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Three-band Ginzburg-Landau model: Length Scales, Leggett's Modes and Type-1.5 Regimes

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The recent discovery of iron pnictide superconductors has resulted in a rapidly growing interest in multiband models with more than two bands. In this work we specifically focus on the properties of three-band Ginzburg-Landau models which do not have direct counterparts in more studied two-band models. First we derive normal modes and characteristic length scales in the conventional $U(1)$ three-band Ginzburg-Landau model as well as in its time reversal symmetry broken counterpart with $U(1) \times Z_2$ symmetry. We show that in the latter case, the normal modes are mixed phase/density collective excitations. The appearance of a massless phase-difference mode associated with fluctuations of the phase difference is also discussed. Next we show that gradients of densities and phase differences can be inextricably intertwined in vortex excitations in three-band models. This can lead to very long-range attractive intervortex interactions and appearance of type-1.5 regimes even when the intercomponent Josephson coupling is large. In some cases it also results in the formation of a domain-like structures in the form of a ring of suppressed density around a vortex across which one of the phases shifts by π . We also show that field-induced vortices can lead to a change of symmetry from $U(1)$ to $U(1) \times Z_2$ in the system. In the type-1.5 regime, it results in a semi-Meissner state where the system has a macroscopic phase separation in domains with broken $U(1)$ and $U(1) \times Z_2$ symmetries.

Superconductivity with two gaps associated with different bands was first theoretically predicted in 1959¹. However it was not until 42 years later, with the discovery of MgB_2 ² that it started to attract a wide interest (for a recent review see³). Because the condensates in two band superconductors are not independently conserved, the system considered in¹ share the same broken $U(1)$ symmetry of the ground state as their single-component counterparts. The interband tunneling results in a system that attains its free energy minimum when the phase difference between the condensates is either zero or π . Nonetheless in 1969 it was discussed that individual phases of the two condensate wave functions are important degrees of freedom, since they give rise to a new kind of collective excitations. These collective excitations are associated with the fluctuations of the relative phase of the two superconducting components around its ground state value: the Leggett's mode⁴, for a recent discussion see⁵. A report of the observation of the Leggett's mode in MgB_2 appeared very recently⁶.

Another example of new physics which can arise in two-band system (as compared to their single-band counterparts) is associated with disparity of the characteristic length scales of density variations. That is, a single quantum vortex in a two-band system, should in general produce two different cores, one associated with each band. As a consequence of this, there appears a regime which was recently termed type-1.5 superconductivity⁷. In that regime the two characteristic length scales of density variations ξ_1 and ξ_2 satisfy the condition $\xi_1 < \sqrt{2}\lambda < \xi_2$. For a subset of parameters in this regime there are thermodynamically stable vortices with non-monotonic interaction. Namely, these vortices exhibit interaction which is long range attractive due to core-core interaction like vortices in type-1 superconductors, and short-range repulsive like vortices in type-2 superconductors. As a consequence of the long range attraction between vortices the system allows an additional "semi-Meissner" phase associated with a macroscopic phase separations in domains of the Meissner state and vortex states see e.g.⁷⁻¹⁴. For a detailed in-

troducton see¹⁵.

In the last three years there has been a rapidly growing interest in multiband superconductivity with more than two components. The interest was sparked by the recent discovery of iron pnictide superconductors¹⁶ and subsequent discussions that superconductivity in these systems may be described by a theory with more than two relevant bands^{17,18}. It was observed that the inclusion of a third band in the theory in several respects leads to qualitatively different physics compared to two-band systems¹⁹⁻²². The new physics arises from the fact that the presence of three or more components can lead to phase frustration. It results from competition of three or more interband Josephson coupling terms, which cannot all simultaneously attain the most energetically favorable phase locking pattern¹⁹⁻²². This frustration leads to Time Reversal Symmetry Breakdown (TRSB)¹⁹⁻²³ (we discuss it more quantitatively below). See also^{24,25} for a different discussion of possible time reversal symmetry breakdown in iron pnictides. Here we show that phase frustration leads to a plethora of new phenomena in the physics of collective excitations and the magnetic response of the three-band Ginzburg-Landau model.

In the TRSB phase the "phase-only" Leggett's modes are transformed into mixed phase-density modes. These mixed normal modes have quite complex structure and, they can possess modes with large characteristic length scales even in the case of strong Josephson coupling. At the transition point to the TRSB regime, the length scale of one of the phase difference modes diverges, rendering one of the Leggett's modes massless (as was also found recently in a London model²⁶, for other recent discussions of Leggett's modes in connection with iron pnictides see^{27,28}). This is in contrast to two-band systems where increasing interband Josephson coupling always diminishes disparities of the density variations^{9,15}. In particular it implies that the type-1.5 regime is possible in three band superconductors even in cases of quite strong interband Josephson coupling. Moreover we show that in three-band systems the Semi-Meissner state can represent not only

a macroscopic phase separation in vortex and Meissner domains but also represent a macroscopic phase separations of domains with different broken symmetries.

I. MODEL

The minimal GL free energy functional to model a three-band superconductor is

$$F = \frac{1}{2}(\nabla \times \mathbf{A})^2 + \sum_{i=1,2,3} \frac{1}{2} |\mathbf{D}\psi_i|^2 + \alpha_i |\psi_i|^2 + \frac{1}{2} \beta_i |\psi_i|^4 + \sum_{i=1,2,3} \sum_{j>i} \eta_{ij} |\psi_i| |\psi_j| \cos(\varphi_{ij}). \quad (1)$$

Here $\mathbf{D} = \nabla + ie\mathbf{A}$ and $\psi_i = |\psi_i|e^{i\varphi}$ are complex fields representing the superconducting components. The phase difference between two condensates is denoted $\varphi_{ij} = \varphi_j - \varphi_i$. The magnetic flux density through the system is given by $\mathbf{B} = (\nabla \times \mathbf{A})$ and the magnetic energy density is $\mathbf{B}^2/2$. Such a multicomponent GL free energy can in certain cases be microscopically derived at temperatures close but not too close to T_c (for a review see²⁹). Indeed the existence of three superconducting bands is not by any means a sufficient condition for a system to have GL expansion like that given in Eq. (1). However many of the questions which we consider below in fact do not require the system to be in the high-temperature region where a GL expansion like Eq. (1) could in certain cases be formally justified. In what follows we will however use the minimal GL model since it provides a convenient framework to discuss this physics qualitatively. In the Eq. (1) the coefficients α_i change signs at some characteristic temperatures which are generally different for all components. Below this temperature $\alpha_i < 0$ and the band is active. Above it, $\alpha_i > 0$ and the band is passive. Passive bands can nevertheless have nonzero superfluid density because of the interband Josephson tunneling terms $\eta_{ij} |\psi_i| |\psi_j| \cos \varphi_{ij}$. Thus it is possible in this model to have only passive bands, and still nonzero superfluid densities due to Josephson terms. In the three component model Eq. (1) there are additional terms allowed by symmetry, e.g. bi-quadratic terms in density (for a review of microscopic derivation of such terms from a weak-coupling two-band theory see²⁹). However the impact of these terms on length scales and vortex physics in three-band model is essentially the same as in the well studied two-band case¹⁵. Since their role is mostly connected with a straightforward renormalization of the length scales we will not repeat this analysis here. Instead we will focus primarily on the Josephson couplings, which can play principally different roles in two- and three- band cases.

