Phase solitons in multi-band superconductors with and without time-reversal symmetry

Shi-Zeng Lin\textsuperscript{1,2,3} and Xiao Hu\textsuperscript{1}

\textsuperscript{1} International Center for Materials Nanoarchitectonics (WPI-MANA), National Institute for Materials Science, Tsukuba 305-0044, Japan
\textsuperscript{2} Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA
E-mail: lin.shizeng@gmail.com

\textit{New Journal of Physics} 14 (2012) 063021 (10pp)
Received 26 March 2012
Published 15 June 2012
Online at \url{http://www.njp.org/}
doi:10.1088/1367-2630/14/6/063021

Abstract. The Josephson-like interband couplings in multi-band superconductivity exhibit degenerate energy minima, which support states with kinks in phase of superconductivity. When the interband couplings in systems of three or more components are frustrated, the time-reversal symmetry (TRS) can be broken, which generates another type of phase kink between the two time-reversal symmetry breaking (TRSB) pair states. In this work, we focus on these novel states of phase kinks, and investigate their stability, similarity, differences and physical consequences. The main results can be summarized as follows: (i) we find a new type of phase slip when the kink becomes unstable. (ii) In the kink region, TRS is broken and spontaneous magnetic fields are induced. (iii) In superconductors with TRSB, composite topological excitations associated with variations of both the superconductivity phase and amplitude can be created by local perturbations or due to proximity effect between normal metals.

\textsuperscript{3} Author to whom any correspondence should be addressed.
1. Introduction

It has been known for a long time that superconductors with different pairing symmetries in contact with one another can form stable domain structures [1, 2]. The properties of domain walls are governed by the pairing symmetries in the domains; thus these heterogeneous systems become vital for understanding the pair symmetry. Meanwhile, there is growing evidence that superconductors may break discrete symmetries in addition to the $U(1)$ (local) gauge symmetry whose loss defines superconductivity [3, 4]. Examples include time-reversal symmetry breaking (TRSB) in some unconventional superconductors [5, 6], which results in unusual phenomena such as the appearance of magnetic flux when the superconductivity is perturbed by nonmagnetic impurities [7]. These superconductors can also form stable domain walls between domains of distinct symmetry-breaking states.

The discovery of MgB$_2$ [8] and iron-pnictide superconductors [9] has opened up intense and exciting discussions of multi-band superconductivity in condensed matter physics. In these systems, the superconductivity in one band is coupled through interband Josephson coupling to that in another band $\gamma_{ij}\Delta_i\Delta_j\cos(\phi_i-\phi_j)$, with $\phi_i$ and $\Delta_i$ being the superconductivity phase and amplitude in the $i$th band, respectively. This gives rise to a collective oscillation of the superconductivity phases, known as the Leggett mode [10].

It is interesting to observe that the interband coupling has degenerate energy minima $\phi_i-\phi_j=2n\pi$ for $\gamma_{ij} < 0$, which supports various topological excitations in the form of phase kinks belonging to the homotopy class $\pi_0(S^0)$, whereas the well-known vortex solution in type II superconductors belongs to the homotopy class $\pi_1(S^1)$. The existence of the kink solution was first discussed by Tanaka [11] for two-component superconductors, and later it was discussed that phase kinks can be excited in nonequilibrium processes such as current injection [12]. The phase kinks have been observed experimentally in layered aluminum mesoscopic rings with two order parameters [13].

In the presence of frustrated interband couplings in superconductors with three or more components, the system may break the time-reversal symmetry (TRS) [14–18]. In the TRSB state, $\Psi \neq e^{i\theta}\Psi^*$ for any phase $\theta$ with $\Psi \equiv (\Psi_1, \Psi_2, \ldots, \Psi_n)$ a vector of the complex order parameters. A phase kink may appear between two degenerate states $\Psi$ and $\Psi^*$. One thus sees that multi-band superconductors support two types of kink solutions of different origins. In a recent paper by Garaud et al [19], composite topological excitations associated with phase kink and vortex in superconductors with TRSB have been found numerically. The stability of these phase kinks, however, remains to be investigated.
In this work, we investigate the stability, similarity, differences and physical consequences of these two types of kink solutions. In superconductors with TRS in bulk, the phase kink breaks TRS at the domain wall, and induces local magnetic flux. Upon elevation of temperatures, kinks become unstable as a consequence of increasing coherence length. At the instability, a phase slippage occurs accompanying a voltage pulse. In contrast, kinks between TRSB pair states remain stable even with increasing coherence length. Moreover, in superconductors with TRS, various types of composite topological excitations associated with the variation of superconductivity phase and amplitude can be created by perturbing the superconductivity locally, such as heating and/or nonmagnetic impurities, and at the interface to a normal metal.

