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Topological solitons in three-band superconductors with broken time reversal symmetry

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We show that three-band superconductors with broken time reversal symmetry allow magnetic flux-carrying stable topological solitons which have only a slightly higher energy than ordinary vortices. Therefore they can be induced by fluctuations or quenching the system through a phase transition. It can provide an experimental signature of the time reversal symmetry breakdown.

Experiments on iron pnictide superconductors suggest the existence of more than two relevant superconducting bands [1, 2]. The new physics which can appear in these circumstances is the possible superconducting states with spontaneously broken time reversal symmetry (BTRS) as a consequence of frustration of competing interband Josephson couplings [2] (other scenario for BTRS state was discussed in [3]). BTRS states also attracted much interest earlier in the context of unconventional spin-triplet superconducting models. There they have a different origin and are described by two-component Ginzburg-Landau models [4]. In those cases the theory predicts domain walls which pin vortices [4]. It was suggested that this can result in formation of experimentally observable vortex sheets if (i) a domain wall itself is pinned by sample inhomogeneities, or (ii) if a domain is dynamically formed inside a current-driven vortex lattice [4].

Here we show that a BTRS state in a three-band superconductor allows formation of metastable topological solitons. Although it is not by any means required to be near T_c for these solitons to exist, we use a static three-band Ginzburg-Landau (GL) free energy density model :

$$F = \frac{1}{2}(\nabla \times \mathbf{A})^2 + \sum_{i=1,2,3} \frac{1}{2}|D\psi_i|^2 + V(\psi_i) - \sum_{i=1,2,3} \sum_{j>i} \eta_{ij} |\psi_i| |\psi_j| \cos(\varphi_i - \varphi_j) \quad (1)$$

Here, $D = \nabla + ie\mathbf{A}$, and $\psi_i = |\psi_i|e^{i\varphi_i}$ are complex fields representing the superconducting components. We choose to work here with a minimal effective potential $V \equiv \sum_{i=1,2,3} \alpha_i |\psi_i|^2 + \frac{1}{2} \beta_i |\psi_i|^4$. Although there could be various other terms allowed by symmetry in (1) they are not qualitatively important for the discussion below. For $\eta_{ij} > 0$, the Josephson interaction term is minimal for zero phase difference, while $\eta_{ij} < 0$ it is minimal for $\varphi_i - \varphi_j = \pi$. When the signs of η_{ij} coefficients are all positive, [we denote it as (+ + +)] the ground state has $\varphi_1 = \varphi_2 = \varphi_3$. Similarly in case (+ - -) one has phase locking pattern $\varphi_1 = \varphi_2 = \varphi_3 + \pi$. However in cases (+ + -) and (- - -) there is a frustration between the phase locking tendencies [*i.e.* one cannot simultaneously satisfy $\cos(\varphi_i - \varphi_j) = \pm 1$]. For example, consider the case $\alpha_i = -1$, $\beta_i = 1$ and $\eta_{ij} = -1$. Without loss of generality lets set $\varphi_1 = 0$ then two ground states are possible $\varphi_2 = 2\pi/3$, $\varphi_3 = -2\pi/3$ or $\varphi_2 = -2\pi/3$, $\varphi_3 = 2\pi/3$. Note that the frustrated phase differences can assume values different from $2\pi n/3$ in case of

differing effective potentials or Josephson coupling strengths. Thus in these frustrated cases there is Z_2 broken symmetry in the system associated with complex conjugation of the all ψ fields. The broken Z_2 symmetry implies existence of domain walls solutions, which are schematically shown on Fig. 1.

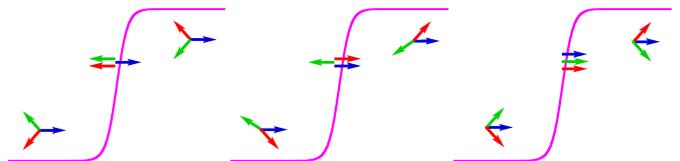


Figure 1. (Color online) – Schematic representation of various Z_2 domain walls in three-band superconductors with different frustrations of phase angles, shown by arrows of different colors. Pink line schematically shows phase difference between red and green arrow, interpolating between the two inequivalent ground states.