Let us first discuss the simplest London approximation *i.e.* $|\psi| = \text{const.}$ Then one can extract gradients of the gauge-

invariant phase differences by rewriting the model as:

$$F = \frac{1}{2 \sum_{i=1,2,3} |\psi_i|^2} \left[\sum_{i=1,2,3} |\psi_i|^2 \nabla \varphi_i + e \sum_{i=1,2,3} |\psi_i|^2 \mathbf{A} \right]^2 + \frac{|\psi_1| |\psi_2|}{4 \sum_{i=1,2,3} |\psi_i|^2} (\nabla(\varphi_1 - \varphi_2))^2 + \frac{|\psi_2| |\psi_3|}{4 \sum_{i=1,2,3} |\psi_i|^2} (\nabla(\varphi_2 - \varphi_3))^2 + \frac{|\psi_1| |\psi_3|}{4 \sum_{i=1,2,3} |\psi_i|^2} (\nabla(\varphi_1 - \varphi_3))^2 + \sum_{i=1,2,3} \sum_{j>i} \eta_{ij} |\psi_i| |\psi_j| \cos(\varphi_i - \varphi_j) + \frac{1}{2} (\nabla \times \mathbf{A})^2 \quad (2)$$

The first term features the phase gradients coupled to the vector potential: this corresponds to the total current in the system. The rest of the terms correspond to counter-flow of carriers in different bands. Since there is no charge transfer in counter-flows there is no coupling to gauge fields. In the limit $\eta_{ij} = 0$ the second, third and fourth term describe neutral superfluid modes with phase stiffnesses $|\psi_i| |\psi_j| / [4 \sum_{i=1,2,3} |\psi_i|^2]$ which were studied in detail in³⁰. When Josephson terms are present they break symmetry by giving preferred values to the phase differences, yet the system can have fluctuations near these values. After this illustration of phase fluctuations, we discuss in the following the fluctuations within the full Ginzburg-Landau model which involves fluctuations of both phases and densities.

Systems with more than two Josephson-coupled bands can exhibit *phase frustration*. For $\eta_{ij} < 0$, a given Josephson interaction energy term is minimal for zero phase difference (we then refer to the coupling as “phase-locking”), while when $\eta_{ij} > 0$ it is minimal for a phase difference equal to π (we then refer to the coupling as “phase-antilocking”). Two component systems are symmetric with respect to the sign change $\eta_{ij} \rightarrow -\eta_{ij}$ as the phase difference changes by a factor π , for the system to recover the same interaction. However, in systems with more than two bands there is generally no such symmetry. For example if a three band system has $\eta > 0$ for all Josephson interactions, then these terms can not be simultaneously minimized, as this would correspond to all possible phase differences being equal to π .

II. GROUND STATE OF A THREE BAND SUPERCONDUCTOR

The ground state values of the fields $|\psi_i|$ and φ_{ij} of system Eq. (1) are found by minimizing its potential energy

$$\sum_i \left\{ \alpha_i |\psi_i|^2 + \frac{1}{2} \beta_i |\psi_i|^4 \right\} + \sum_{j>i} \eta_{ij} |\psi_i| |\psi_j| \cos(\varphi_{ij}). \quad (3)$$

Minimizing the potential energy Eq. (3) can not in general be done analytically. Yet, some properties can be derived from

qualitative arguments. In terms of the sign of the η 's, there are four principal situations:

Case	Sign of $\eta_{12}, \eta_{13}, \eta_{23}$	Ground State Phases
1	---	$\varphi_1 = \varphi_2 = \varphi_3$
2	--+	Frustrated
3	-++	$\varphi_1 = \varphi_2 = \varphi_3 + \pi$
4	+++	Frustrated

The case 2) can result in several ground states. If $|\eta_{23}| \ll |\eta_{12}|, |\eta_{13}|$, then the phase differences are generally $\varphi_{ij} = 0$. If on the other hand $|\eta_{12}|, |\eta_{13}| \ll |\eta_{23}|$ then $\varphi_{23} = \pi$ and φ_{12} is either 0 or π . For certain parameter values it can also have compromise states with φ_{ij} not being integer multiples of π .

The case 4) can give a wide range of ground states, as can be seen in Fig. 1. As η_{12} is scaled, ground state phases change continuously from $(-\pi, \pi, 0)$ to the limit where one band is depleted and the remaining phases are $(-\pi/2, \pi/2)$.

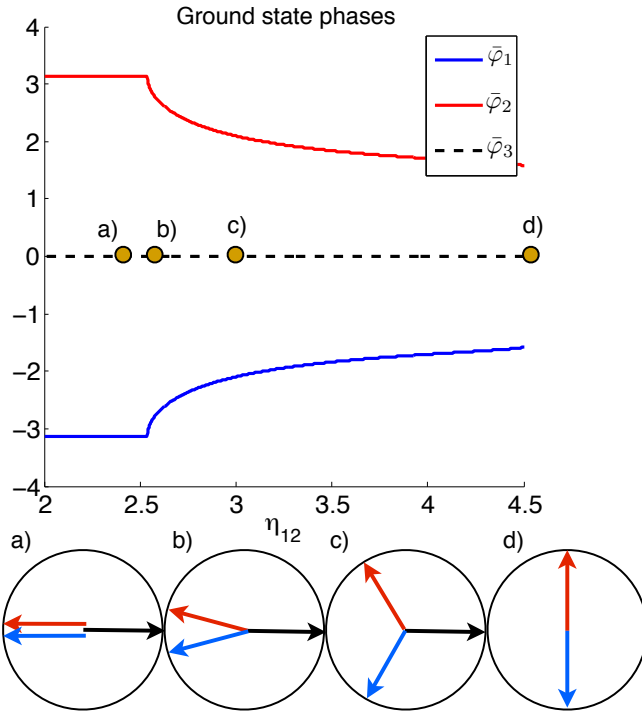


Figure 1. Ground state phases of the three components as function of η_{12} (here $\varphi_3 = 0$ fixes the gauge). The GL parameters are $\alpha_i = 1$, $\beta_i = 1$, $\eta_{13} = \eta_{23} = 3$. For intermediate values of η_{12} the ground state exhibits discrete degeneracy (symmetry is $U(1) \times Z_2$ rather than $U(1)$) since the energy is invariant under the sign change $\varphi_2 \rightarrow -\varphi_2$, $\varphi_3 \rightarrow -\varphi_3$. For large η_{12} we get $\varphi_2 - \varphi_3 = \pi$ implying that $|\psi_3| = 0$ and so there is a second transition from $U(1) \times Z_2$ to $U(1)$ and only two bands at the point d). Here, the phases were computed in a system with only passive bands, though systems with active bands exhibit the same qualitative properties except for the transition to $U(1)$ and two bands only (*i.e.* active bands have non-zero density in the ground state).

An important property of the potential energy Eq. (3) is that it is invariant under complex conjugation of the fields. That

is, the potential energy does not change if the sign of all phase differences is changed, $\varphi_{ij} \rightarrow -\varphi_{ij}$. Thus, if any of the phase differences φ_{ij} is not an integer multiple of π , then the ground state possesses an additional discrete Z_2 degeneracy. For example for a system with $\alpha_i = -1$, $\beta_i = 1$ and $\eta_{ij} = 1$, two possible ground states are given by $\varphi_{12} = 2\pi/3$, $\varphi_{13} = -2\pi/3$ or $\varphi_{12} = -2\pi/3$, $\varphi_{13} = 2\pi/3$. Thus in this case, the symmetry is $U(1) \times Z_2$, as opposed to $U(1)$. As a result, like any other system with Z_2 degeneracy, the theory allows an additional set of topological excitations: domain walls interpolating between the two inequivalent ground states. Under certain conditions the system also does allow composite topological excitations which are bound states of closed domain walls and vortices³¹.

