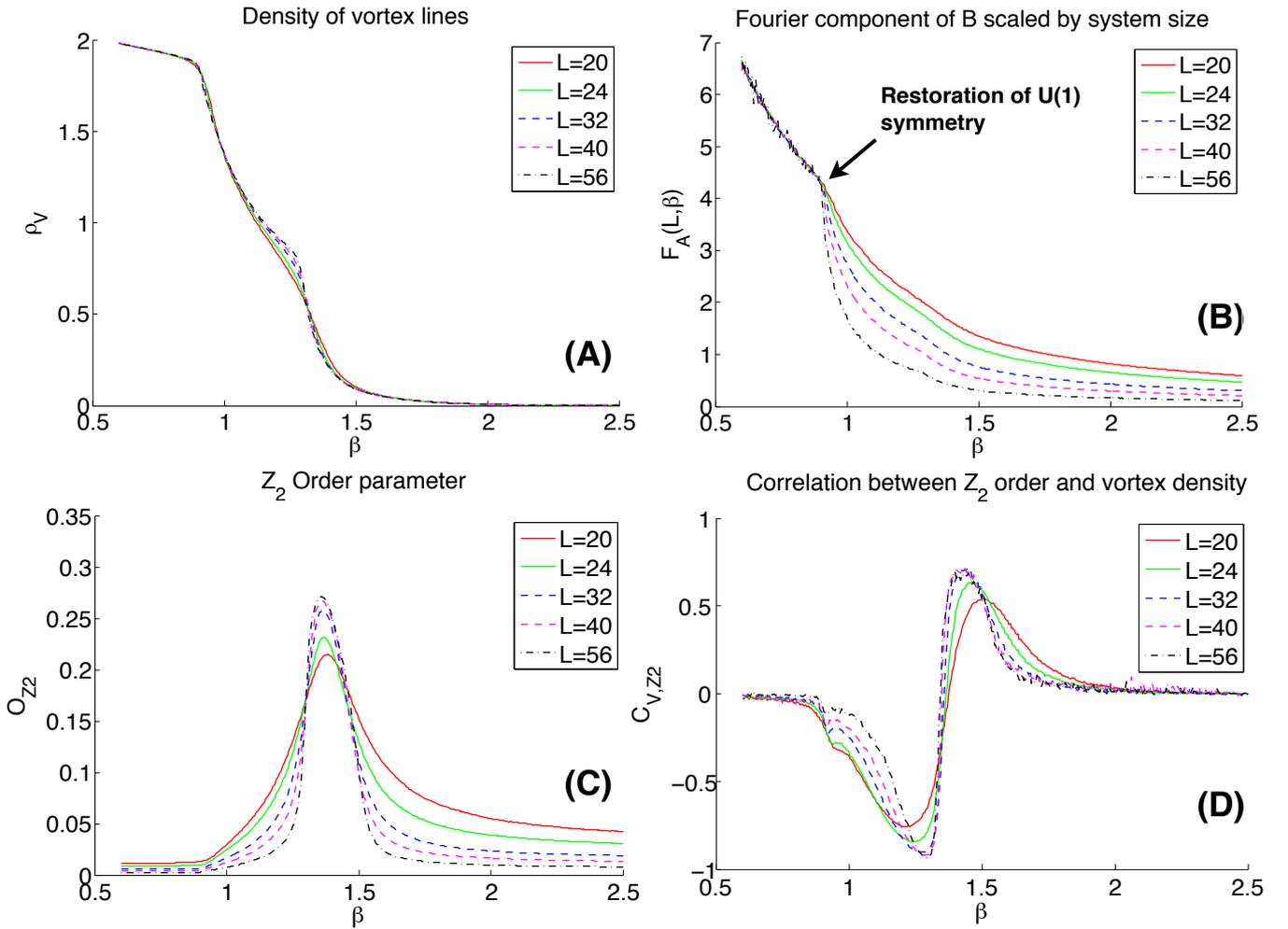


Figure 3. Summary of the simulation results. (A) The density of thermally induced vortices (ρ_V , Eq. 14). It approaches zero at low temperature, but starts to increase substantially at $\beta \approx 1.5$. (B) The Fourier components of the magnetic field scaled by system size ($F_A(L, K)$, Eq. 13) collapse onto the same curve, indicating that the system is non-superconducting for $\beta < \beta_c \approx 0.9$. (C) The order parameter of the broken time-reversal symmetry O_{Z2} (Eq. 9) 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_{Z2} (Eq. 15) 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.

negative, suggesting that further 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 “anti-locking”, i.e. $\varphi_1 - \varphi_2 = \pi$. Likewise, depleting $|\psi_3|$ beyond a certain point contributes to destroying the Z_2 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 see²³).

In conclusion, it is well known that broken symmetries can

be restored by 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 frustrated interband interaction as an example. These models are currently discussed in connection $Ba_{1-x}K_xFe_2As_2$. A transition of the type discussed here could potentially be realised in these systems at a certain doping. 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.

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