2. Kink solutions

We start from the standard multi-band Ginzburg–Landau (GL) theory with Josephson-like interband couplings [20, 21], which is adequate for discussions on physics addressed here

$$\mathcal{F} = \sum \left[ \alpha_j |\Psi_j|^2 + \beta_j |\Psi_j|^4 + \frac{1}{2m_j} \left| (-i\nabla - A) \Psi_j \right|^2 \right] + \frac{1}{8\pi} (\nabla \times A)^2 + \sum_{l \neq j} \gamma_{lj} \left( \Psi_l \Psi_j^* + c.c. \right),$$

(1)

where symbols are conventionally defined [22]. Throughout the paper, we use the units $\hbar = 2e = c = 1$. $\gamma_{lj}$ for $l \neq j$ is the interband coupling, which can be either repulsive or attractive depending on the strengths of the Coulomb and electron–phonon interactions. The interband repulsion may cause frustration of the superconductivity in different bands and results in TRSB [14–18]. For MgB$_2$, the interband coupling is commonly accepted as attractive $\gamma_{12} < 0$, while for iron-pnictide superconductors, there is growing evidence that some of $\gamma_{ij}$ are positive and the system favors s± pair symmetry [23, 24].

The kinetic energy in equation (1) can be rewritten as $\frac{\hbar^2 j}{4\pi} |\xi_j|^2 (\nabla + i A)^2 |\Psi_j|^2$, where $\xi_j = \sqrt{1/2m_j} |a_j|$ and $H_{ij}$ are the coherence length and thermodynamic critical field in respective single-band condensates ($\gamma_{ij} = 0$). When the width of the kink $\lambda_k$ (derived below) is much larger than $\xi_j$, $\lambda_k \gg \xi_j$, the suppression of the amplitude of the order parameters by the phase kink is weak, and the order parameter is approximately constant in space. In this case, we can concentrate on the phase variables of the order parameters.

First we consider the phase kink between domains with TRS in one dimension, where we can take the gauge $A = 0$. The minimal model for this domain structure is of two bands. Since the sign of $\gamma_{12}$ can be gauged away in this case, we consider $\gamma_{12} < 0$ without loss of generality. We also assume an identical amplitude of order parameter $\Delta_1 = \Delta$ for simplicity. The variation of the phase difference $\phi_{12} = \phi_1 - \phi_2$ is described by the sine-Gordon equation [11]

$$\partial_s^2 \phi_{12} + 2\gamma_{12}(m_1 + m_2) \sin \phi_{12} = 0,$$

(2)

and $\partial_s \phi_1 = -m_1 \partial_s \phi_2 / (m_1 + m_2)$. The width of the kink is $\lambda_k = 1/\sqrt{-2\gamma_{12}(m_1 + m_2)}$, which is temperature independent. The condition that $\lambda_k \gg \xi_j$ then becomes $|\gamma_{ij}| \ll \alpha_j$. A typical phase kink is shown in figure 1 (middle). The TRS is broken at the domain wall, while it is preserved in the domains. There are finite phase differences between the right and left domains in both components.

Now we consider the kink solution of a superconductor of three or more components with frustrated interband couplings, where TRS is broken in bulk. As a minimal model,
we treat a superconductor with three equivalent bands $\alpha_j = \alpha$, $\gamma_j = \gamma > 0$ and $m_i = m$. The two degenerate ground states $\hat{\Psi} = \Delta(1, e^{i2\pi/3}, e^{i4\pi/3})$ and $\hat{\Psi}^* = \Delta(1, e^{-i2\pi/3}, e^{-i4\pi/3})$ as a consequence of TRSB are displayed in figure 1 (right). For constant amplitudes of order parameters at $\gamma \ll \alpha$, the phase kink is described by $\partial_x \phi_1 = 0$, $\partial_x (\phi_{12} + \phi_{13}) = 0$ and
\begin{equation}
\frac{1}{2m\gamma} \partial_x^2 \phi_{12} + \sin \phi_{12} + \sin (2\phi_{12}) = 0.
\end{equation}