We are interested in determining quantitatively (i) the ground state densities and phase differences and (ii) the characteristic length scales at which a perturbed field recovers its ground state values. These quantities are derived from a perturbative expansion around the ground state. Consider the following expansion of the fields entering the Ginzburg-Landau free energy functional Eq. (1), around the ground state

$$\psi_i = (u_i + \epsilon_i(r)) \exp \{i(\bar{\varphi}_i + \phi_i(r))\},$$

$$\mathbf{A} = \left(\frac{a(r)}{r} \right) (\sin \theta, \cos \theta). \quad (4)$$

The ground state densities and phases are denoted u_i and $\bar{\varphi}_i$ respectively. Since we are interested in vortex excitations, let's consider an axially symmetric configuration by requiring that the field fluctuations $\epsilon_i(r)$, $\phi_i(r)$ and $a(r)$, depend only on the radial coordinate. The expansion Eq. (4) is inserted into the free energy Eq. (1) which is then sorted by growing orders in the fluctuations, namely $F = F^{(0)} + F^{(1)} + F^{(2)} + \dots$. The condensation energy is given by $F^{(0)}$.

A. Ground state

The ground state can be represented by the vector of the zeroth order degrees of freedom of Eq. (4),

$$\gamma^{(0)} = (u_1, u_2, u_3, \bar{\varphi}_1, \bar{\varphi}_2, \bar{\varphi}_3)^T. \quad (5)$$

The fluctuation amplitudes are collected in the 6 entry vector

$$\gamma^{(1)} = (\epsilon_1, \epsilon_2, \epsilon_3, \phi_1, \phi_2, \phi_3)^T. \quad (6)$$

The gauge field fluctuation a decouples from the other fluctuations. The term in the GL free energy which is linear in the fluctuations reads

$$F^{(1)} = \sum_i 2u_i \epsilon_i (\alpha_i + \beta_i u_i^2) + \sum_{j>i} \eta_{ij} (u_i \epsilon_j + u_j \epsilon_i) \cos \bar{\varphi}_{ij} + \sum_{j>i} \eta_{ij} u_i u_j (\phi_j - \phi_i) \sin \bar{\varphi}_{ij}. \quad (7)$$

where $\bar{\varphi}_{ij}$ denote phase differences of the ground state. Eq. (7) is a linear (in the fluctuations) system of 6 equations. Since we consider fluctuations near the ground state it has

to be zero for any arbitrary fluctuation. Indeed, by definition, no fluctuation can decrease the energy of the ground state. Positive definiteness implies that all the prefactors of the fluctuations are zero. Thus expanding Eq. (7) and collecting the prefactors of the fluctuation amplitudes gives the system of 6 equations which determine the ground state vector $\gamma^{(0)} = (u_1, u_2, u_3, \bar{\varphi}_1, \bar{\varphi}_2, \bar{\varphi}_3)^T$. The system reads explicitly

$$0 = \alpha_1 u_1 + \beta_1 u_1^3 + \frac{\eta_{12}}{2} u_2 \cos \bar{\varphi}_{12} + \frac{\eta_{13}}{2} u_3 \cos \bar{\varphi}_{13} \quad (8a)$$

$$0 = \alpha_2 u_2 + \beta_2 u_2^3 + \frac{\eta_{12}}{2} u_1 \cos \bar{\varphi}_{12} + \frac{\eta_{23}}{2} u_3 \cos \bar{\varphi}_{23} \quad (8b)$$

$$0 = \alpha_3 u_3 + \beta_3 u_3^3 + \frac{\eta_{13}}{2} u_1 \cos \bar{\varphi}_{13} + \frac{\eta_{23}}{2} u_2 \cos \bar{\varphi}_{23} \quad (8c)$$

$$0 = -\eta_{12} u_1 u_2 \sin \bar{\varphi}_{12} - \eta_{13} u_1 u_3 \sin \bar{\varphi}_{13} \quad (8d)$$

$$0 = \eta_{12} u_1 u_2 \sin \bar{\varphi}_{12} - \eta_{23} u_2 u_3 \sin \bar{\varphi}_{23} \quad (8e)$$

$$0 = \eta_{13} u_1 u_3 \sin \bar{\varphi}_{13} + \eta_{23} u_2 u_3 \sin \bar{\varphi}_{23}. \quad (8f)$$

Except under very specific conditions this cannot be solved analytically. In this paper we aim at the most general structure of the ground state, so no further assumptions will be made and the problem is solved using numerical methods (we here used Newton-Raphson algorithm). For numerical calculations of the ground state values of the fields, it is convenient to fix the gauge by for example imposing $\bar{\varphi}_1 = 0$.

B. Length scales

Once the ground state $\gamma^{(0)}$ is known, relevant information about the physics of the system can be extracted from the quadratic order $F^{(2)}$ of the fluctuation expansion (note that this is equivalent to considering linearized GL equations). The fluctuations are described by a system of Klein-Gordon equations for the 6 condensate fluctuations (3 densities plus 3 phases), supplemented by a Proca field equation which describes fluctuations of the gauge field. For studying the system it may be convenient to switch to a slightly different basis

$$\gamma^{(1)} = (\epsilon_1, \epsilon_2, \epsilon_3, \pi_1, \pi_2, \pi_3)^T \text{ where } \phi_i \equiv \frac{\pi_i}{u_i} \quad (9)$$

since in this basis, the (squared) mass matrix of the Klein-Gordon system is symmetric. The results will be straightforwardly switched back to the basis ϕ . The total functional at this order reads

$$F^{(2)} = E_{\text{Klein-Gordon}} + E_{\text{Proca}}, \quad (10)$$

where

$$E_{\text{Klein-Gordon}} \equiv \frac{1}{2} (\gamma^{(1)})'^2 + \gamma^{(1)} \mathcal{M}^2 \gamma^{(1)} \\ E_{\text{Proca}} \equiv \frac{1}{2} \left(\frac{a'}{r} \right)^2 + \frac{e^2}{2} \sum_i u_i^2 a. \quad (11)$$

Here ' denotes the differentiation with respect to the radial coordinate r . The (squared) mass matrix \mathcal{M}^2 of the Klein-

Gordon system can easily be read from

$$\gamma^{(1)} \mathcal{M}^2 \gamma^{(1)} = \sum_i \epsilon_i^2 (\alpha_i + 3\beta_i u_i^2) + \sum_{j>i} \eta_{ij} \epsilon_i \epsilon_j \cos \bar{\varphi}_{ij} \\ + \sum_{j>i} \eta_{ij} \left\{ (u_i \epsilon_j + u_j \epsilon_i) \left(\frac{\pi_j}{u_j} - \frac{\pi_i}{u_i} \right) \sin \bar{\varphi}_{ij} \right. \\ \left. - \frac{u_i u_j}{2} \left(\frac{\pi_j}{u_j} - \frac{\pi_i}{u_i} \right)^2 \cos \bar{\varphi}_{ij} \right\}, \quad (12)$$

simply by identifying the prefactors of the perturbations and filling the corresponding entries in the mass matrix. Before discussing in detail this mass matrix, let us consider the Proca equation, for the mass of the gauge field. It is the easiest length scale to derive, since the Proca equation for the gauge field fluctuation Eq. (11) decouples from all other. The London penetration depth of the magnetic field λ is the inverse mass of the gauge field, namely

$$\lambda \equiv \frac{1}{m_{\text{Proca}}} = \frac{1}{e \sqrt{\sum_i u_i^2}}. \quad (13)$$