Let us now outline basic properties of the model (1). Without intercomponent Josephson coupling and $\alpha_i < 0$, its symmetry is $[U(1)]^3$. Then it allows three kinds of fractional flux vortices with logarithmically diverging energy [5] characterized by a phase winding in (*i.e.* integral over a phase gradient around a vortex) $\Delta\varphi_i \equiv \oint_{\sigma} \nabla\varphi_i = 2\pi$. Such a vortex carries a fraction of magnetic flux quanta (Φ_0), given by $\Phi_i = |\psi_i|^2 / (|\psi_1|^2 + |\psi_2|^2 + |\psi_3|^2) \Phi_0$. However a bound state of three such vortices ($i = 1, 2, 3$) has a finite energy. The finite-energy bound state is a “composite” vortex which has one core singularity where $|\psi_1| + |\psi_2| + |\psi_3| = 0$. Around this core all three phases have similar winding $\Delta\varphi_i = 2\pi$. Thus it is a logarithmically bound state of fractional vortices whose flux adds up to one flux quantum Φ_0 . In case of non-zero Josephson coupling fractional vortices are bound much stronger since they interact linearly [5].

We show below that the model (1) remarkably has a different kind of stable topological excitations distinct from vortices. Note that in two-component superconductors Skyrmion and Hopfion topological solitons can be represented as bound states of two spatially separated fractional vortices [6]. Likewise we can represent a topological soliton carrying N flux quanta (*i.e.* with each phase winding $2\pi N$) in a three component superconductor like a stable bound state of *spatially separated* $3N$ fractional vortices. Below we will call it “ $GL^{(3)}$ soliton”. At first glance, split fractional vortices could not be stable in the model (1) because of the strong linear attractive interaction between fractional vortices caused by Josephson

couplings. However we show that such solutions exist as topologically nontrivial *local* minima in the energy landscape of the model (1). These solutions may also be viewed as combinations of fractional vortices and closed domain walls.

Domain walls can form dynamically by a quench, but due to its line tension a single Z_2 closed domain wall (*i.e.* a domain wall loop) should rapidly collapse. Because of the field gradients, the superfluid density is suppressed on a domain wall. Therefore it can pin vortices. Furthermore at a domain wall one has energetically unfavorable values of cosines of phase differences $\cos(\varphi_i - \varphi_j)$. Thus Josephson terms immediately at the domain wall energetically prefer to *split* integer flux vortices into fractional flux vortices since it allows to attain more favorable phase difference values in between the split fractional vortices. (Note that, away from domain walls, Josephson terms give in contrast attractive interaction between fractional vortices). We find that if the magnetic field penetration length is sufficiently large, then there is a length scale at which repulsion between the fractionalized vortices pinned by domain wall counterbalances the domain wall's tension. It thus results in a formation of a stable topological soliton made up of $3N$ fractional vortices. Thus these topological solitons represent a closed Z_2 domain wall along which there are N points of zeros of each condensate $|\psi_i|$. Around each of these zeros the phase φ_i changes by 2π . The total phase winding around the soliton is $\oint \nabla\varphi_1 dl = \oint \nabla\varphi_2 dl = \oint \nabla\varphi_3 dl = 2\pi N$. Therefore it carries N flux quanta.

Since it is a complicated nonlinear problem, no analytical tools are available and thus a conclusive answer if these solitons are stable could only be obtained numerically. We performed a numerical study based on energy minimization using a Non-Linear Conjugate Gradient algorithm showing the existence and stability of the $GL^{(3)}$ solitons. Technical details of numerical calculations are available as supplementary online material. The general tendency which we observed is, that in contrast to most of the known topological solitons, they are more stable at higher topological charges. In fact we did not find any stable solitons for the lowest topological charge corresponding to enclosed one quanta of magnetic flux ($N = 1$). The lowest topological charge solutions we found carry two flux quanta, and thus consist of six fractional vortices residing on a closed domain wall. The Fig. 2 shows the $N = 2$ soliton in a superconductor with two passive bands (thus in this respect, similar to the models which are believed to be relevant for iron pnictide) coupled to an active band. Although it consists of six fractional vortices, one of the bands in this example has larger density and thus the magnetic field has two pronounced peaks near singularities in the main band. This is because the fractional vortices in that band carry the largest amount of the magnetic flux $\Phi_3 = |\psi_3|^2 / [|\psi_1|^2 + |\psi_2|^2 + |\psi_3|^2]$. So the magnetic field profile of this soliton resembles a vortex pair. We similarly found $N = 2$ solitons for superconductor with three passive bands and for three active bands which was not qualitatively different from the one shown on Fig. 2.