The potential associated with equation (3) $V_p = \cos \phi_{12} + \cos(2\phi_{12})/2$ has many degenerate minima $\phi_{12,m} = \pm 2\pi/3 + 2\pi n$. One can construct a kink solution between any pair of the energy minima. Their stability and magnetic response are qualitatively the same. To be specific, we only consider the following kink solution, which can be found analytically using the Bogomolny inequality [25]
\begin{equation}
\phi_{12} = 2 \arctan \left[ \sqrt{3} \tanh \left( -\frac{\sqrt{3}m\gamma}{2x} \right) \right],
\end{equation}
and the associated energy is
\begin{equation}
E_k = \frac{4}{3} \sqrt{m\gamma} (3\sqrt{3} - \pi).
\end{equation}

In one dimension (1D), there is no supercurrent in the domain wall due to the current conservation $\partial_t J_s = 0$. In higher dimensions, the supercurrent and the associated magnetic field are induced at the domain wall as a result of TRSB. We consider a closed domain wall described by either equation (2) or (4) in a 2D superconductor. To investigate the dynamic evolution of the domain wall, we solve the time-dependent GL equation (TDGL) numerically [26]
\begin{equation}
\frac{\hbar^2}{2m_j D_j} \left( \partial_t + i \frac{2e}{\hbar} \Phi \right) \Psi_j = -\frac{\delta F}{\delta \Psi_j^*},
\end{equation}
New Journal of Physics 14 (2012) 063021 (http://www.njp.org/)
Figure 2. Numerical results of the magnetic field distribution: (a) a circular domain wall in a two-band superconductor; (b) a circular domain wall between two TRSB pair states in a three-band superconductor. For (a), \( \alpha_j = -20, \gamma_{12} = -1, \beta_j = 1, m_1 = 1 \) and \( m_2 = 3 \) in the numerical calculations; for (b), \( \alpha_j = 0, \beta_j = m_j = p_j = 1, \gamma_{12} = 1, \gamma_{13} = 1.2 \) and \( \gamma_{23} = 1.5. \)

\[
\sigma c \left( \frac{1}{c} \delta_j A + \nabla \Phi \right) = -\frac{\delta F}{\delta A},
\]

with \( D_j \) being the diffusion constant, \( \sigma \) the normal conductivity and \( \Phi \) the electric potential.

In simulations, we prepare a closed domain wall with square or rectangular shapes as the initial conditions. In order to minimize its energy, the domain wall organizes itself into a circular shape irrespective of its initial shape during the time evolution in simulations. Magnetic fields appear spontaneously at the domain wall with alternating directions, as shown in figures 2(a) and (b). As revealed by numerical simulations, for phase kinks in superconductors with TRS (see equation (2)), the induced magnetic field changes polarization in both the radial and azimuthal directions as shown in figure 2(a). In contrast, for kinks between TRSB pair states (see equation (4)), the magnetic field changes polarization only in the azimuthal direction as shown in figure 2(b). One may treat the domain wall at the left semicircle as a phase kink; then the domain wall at the right semicircle is an anti-kink. They attract each other, which causes the whole circular domain wall to collapse, and renders a uniform state. Since the attraction between two domain walls becomes exponentially weak at a large separation, the lifetime of the domain walls increases with the size of the domain enclosed. This allows for possible experimental detections of the induced magnetic flux after quenching when domain walls are excited by chance.

3. Stability of the kink solution

We proceed to investigate the stability of the kink solution in equation (2) taking into account the suppression of amplitude of the order parameter by the phase kink. The magnitude of the suppression depends on the ratio of the kink width \( \lambda_k \) to the coherence length \( \xi \) as briefly mentioned above. As the coherence length increases when the temperature is elevated while the
Figure 3. (a) Suppression of the amplitude of superconductivity at the domain wall when the temperature denoted by \( \alpha \) is increased in a two-band superconductor with \( \gamma_{12} = -0.9 \). (b) Phase diagram for the stability of the phase kink. (c) Structure of the phase kink in the presence of supercurrent. Here \( \alpha_j = -7 \), \( \gamma_{12} = -0.5 \) and the supercurrent \( J_s = 2.94 \). (d) Stability of the phase kink upon current injection, with \( \alpha_j = -7 \), \( \beta_j = 1 \) and \( m_j = 2 \).