Length scales associated with condensate's degrees of freedom are obtained in a more complicated way. Indeed they are given by the eigenvalue spectrum of a system of 6 coupled (static) Klein-Gordon equations, whose (squared) mass matrix \mathcal{M}^2 is derived from Eq. (12). It may be instructive to have this mass matrix explicitly. First of all, let us remark that fluctuations can be separated in two groups, the 'density amplitude' $\vec{f} = (f_1, f_2, f_3)^T$, and the 'normalized phase amplitudes' $\vec{\pi} = (\pi_1, \pi_2, \pi_3)^T$. This mass matrix is a real symmetric matrix, which is not diagonal and whose eigenvalues are the (squared) masses of the normal modes. The eigenspectrum of \mathcal{M}^2 , defines the (squared) masses of the physical modes. The inverses of each of the masses gives the characteristic length scales of the theory. For example in a single component theory the inverse mass of the fluctuations of the modulus of the order parameter $|\psi|$ is the coherence length (up to a factor of $\sqrt{2}$ depending on used units). In a two-component theory the fluctuations in the phase difference (the Leggett's mode) are characterized by a mass, the inverse of which sets the length scale at which a perturbed phase difference recovers its ground state values. In two-component models the density modes are mixed: *i.e.* the characteristic length scales of the density fields are associated with the linear combinations of the fields^{9,13,15}. Physically this means that disturbing one density field necessarily perturbs the other. It also implies that, say in a vortex, the long-range asymptotic behavior of both density fields is governed by the same exponent, corresponding to a mixed mode with the lowest mass.

We will see that in the three-component case a new situation can arise where the normal modes are associated with mixed density and phase modes. In the basis $(\vec{f}, \vec{\pi})$, the (squared) mass matrix can be written in terms of 4 sub-matrices

$$\gamma^{(1)} \mathcal{M}^2 \gamma^{(1)} = (\vec{f}, \vec{\pi}) \begin{pmatrix} M_{ff} & M_{f\pi} \\ M_{\pi f} & M_{\pi\pi} \end{pmatrix} \begin{pmatrix} \vec{f} \\ \vec{\pi} \end{pmatrix}. \quad (14)$$

Where M_{ff} and $M_{\pi\pi}$ are the self-coupling of density and

phase fluctuations, while $M_{f\pi}$ and $M_{\pi f}$ blocks control the mixing of density modes and phase modes.

$$\begin{aligned}
 M_{ff} &= \begin{pmatrix} \alpha_1 + 3\beta_1 u_1^2 & \bar{\eta}_{12} & \bar{\eta}_{13} \\ \bar{\eta}_{12} & \alpha_2 + 3\beta_2 u_2^2 & \bar{\eta}_{23} \\ \bar{\eta}_{13} & \bar{\eta}_{23} & \alpha_3 + 3\beta_3 u_3^2 \end{pmatrix}, & M_{\pi\pi} &= \frac{-1}{2} \begin{pmatrix} 2 \frac{u_2 \bar{\eta}_{12} + u_3 \bar{\eta}_{13}}{u_1} & -\bar{\eta}_{12} & -\bar{\eta}_{13} \\ \bar{\eta}_{12} & 2 \frac{u_1 \bar{\eta}_{12} + u_3 \bar{\eta}_{23}}{u_2} & -\bar{\eta}_{23} \\ -\bar{\eta}_{13} & -\bar{\eta}_{23} & 2 \frac{u_1 \bar{\eta}_{13} + u_2 \bar{\eta}_{23}}{u_3} \end{pmatrix}, \\
 M_{f\pi} = M_{\pi f}^T &= \begin{pmatrix} -\frac{\hat{\eta}_{12} u_2 + \hat{\eta}_{13} u_3}{u_1} & \hat{\eta}_{12} & \hat{\eta}_{13} \\ -\hat{\eta}_{12} & \frac{\hat{\eta}_{12} u_1 - \hat{\eta}_{23} u_3}{u_2} & \hat{\eta}_{23} \\ -\hat{\eta}_{13} & -\hat{\eta}_{23} & \frac{\hat{\eta}_{13} u_1 + \hat{\eta}_{23} u_2}{u_3} \end{pmatrix}, & & (15)
 \end{aligned}$$

where for having more compact expression we introduce new notations $\bar{\eta}_{ij} = \frac{\eta_{ij}}{2} \cos \bar{\varphi}_{ij}$, and $\hat{\eta}_{ij} = \frac{\eta_{ij}}{2} \sin \bar{\varphi}_{ij}$. Finally in order to derive the length scales associated with the condensate fluctuations, one has to diagonalize the matrix \mathcal{M}^2 . Its eigenspectrum is the set of 6 squared masses \mathcal{M}_i^2 , whose corresponding lengths $\ell_i = 1/\mathcal{M}_i$ are the physical length scales of a three band superconductor. In appendix A we also show these length scales are expressed in different units. There is a spontaneously broken $U(1)$ symmetry associated with the simultaneous equal changes of all phases. The mass of this mode is zero and the eigenvector associated with this $U(1)$ zero mode can easily be decoupled. Thus one can reduce the size of the system. However we prefer not to decouple this mode from the mass spectrum, since it provides a measure of the error of the numerical resolution of masses of other modes. The corresponding degree of freedom is described by the first term in Eq. (2), it is a $U(1)$ Goldstone boson which, due to its coupling to the gauge field \mathbf{A} yields a massive vector field with the mass m_{Proca} via the Anderson-Higgs mechanism.

Unfortunately the eigenbasis of \mathcal{M}^2 cannot be known analytically, in the general case. We calculate it numerically below.

C. Numerical results

Fig. 2 shows the ground state, eigenspectrum and eigenvectors of the (squared) mass matrix in a frustrated three-band superconductor as a function of the Josephson couplings. The coupling η_{12} is fixed, while the horizontal axis gives the coupling coefficients η_{13} and η_{23} . Each eigenvector is a linear combination of the degrees of freedom that comprises a physical mode, which variation length scale is given by the square root of the inverse of the corresponding eigenvalue in the eigenspectrum. The system crosses over from $U(1)$ to $U(1) \times Z_2$ TRSB state at $\eta_{13} = \eta_{23} \approx -3.69$. Interestingly, in the $U(1)$ regime, the density modes are mixed. However, as can be seen from the eigenvectors, there is no mixing between density modes and the phase modes. Thus, perturbations of the densities and of the phases recover independently from each other. The fluctuations of the phase modes are the three-component generalization of the standard Leggett's modes. In

the $U(1) \times Z_2$ regime the situation is opposite, and all eigenvectors are mixed in density and phase. This indicates that any perturbation of the densities creates a perturbation to the phases, and vice versa.

There is a point where a Leggett's mode becomes massless, as was also pointed out recently in the phase-only model in²⁶. This occurs at the transition from $U(1)$ to $U(1) \times Z_2$. In Fig. 2 panel (c) the eigenvalue 5 does indeed go to zero, indicating that the mass vanishes. The corresponding eigenvector can be seen in panel (h). In the $U(1)$ regime it corresponds to perturbation of the phases 1 and 2. The physical implication is that the recovery of a perturbation at this point is governed not by an exponential, but by a power law. It is only a point in the parameter space where this mass is zero. However there is a finite area in the parameter space around that point where although the mode is massive, the length scale associated with this it is anomalously large as a consequence of the frustration between Josephson couplings.