We find that solutions with larger number of flux quanta

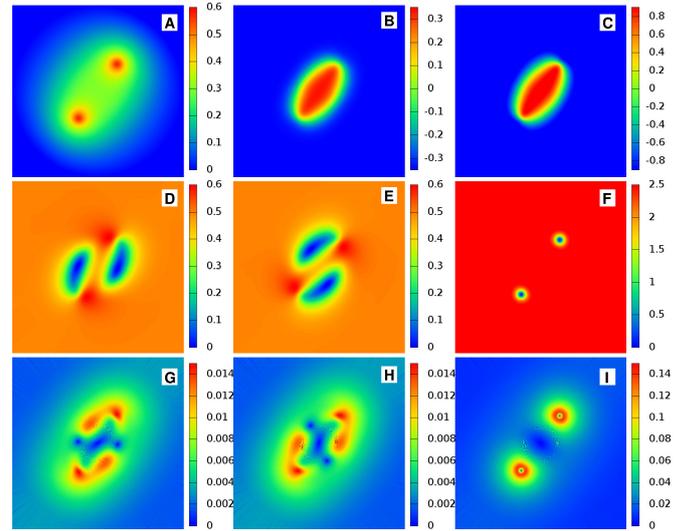


Figure 2. (Color online) – $N = 2$ topological solitons for two similar passive bands $(\alpha_i, \beta_i) = (1, 1)$ with interband coupling $\eta_{12} = -3$. These bands have Josephson coupling $\eta_{13} = \eta_{23} = 1$ to the third band, which is active $(\alpha_3, \beta_3) = (-2.5, 1)$. The system is type-II with $e = 0.07$ (we use coupling constant e in (1) to parametrize inverse penetration length). The panel A displays the magnetic field B . Panels B and C respectively display $(\psi_1^* \psi_2 - \psi_1 \psi_2^*)/2i$ and $(\psi_1^* \psi_3 - \psi_1 \psi_3^*)/2i$, showing the phase difference between two condensates. Second line, shows the densities of the different condensates $|\psi_1|^2$ (D), $|\psi_2|^2$ (E), $|\psi_3|^2$ (F). The third line displays the supercurrent densities associated with each condensate $|J_1|$ (G), $|J_2|$ (H), $|J_3|$ (I). Phase differences on panels B and C show that there is a closed domain-wall since there are two areas with different phase-lockings (blue and red) associated with two possible ground states. The solution consists of $N = 2$ vortices which are fractionalized: indeed, the panels D, E and F show separated highly asymmetric pairs of singularities of different condensates. Note the very complicated geometry of supercurrent densities shown on panels G, H and I.

tend to have ring-like shapes. The Fig. 3 gives an example of a solution with $N = 8$ flux quanta. Note that this object will have a very distinct magnetic signature which can be distinguished by scanning SQUID or Hall or magnetic force microscopy. Despite the fact that this object is a bound state of 24 fractional vortices, the magnetic field has only 8 pronounced maxima. They coincide with the position of the 8 singularities in the band with the largest density.

The magnetic structure of the soliton always clearly reflects the relative densities the bands. When the ground state densities in each band are equal, the magnetic field has a uniform ring-like geometry as shown on Fig. 4.

When disparity of the densities in different bands is small there is also a family of N quanta solitons which have $2N$ pronounced maxima in the magnetic field. An example with $N = 4$ is shown on Fig. 5.