When the temperature increases, the amplitude of the superconductivity at the domain wall decreases as depicted in figure 3(a). At a threshold \( \alpha \) for a given value of \( \gamma_{12} \) (symbols in figure 3(b)), the phase kink becomes unstable and the system evolves into a uniform state, during which a voltage pulse appears. Therefore, the phase kinks in superconductors with TRS are stable only for weak interband couplings.

A superconducting wire with a phase kink can be alternatively considered as a Josephson junction since the superconductivity is suppressed at the domain wall. In the ground state, the
phase difference between two domains is finite, thus it is a realization of $\phi$-junction [27] or $\pi$-junction [28] if the two bands are identical. When current is injected into the wire, the phase kink is deformed due to the phase gradient created by the injected current. At a threshold current, the phase kink becomes unstable, and the system evolves into a uniform superconducting state, during which a voltage pulse appears, similar to the case with increasing temperature. The threshold current is still much smaller than the depairing current of the uniform state. One may regard the threshold current as a critical current for the present Josephson junction.

We perform numerical calculations on the critical current of a superconducting wire with a phase kink, introducing supercurrent into the system by twisting the phases at the two edges of the wire far away from the phase kink. The kink structure is deformed into the shape depicted in figure 3(c) by the current injection. The critical current for the kink state decreases with $|\gamma_{12}|$ as shown in figure 3(d), since the kink state gradually loses its stability as $|\gamma_{12}|$ increases as discussed above. At the critical current, we observe a phase slip with a voltage pulse and finally the system reaches a uniform state.

The phase kink in equation (4) between two TRSB pair states of a three-component superconductor is stable because the system takes different states in the left and right domains, and one cannot transform one state to the other by adjusting superconductivity at the domain wall. This kink is thus protected by symmetry and is very different from those with bulk TRS as in equation (2), where the states in the left and right domains are essentially the same except for a common phase factor, as shown in figure 1 (middle), and the system evolves into a uniform state by rotating the phase of domains globally at the instability of the kinks.

4. Consequences of time-reversal symmetry breaking

We have shown that spontaneous magnetic flux and voltage pulse appear during the nonequilibrium evolution of the superconductivity phase when a phase kink becomes unstable. Here we discuss possible experimental observations on stable phase kinks at equilibrium. In the presence of a phase kink, the TRS is violated at the domain wall, namely $\phi_1 - \phi_2 \neq 0$ or $\pi$. The variation of the superconductivity amplitude is coupled with that of the superconductivity phase, which can be checked by expanding the interband coupling term $\gamma_{ij} \Delta_i \Delta_j \cos(\phi_i - \phi_j)$ to the quadratic order of phase difference. When the superconductivity is suppressed locally by nonmagnetic impurities, by proximity effect at the sample edge or by heating, variations in superconductivity phases are induced, which in turn excite supercurrent and magnetic flux, as was confirmed numerically.

We study the proximity effect between a superconducting strip and a normal metal when a phase kink is present in the superconductor. In order to describe the proximity effect correctly, a boundary condition between a multi-band superconductor and normal metals should be formulated. The boundary condition in terms of the Usadel equation has been derived in [29]. In the framework of phenomenological GL theory, the boundary condition for a single-band superconductor can be generalized straightforwardly to a multi-band one [22]

$$(-i \nabla - A) \Psi_j = \sum_k p_{jk} \Psi_k,$$

where the off-diagonal coefficient $p_{jk}$ with $j \neq k$ accounts for the interband coupling, whereas the diagonal coefficient $j = k$ represents suppression of superconductivity as a consequence of the leakage of Cooper pairs at the interface. We minimize the GL energy numerically, and
Figure 4. Numerical results of the magnetic field distribution: (a) a two-band superconducting strip with a phase kink in contact with a normal metal; (b) a three-band superconductor with TRSB in contact with a normal metal; and (c) a three-band superconductor with TRSB with an impurity. For (a), $\alpha_j = -20$, $\gamma_{12} = -1$, $\beta_j = 1$, $m_1 = 1$ and $m_2 = 3$, with proximity lengths $p_{jj} = 2$ and $p_{j\neq i} = \infty$; for (b), $\alpha_j = 0$, $\beta_j = m_j = 1$, $\gamma_{12} = 1$, $\gamma_{13} = 1.2$ and $\gamma_{23} = 1.5$, $p_{ji} = 1$ and $p_{j\neq i} = \infty$; and for (c), the same as panel (b) except for $\alpha_j = 0.5$ inside the impurity area, and $p_{ji} = \infty$.