III. VORTEX MATTER IN THREE-BAND TYPE-1.5 SUPERCONDUCTORS

A. Topological defects in three-band Ginzburg-Landau model

Lets us start with outlining the basic properties of the vortex excitations. In case of a $[U(1)]^3$ Ginzburg-Landau model (*i.e.* when $\eta_{ij} = 0$) there are three "elementary" vortex excitations associated with 2π winding in only one of the phases : $\oint_{\sigma} \nabla \varphi_i = 2\pi$, where σ is a closed path around a vortex core. Such a vortex carries a fraction of flux quantum as can be seen from the following argument^{30,32}: the supercurrent in case when there is a phase winding in only one phase is

$$\mathbf{J}_i = \frac{ie}{2} [\psi_i^* \nabla \psi_i - \psi_i \nabla \psi_i^*] - e^2 \sum_k |\psi_k|^2 \mathbf{A} \quad (16)$$

Expressing \mathbf{A} via gradients and choosing the contour σ far from the vortex core gives the following equation for the mag-

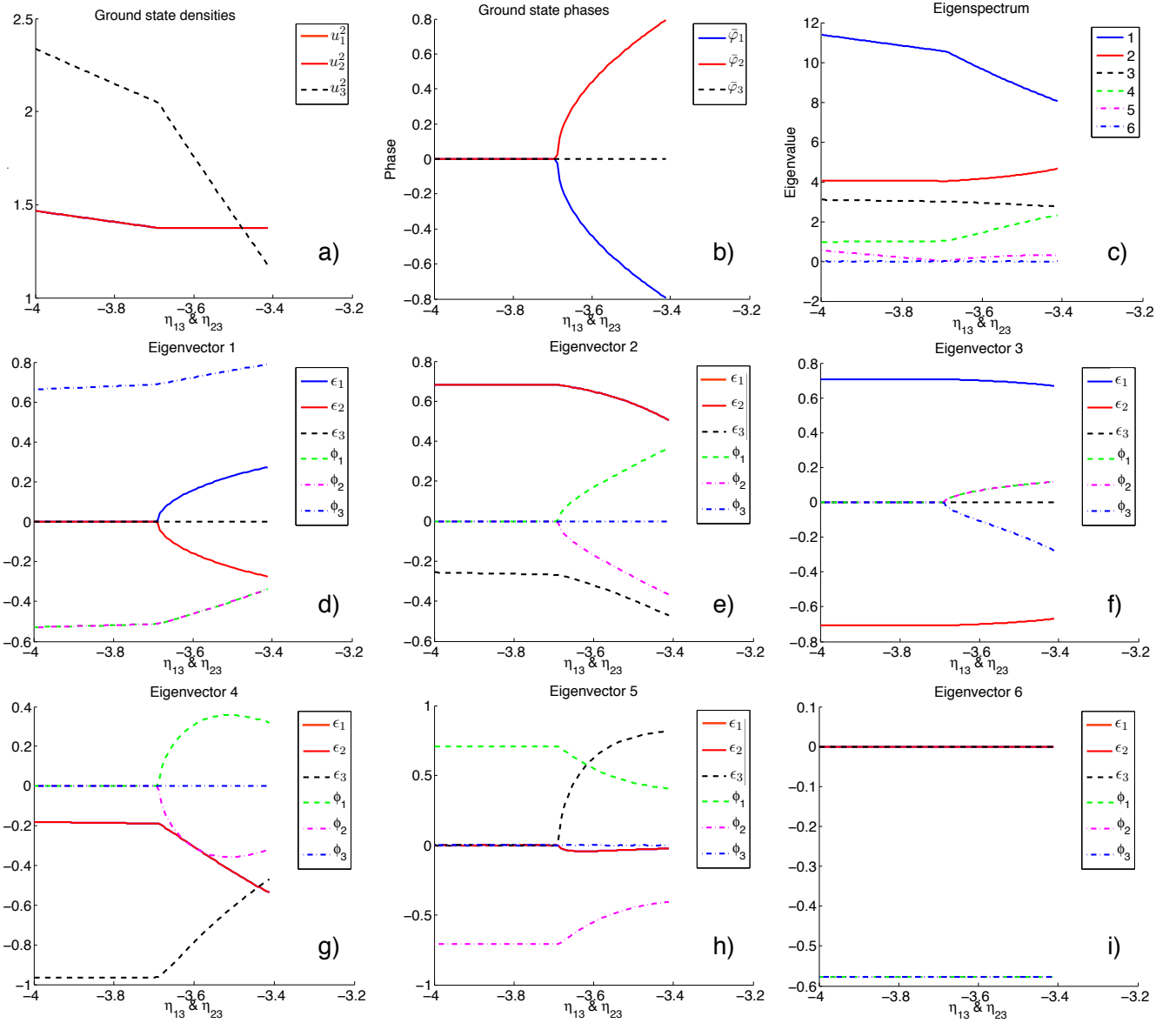


Figure 2. Ground state, eigenspectrum and eigenvectors of the mass matrix. The x-axis gives the two parameters $\eta_{13} = \eta_{23}$ while the other parameters are $\alpha_1 = -3$, $\beta_1 = 3$, $\alpha_2 = -3$, $\beta_2 = 3$, $\alpha_3 = 2$, $\beta_3 = 0.5$, $\eta_{12} = 2.25$. The eigenvectors are sorted according to corresponding eigenvalue, starting with the largest. The smallest eigenvalue is the zero mode associated with the spontaneously broken $U(1)$ symmetry. At $\eta_{13} = \eta_{23} \approx -3.69$ there is a transition from $U(1)$ to $U(1) \times Z_2$. The eigenvalue 5 (c) becomes zero at the transition point, so there appears a divergent length scale at this point which correspond to the eigenvector shown on panel (h) *i.e.* the phase difference mode becomes a scaleless collective excitation. Observe that in the $U(1)$ region, the eigenvectors exhibit no mixing between densities and phases, whilst in the $U(1) \times Z_2$ region there is in fact not a single eigenvector that is not a mixing of phases and densities. Then, perturbation of densities are generically associated with perturbations of the phase differences in this regime.

netic flux

$$\begin{aligned} \Phi_i &= \oint_{\sigma} \mathbf{A} d\mathbf{l} = \frac{u_i^2}{\sum_{k=1,2,3} u_k^2} \frac{1}{e} \oint_{\sigma} \nabla \phi_i \\ &= \frac{u_i^2}{\sum_{k=1,2,3} u_k^2} \Phi_0 \end{aligned} \quad (17)$$

where Φ_0 is a flux quantum. Such a fractional vortex in the $[U(1)]^3$ case has logarithmically divergent energy. Thus in

external field a bulk three-component superconductor should form “composite” integer flux vortices which have phase winding in all components: $\oint_{\sigma} \nabla \varphi_1 = 2\pi$, $\oint_{\sigma} \nabla \varphi_2 = 2\pi$, $\oint_{\sigma} \nabla \varphi_3 = 2\pi$. When Josephson coupling is non-zero, then energy of a fractional vortex diverges linearly³² and thus a single integer flux vortex in a bulk superconductor can be viewed as a strongly bound state of three co-centered fractional flux vortices. Note that such a bound state will in gen-

eral have three different sizes of vortex cores. The characteristic length scales of the density recovery in the vortex cores are determined by the inverse masses of normal modes calculated above. Note also that the role of Josephson interaction on vortices is different in the presence of domain walls in three-band $U(1) \times Z_2$ superconductors. Immediately at the domain wall the Josephson terms have energetically unfavourable values of the phase differences. Thus, if a composite vortex is placed on such a domain wall, the Josephson interaction can force a splitting of this vortex into fractional flux vortices, because the splitting will allow to attain a more favorable configuration of the phase differences³¹.