We investigated numerically more than 500 parameter sets in three-component BTRS GL models. For all type-II three-component BTRS GL models we found stable $GL^{(3)}$ solitons, provided the topological charge was large enough. The solu-

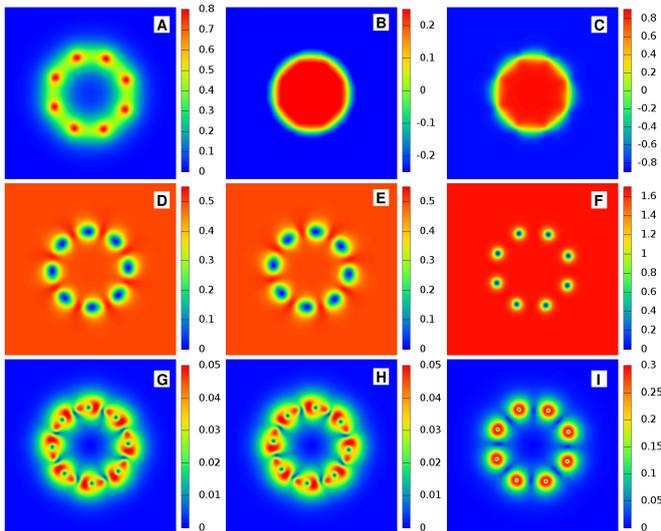


Figure 3. (Color online) – $N = 8$ quanta soliton for the same parameter set as in Fig. 2 except that $e = 0.3$ and $(\alpha_3, \beta_3) = (-1.5, 1)$, giving less disparity in the ground state densities (displayed quantities are the same as in Fig. 2). The cores of vortices in each band do not coincide. Note the complicated structure of currents in each band.

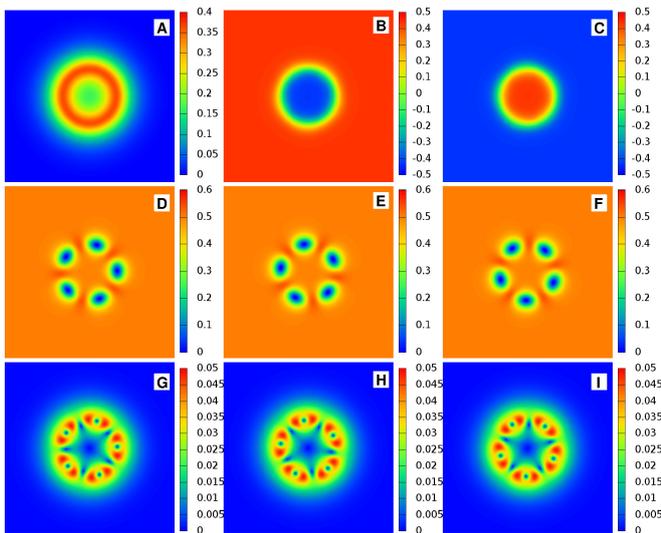


Figure 4. (Color online) – $N = 5$ quanta soliton with $e = 0.3$. With three identical passive bands $(\alpha_i, \beta_i) = (1, 1)$, with superconductivity induced by repulsion $\eta_{ij} = -3$ between the three condensates. Displayed quantities are the same as in Fig. 2.

tion existed in BTRS states irrespectively of whether bands are active or passive and for very different effective potentials and interband coupling strengths. It indicates that these solitons should be rather generic excitations in three-component type-II BTRS superconductors. Fig. 6 shows the energy and stability of the solitons for different values of the coupling constant e (in our parametrization e controls the inverse magnetic field penetration length). It reflects the generic tendency which we find, that the solitons are more stable in more type-II