The results are presented in figure 4(a). Spontaneous magnetic field is induced at the interface between the normal metal and superconductor at the position of the domain wall, which is strong enough (in figure 4(a), $H \sim 10^{-5}H_c$) to be measured experimentally by scanning SQUID, Hall or magnetic force microscopy. The magnetic field has opposite signs at the two interfaces, leaving a zero integration over the sample.

In TRSB superconductors, stable domain walls associated with the variation of the superconductivity phase and amplitude can be created by local perturbations, because the phase is coupled with the amplitude when TRS is violated. In figure 4(b), we consider the proximity effect between a three-band superconductor with TRSB and a normal metal. Magnetic fluxes appear at the corners of the superconductor, associated with sharp changes in phase gradients. In figure 4(c), we introduce an impurity by modifying $\alpha_i$ locally. We see that magnetic flux is induced around the impurity. For superconductors with TRS, no magnetic field can be induced by the proximity effect or impurities, which implies a possible way of detecting the TRSB in experiment.

5. Discussions

In multi-band superconductors with Josephson-like interband coupling, the phase kinks as topological excitations can exist because of the multiple degenerate energy minima associated
with the interband Josephson coupling. The phase kink suppresses the superconductivity nearby depending on the ratio of the width of the phase kink to the superconducting coherence length, which causes instability when the suppressed superconductivity is insufficient to maintain the phase coherence for the phase kink. The existence of a phase kink does not require breaking of additional symmetry besides $U(1)$. Instead, the presence of a phase kink violates the TRS locally. When bulk multi-band superconductors break TRS, a new type of phase kink can be formed between the two TRSB pair states. The topological solutions (phase kinks) in multi-band superconductors discussed in this work are different from the topological superconductors realized in materials with strong spin–orbit couplings.

In 1D, both the phase kink in a superconductor with TRS and that between TRSB pair states are stable. In 2D, because of the attraction between opposite kinks, the domain wall collapses and the system reaches a uniform state. This is in accordance with Derrick’s theorem [30], i.e. for an infinite system, the kink state is only stable in 1D. Kinks can be pinned by the pinning centers where the superfluid densities are small, since the loss of superconductivity condensation energy can be reduced by adapting the domain wall to the pinning centers. This may prevent the domain wall from collapsing and stabilize the kink in 2D. The kink can also be stabilized when vortices are present as discussed by Garaud et al [19]. Domain walls created by local heating or impurities in superconductors with TRSB are stable in 2D and 3D since they are enforced by external perturbations.

Let us discuss the realization of the phase kink in equation (2). In iron-pnictide superconductors, interband scatterings are strong [31], and thus the phase kinks are unlikely to be realized. While for the well-known two-band superconductor MgB$_2$ and V$_3$Si, it is revealed that interband scatterings are weak [32, 33], which may allow for the excitation of stable phase kinks in the low-temperature region. In contrast, for the realization of a kink in equation (4), we need multi-band superconductors with TRSB. As discussed in [18], the TRSB state can be achieved by chemical doping in iron-pnictide superconductors. Moreover, phase kinks can also be realized in hybrid structures with two superconducting films coupled with Josephson coupling. Recently, Vakaryuk et al [34] proposed to realize the phase kinks in superconductors with the $s^\pm$ pairing symmetry by exploiting the proximity effect to a conventional s-wave superconductor.

Acknowledgments

The authors are grateful to L N Bulaevskii and Z Wang for discussions. This work was supported by WPI Initiative on Materials Nanoarchitectonics and Grants-in-Aid for Scientific Research (no. 22540377), MEXT, Japan and was partially supported by CREST, Japan Science and Technology Agency (JST). SZL was partially supported by the Los Alamos National Laboratory under contract no. E8L5-000100LB.

References

[1] Tsuei C C, Kirtley J R, Chi C, Yu-Jahnnes L S, Gupta A, Shaw T, Sun J Z and Ketchen M B 1994 Phys. Rev. Lett. 73 593
[2] Ng T K and Nagaosa N 2009 Europhys. Lett. 87 17003
[3] Sigrist M and Ueda K 1991 Rev. Mod. Phys. 63 239
[4] Sigrist M, Ogawa N and Ueda K 1991 J. Phys. Soc. Japan 60 2341

New Journal of Physics 14 (2012) 063021 (http://www.njp.org/)