B. Qualitative argument on the vortex states in frustrated three-band superconductors

The ground state of a phase frustrated superconductor is in many cases non-trivial, with phase differences being compromises between the various interaction terms. Inserting vortices in such a system can shift the balance between different competing couplings, since vortices can in general have different effects on the different bands. In particular, since the core sizes of vortices are not generally the same in all bands, vortex matter will typically deplete some components more than others and thus can alter the preferred values of the phase difference. So the minimal potential energy inside a vortex lattice or cluster may correspond to a different set of phase differences than in the vortexless ground state. In this subsection we give a qualitative description of it, using an ansatz-based argument. In the following section we study this question numerically without involving an ansatz.

The qualitative argument is as follows. Consider the phase-dependent potential terms in the free energy Eq. (1) which are of the form

$$\eta_{ij} u_i u_j f_i(\mathbf{r}) f_j(\mathbf{r}) \cos(\varphi_{ij}(\mathbf{r})), \quad (18)$$

where u_i are ground state densities and each $f_i(\mathbf{r})$ represent an ansatz which models how superfluid densities are modulated due to vortices. Consider now a system where N vortices are uniformly distributed in a domain Ω . The phase dependent part of the free energy is

$$U_\varphi = \left[\sum_{i>j} \eta_{ij} u_i u_j \right] \int_{\Omega} d\mathbf{r} f_i(\mathbf{r}) f_j(\mathbf{r}) \cos(\varphi_{ij}(\mathbf{r})). \quad (19)$$

If φ_{ij} is varying slowly in comparison with the inter vortex distance, then it can be considered constant in a uniform distribution of vortices (as a first approximation). In that case Eq. (19) can be approximated by

$$U_\varphi \simeq \sum_{ij} \tilde{\eta}_{ij} u_i u_j \cos(\varphi_{ij}) \text{ where } \tilde{\eta}_{ij} = \eta_{ij} \int_{\Omega} d\mathbf{r} f_i(\mathbf{r}) f_j(\mathbf{r}) \quad (20)$$

If on the other hand φ_{ij} varies rapidly, then it is not possible to define $\tilde{\eta}_{ij}$ without a spatial dependence. Then φ_{ij} will depend

on $\tilde{\eta}_{ij}(\mathbf{r})$ which is related to the local modulation functions $f_i f_j$ and vary with a length scale given by the mass matrix Eq. (12).

Thus, $\tilde{\eta}$ is the effective inter-band interaction coupling resulting from density modulation. Since in general, $f_i \neq f_j$ (unless the two bands i, j are identical), one must take into account the modulation functions f_i when calculating the phase differences. In particular, if the core size in component i is larger than in component j , then $\int d\mathbf{r} f_i f_k < \int d\mathbf{r} f_j f_k$ and therefore the phase differences φ_{ij} minimizing Eq. (20) depend on f_i , and consequently on the density of vortices. Roughly speaking, introducing vortices in the system is equivalent to relative effective decrease of some of the Josephson coupling constants.

Because the problem is nonlinear, the modulation functions f_i generally depend on φ_{ij} since the vortex core shape depends on the inter band interactions. As a result, an exact solution to this problem can only be found by numerical methods. Below, we address this problem by finding numerically vortex clusters solutions. Some qualitative statements can nonetheless be made about these systems:

- If band i is associated with larger vortex cores than band j , then with increasing density of vortices, the effective Josephson coupling $\tilde{\eta}_{ik}$ is depleted faster than $\tilde{\eta}_{jk}$.
- The average intercomponent phase difference in a vortex cluster depends on the parameters $\tilde{\eta}_{ij}$. So the intercomponent phase differences inside a vortex cluster can be different from the vortexless ground state. Superconductors with $U(1) \times Z_2$ symmetry and disparity of core sizes will therefore generally exhibit perturbation of the phase differences due to vortices.
- The symmetry of the system depends on the inter-band interactions, so vortex matter can induce a phase transition between $U(1)$ and $U(1) \times Z_2$ states or vice versa

This physics depends on the spatial distribution of vortices in the system.

If vortices are uniformly distributed in the sample, as is generally the case in clean type-2 superconductors, then the effective inter-band interaction strengths $\tilde{\eta}_{ij}$ are depleted in the same way everywhere in the sample. A change in symmetry $U(1) \rightarrow U(1) \times Z_2$ would then occur in the whole system at a certain value of applied external field.

It also opens a possibility of a type-1.5 regime qualitatively different in three-band systems than in their two band counter parts. Indeed, because of the non-monotonic interactions, the superconductor possesses macroscopic separation of Meissner domains and vortex clusters. In the three-band case, these phases can exhibit different broken symmetries. For example, Meissner domains with the $U(1)$ symmetry and vortex clusters having a different symmetry, $U(1) \times Z_2$. The $U(1) \times Z_2$ broken symmetry arising here because of the renormalization by vortices of the effective coupling constants $\tilde{\eta}_{ij}$. If there is a symmetry change $U(1) \rightarrow U(1) \times Z_2$ associated with vortex clusters in the system then there will be two kinds of vortex clusters corresponding to with Z_2 states. They will coexist with the Meissner states voids which do not have the

broken Z_2 symmetry. Clearly, because of this additional discrete symmetry, inter-cluster interaction should generally be affected by whether the clusters are in the same, or in different Z_2 states. When the magnetic field increases vortex clusters will merge and the entire system will be in the state with broken $U(1) \rightarrow U(1) \times Z_2$ symmetry.

C. Numerical results

We used numerical computations to examine the questions which were raised about vortex matter in the previous sections. The free energy functional Eq. (1) is minimized in presence of vortex matter. In these simulations the variational problem was defined using a finite element formulation provided by the Freefem++³³ library framework, using a Non-linear Conjugate Gradient method. Reader interested in more technical details can refer to the appendix B. From this numerical data, several observations about vortex matter in three-band systems can be made.

1. Vortex clusters with broken Z_2 symmetry

We have simulated vortex clusters in a type-1.5 regime in the system given in Fig. 2 for $\eta_{13} = \eta_{23} = -3.7$, *i.e.* in the $U(1)$ region but close to the transition to broken time reversal symmetry. Thus, if the vortex core size in component 3 is larger than in the bands 1 and 2, then we should expect the breakdown of time reversal symmetry, for a sufficiently high density of vortices. Fig. 3 shows that this is indeed the case. In the ground state, all phases are equal ($\bar{\varphi}_1 = \bar{\varphi}_2 = \bar{\varphi}_3$), but once vortex clusters are present, these phases are no longer preferable and two other equivalent phase locking states develops. As the density of the third band is depleted, phase differences come to be increasingly dominated by the inter-band coupling between the two other bands. This coupling term not being minimal for $\varphi_1 = \varphi_2$.

2. Long-range intervortex forces

Vortex matter in this system is associated with substantial variations of the intercomponent phase differences. As discussed above, in three-band system there is a phase difference mode that becomes massless as we approach the transition to a TRSB state. Thus in the vicinity of this point the mass of the corresponding mode can be very small and then characteristic lengths of its variation, very large. This provides an additional mechanism that can lead to vortex interactions at very large distances. Fig. 4 displays the same system as in Fig. 3, but with two vortex clusters rather than one. A clearly visible perturbation of the phase differences extends from the clusters well outside the region with magnetic field and far beyond the area with significant density suppression, providing a mechanism for long range inter cluster interaction.