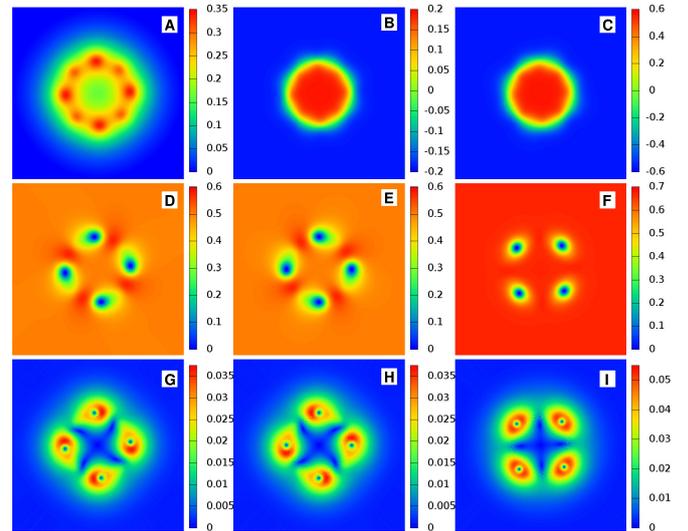


Figure 5. (Color online) – $N = 4$ quanta soliton for two similar passive bands coupled to a third active band. The parameter set used here is the same as in Fig. 3 except $(\alpha_3, \beta_3) = (-0.5, 1)$ and $e = 0.2$. Displayed quantities are the same as in Fig. 2.

regimes and also at higher topological charges.

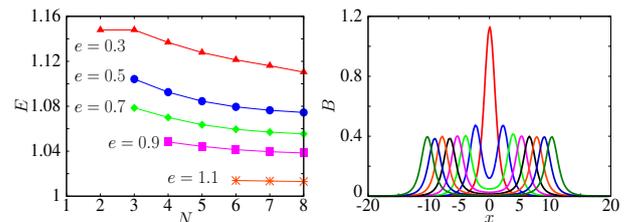


Figure 6. (Color online) – Energies of the solitons per flux quanta, in the units of the energy of a single ordinary vortex (left). When the electric charge increases (*i.e.* the penetration length decreases) solitons with smaller N become unstable. The right panel shows crosssections of the magnetic field for solitons with $N \in [2, 8]$ (double-peak curves). The central curve corresponds to a crosssection of a regular $N = 1$ vortex. The parameters of the Ginzburg-Landau model used here are the same as in Fig. 4, which gives nearly axially-symmetric magnetic field.

Lets us now address the physical observability of these solitons. First in all the cases which we studied in the model (1), the solitons with N flux quanta were more energetically expensive than N isolated one-quanta vortices. However they are protected by an energy barrier against decay into ordinary vortices. Note that because the solitons are obtained as solutions of the energy minimization problem, they are guaranteed to be stable against infinitesimally small perturbations. However, since they are more energetic than vortices, *strong enough* perturbation should destabilize them. This stability question is addressed numerically in the Supplementary material. For strongly type-II regime the potential barrier can be estimated as the energy needed to disconnect the domain wall. For a soliton in a three-dimensional sample with phase wind-

ing in the xy -plane the potential barrier can be estimated as $[\text{coherence length}]^2 \times [\text{sample size in the direction of applied magnetic field}] \times [\text{condensation energy density}]$.

Being more expensive than vortices, these objects cannot form as a ground state in low external field [7]. However as demonstrated in Fig. 6 they are not much more energetically expensive than vortices. In fact the corresponding energy differences can be just a few percent. Thus they can be excited by either by (a) thermal fluctuations or (b) by quenching in a sample subjected to a magnetic field. To address the scenario (b) of possible formation of these solitons in a post-quench relaxation, we have to assess ‘‘capture basin’’ of these solutions (*i.e.* how large is the area in the free energy landscape from which an excited system would relax into the local mini-

um corresponding to a soliton. Although studying real post-quench relaxation dynamics is beyond the scope of this paper, nonetheless we can directly assess the capture basin of the solutions from the evolution of the system in our relaxation scheme (see also remark [8]). We investigated several hundreds regimes and found that solitons typically easily form when a system is relaxed from various higher energy states. This indicates that the capture basin of these solutions is typically very large. We find that these defects in fact very easily form during a rapid expansion of vortex lattice (which should occur when magnetic field is rapidly lowered, or if a system is quenched through H_{c2}). A typical example is shown on Fig. 7. Animations of these processes are available as a supplementary online material [9].

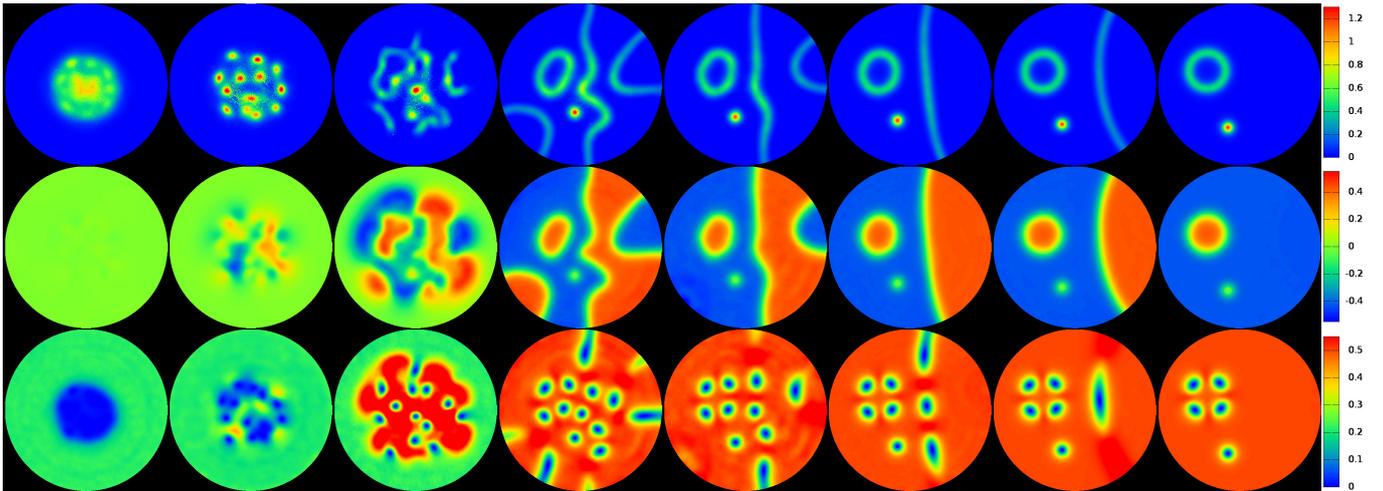


Figure 7. (Color online) – The soliton formation during energy relaxation of an initial state of expanding group of vortices in a circular system with open boundary conditions. First line displays the energy density. Second line shows the phase difference between condensates $(\psi_1^* \psi_2 - \psi_1 \psi_2^*)/2i$. When domain walls form they separate two inequivalent ground states (blue and red). Third line is the density of the first condensate $|\psi_1|^2$. Initial configuration has a high density of 13 vortices in the center. Repulsive type-II interaction makes all vortices move away from each other and escape the sample. In the process of energy minimization domain walls and $GL^{(3)}$ solitons form. Domain wall connected to boundaries quickly disappear. The final picture shows the resulting long-living state of a well separated $N = 4$ $GL^{(3)}$ soliton and a vortex. Parameter set used here is the same as in Fig. 4, with $e = 0.4$.

In conclusion, we have shown that BTRS state of a three-band superconductor can be detected through its magnetic response. Namely we have demonstrated that in this state the system has two kinds of flux carrying topological defects : ordinary vortices and also a different kind of topological solitons. These solitons are only slightly more energetically expensive than vortices (in some cases we found the energy difference as small as $10^{-2}E_v$ where E_v is the energy of a vortex). They should form during a post-quench relaxation of a BTRS superconductor in an external field, since they represent local minima with a wide capture basin in the free energy landscape. *I.e.* a system should relax to these local minima from a wide variety of excited states. Then these solitons can be observed in scanning SQUID, Hall, or magnetic force microscopy measurements. They can provide an experimental signature of possible BTRS states in iron pnictide superconductors. A tendency for vortex pair formation, yielding

magnetic profile similar to that shown on Fig. 2 was observed in $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$, [10] as well as vortex clustering in $\text{BaFe}_{2-x}\text{Ni}_x\text{As}_2$ [11]. These materials have strong pinning which can naturally produce disordered vortex states [11], although a possibility of ‘‘type-1.5’’ scenario for these vortex inhomogeneities was also voiced in [11]. The vortex pairs observed in [10] can be discriminated from $N = 2$ solitons (such as that shown on Fig. 2), by quenching the system and observing whether or not it forms vortex triangles, squares, pentagons etc corresponding to higher- N solitons.

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