3. Vortex fractionalization in clusters

Fig. 3 and Fig. 4 also exhibit flux fractionalization. As previously mentioned, the model Eq. (1) allows fractional vortex solutions, where only one of the phases φ_i winds 2π around some point while the rest doesn't. The flux carried by a single fractional vortex is given by Eq. (17). Two forces hold fractional vortices together as a one-quantum composite vortex, in the three-component model. First is the interaction with the gauge field, which gives logarithmic interaction at long range^{30,32}. The second is the Josephson coupling, which is asymptotically linear. In non-frustrated superconductors the Josephson coupling gives attractive interaction between fractional vortices, but in frustrated systems this interaction can be repulsive, resulting in fractionalization of vortices³¹.

Consider the system in Fig. 3 and Fig. 4. The ground state corresponds to $\bar{\varphi}_1 = \bar{\varphi}_2 = \bar{\varphi}_3$. Since there is an energy cost associated with gradients of the phase difference, these are expected to change slowly. Thus, far away from the cluster, the state is simply the ground state. Deep inside the cluster phase differences attain a broken $U(1) \times Z_2$ state, depending on the density of vortex matter. If the vortex density is very high, then $|\psi_3|$ is very small, and we expect inside the cluster $\varphi_{12} \rightarrow \pi$ (provided that the cluster is large). While φ_{12} varies slowly, the density in $|\psi_3|$ recovers more rapidly at the boundary of the cluster. Thus, there may be an area where $|\varphi_{12}| < \pi/2$ while $|\psi_3|$ is small. Consequently the interaction between fractional vortices in the bands 1 and 2 due to Josephson coupling is repulsive in this area. Also when the magnitude $|\psi_3|$ is very small or zero, the Josephson inter-band coupling ψ_{23} and ψ_{13} which provides attractive interaction between the fractional vortices is weaker or essentially disappears. Thus, the interaction of the fractional vortices is governed by the coupling to the gauge field, which gives attractive interaction, and the remaining Josephson coupling, which in this case gives repulsive interaction. As a result, in that region the integer flux vortices split into fractional ones.

This effect is found in numerical simulations of vortex clusters. Looking carefully at Fig. 3 and Fig. 4 we can see that the vortex cores in the bands 1 and 2 do not generally coincide. From panel g) we can read off that, at the boundary of the cluster, the phase difference between the components 1 and 2 is given by $|\psi_1||\psi_2|\sin(\varphi_{12}) \approx -0.7 \rightarrow |\varphi_{12}| \approx 0.5 \rightarrow \cos(\varphi_{12}) \approx \sqrt{3}/2 > 0$. Thus, in that region, the Josephson term associated with components 1 and 2 gives a positive energy contribution resulting in repulsive interaction between fractional vortices in components 1, 2 and so fractionalization of vortices. Indeed, fractionalization occurs for all vortices except those in the center of the large 8 or 9 quanta clusters. We observe in large systems, that fractionalization is important at the boundary of the clusters and becomes less pronounced for vortices located deep inside. The magnetic field is significantly smeared out, as a result of this fractionalization.

The fractionalization at the cluster's boundary has a similar origin as the physics which stabilizes topological solitons in the TRSB states in three-band superconductors³¹. The difference is however that the topological solitons discussed in³¹ are stable bound states of Z_2 domain walls and fractional vortices,

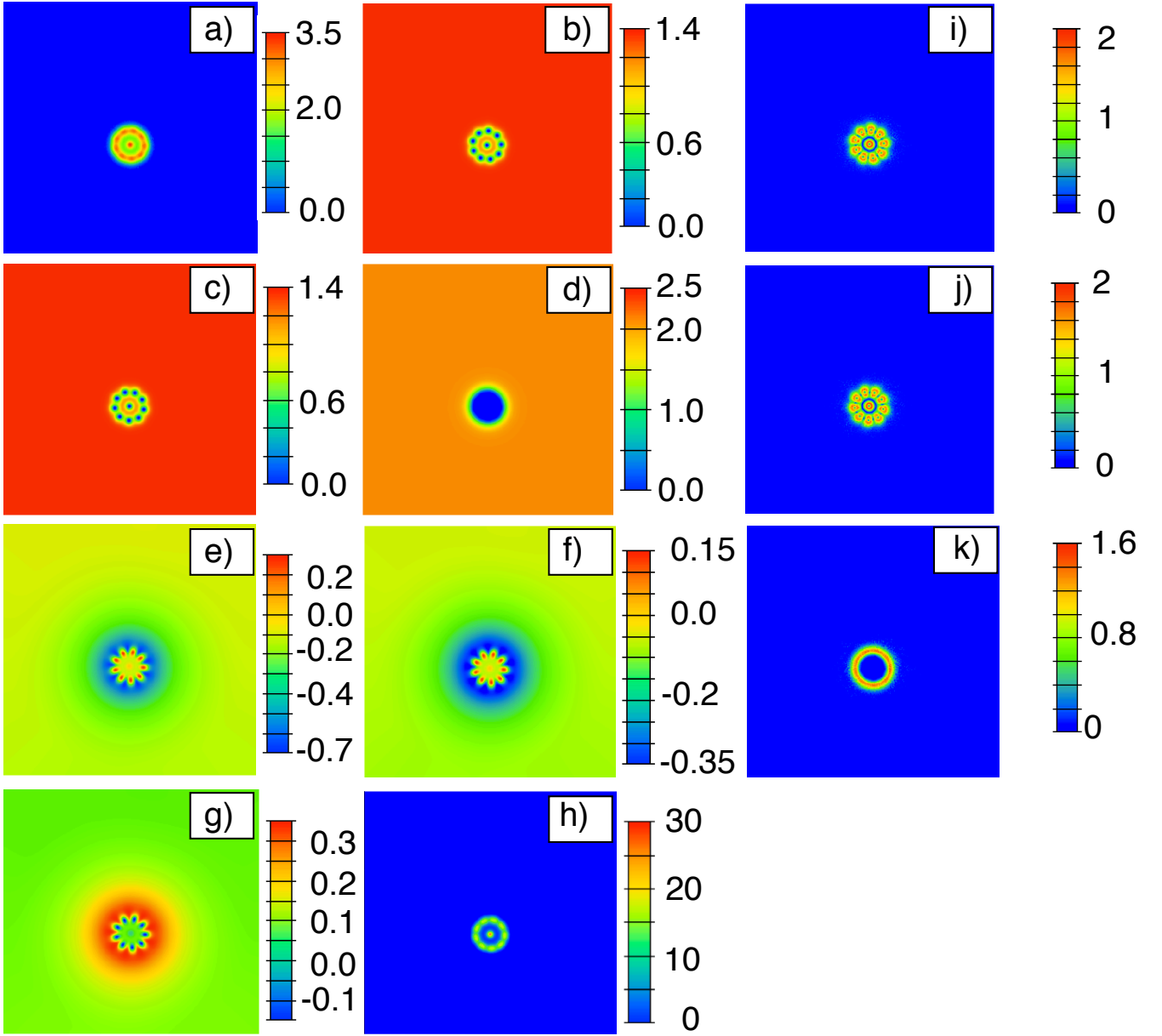


Figure 3. Vortex cluster exhibiting an internal Z_2 state in a frustrated three-band superconductor. The panel displays the following quantities. a) is the magnetic field, and the densities of the different condensates are b) $|\psi_1|^2$, c) $|\psi_2|^2$, d) $|\psi_3|^2$. To monitor the relative phase differences, we use e) $|\psi_1||\psi_2|\sin(\varphi_{12})$, f) $|\psi_1||\psi_3|\sin(\varphi_{13})$, g) $|\psi_2||\psi_3|\sin(\varphi_{23})$. Panel h) is the energy density and the supercurrents in each condensate are displayed on i) J_1 , j) J_2 , k) J_3 . The GL parameters used for this simulation are $\alpha_1 = -3$, $\beta_1 = 3$, $\alpha_2 = -3$, $\beta_2 = 3$, $\alpha_3 = 2$, $\beta_3 = 0.5$, $\eta_{12} = 2.25$, $\eta_{13} = -3.7$, $\eta_{23} = -3.7$. Thus, they correspond to the $U(1)$ region in Fig. 2, but close to the transition point to $U(1) \times Z_2$ symmetry. In the ground state, all the phases are locked ($\bar{\varphi}_1 = \bar{\varphi}_2 = \bar{\varphi}_3$) as a consequence of the Josephson couplings $\eta_{12} = \eta_{13} = -3.7$ dominating the interaction. Inside the vortex cluster the third condensate is depleted, so the coupling terms $\eta_{i3}|\psi_i||\psi_3|\cos(\varphi_{i3})$, $\{i = 1, 2\}$ become much weaker while the term $|\psi_1||\psi_2|\eta_{12}\cos(\varphi_{12})$ becomes dominant. In sufficiently dense vortex matter, the ground state is changed due to the dominating antilocking interaction between the components 1 and 2. This results in a $U(1) \times Z_2$ state inside the vortex cluster, as can be seen from the phase differences plots shown in panels e), f), g). (Note that in the very center of the vortex cluster this quantity is small because of small values of the prefactors $|\psi_i||\psi_j|$.) A closer inspection of the density panels b) and c) reveals that vortex cores in both densities do not necessarily superimpose (it can also be seen from the supercurrents on panels i) and j) and so they are fractional vortices. This fractionalization occurs at the boundary of the cluster, while the vortex in the middle is a composite one-quantum vortex.

while here there is not a Z_2 domain wall, but fractionalization comes as a result of complicated behaviour of the fields at a cluster boundary which is an interface between $U(1)$ and

$U(1) \times Z_2$ states.

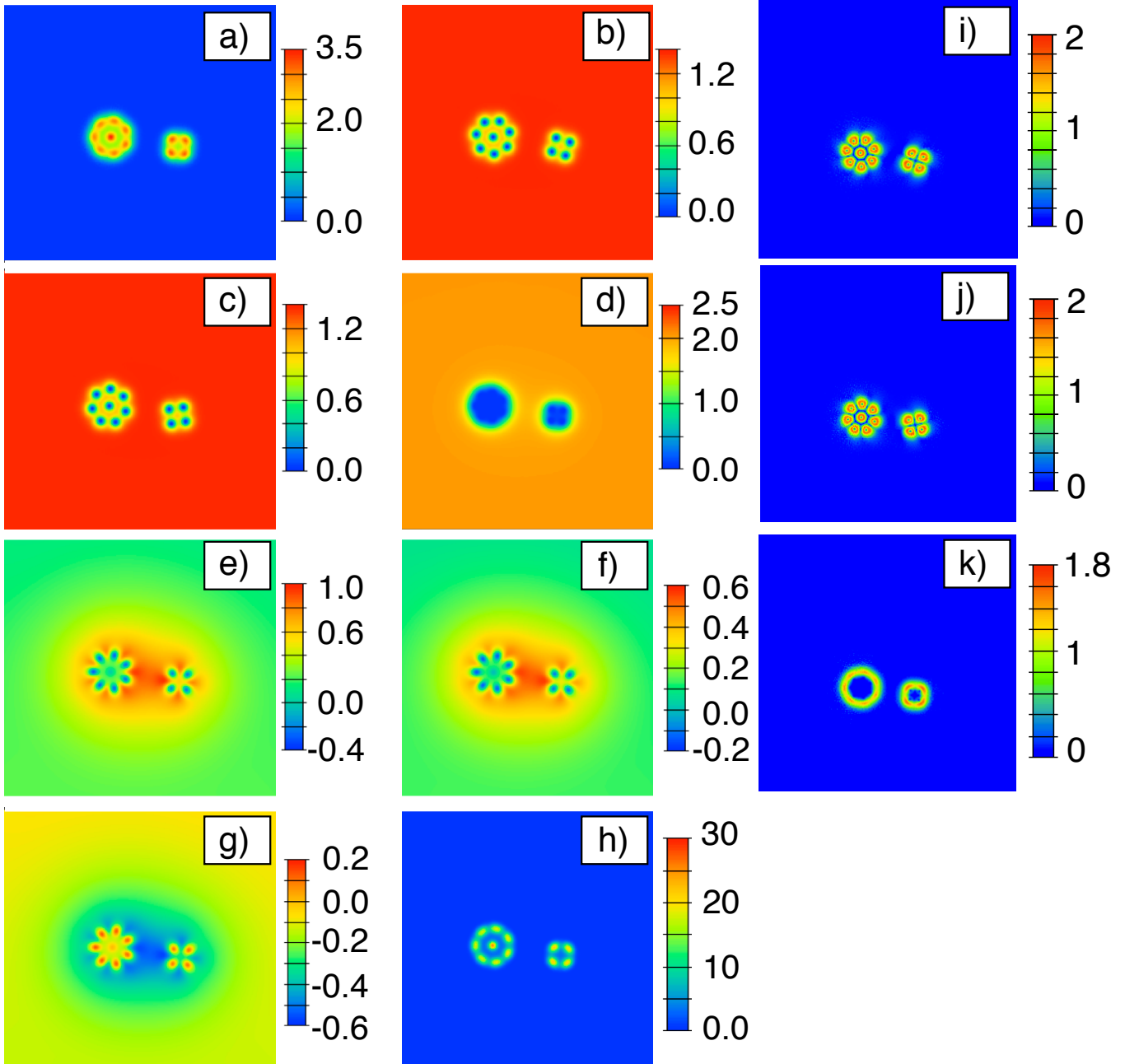


Figure 4. Interacting vortex clusters with internal Z_2 symmetry in a frustrated superconductor. The snapshot represents a state where the energy is well minimized with respect to all variables except the relative positions of the weakly interacting well-separated clusters. The GL parameters and displayed quantities in the panels are the same as in Fig. 3. The analysis of the eigenvalues in Fig. 2 shows that there is a mode with a very small mass, associated with the eigenvector $[0, 0, 0, 1, -1, 0]$. It corresponds to the mode which is associated with phase difference fluctuations and it has the largest recovery length scale. This is indeed visible in the plots e), f), and g). The phase difference φ_{12} (e) recovers much more slowly than the magnetic field (a) and the condensate densities (b-d). Clusters clearly interact at a distance greatly exceeding the length scales of density modulation and the magnetic penetration depth, as this mode stretches out between them.

4. π -walls

Another phenomena associated with frustrated superconductors are objects which we term “ π -walls”. In certain parameter regions, vortices and vortex clusters are surrounded

by a domain-wall-like object with substantially suppressed density across which the phase of one of the condensates jumps by π .

An example of such an object is displayed in Fig. 5. The density in the third band is small in comparison to the other

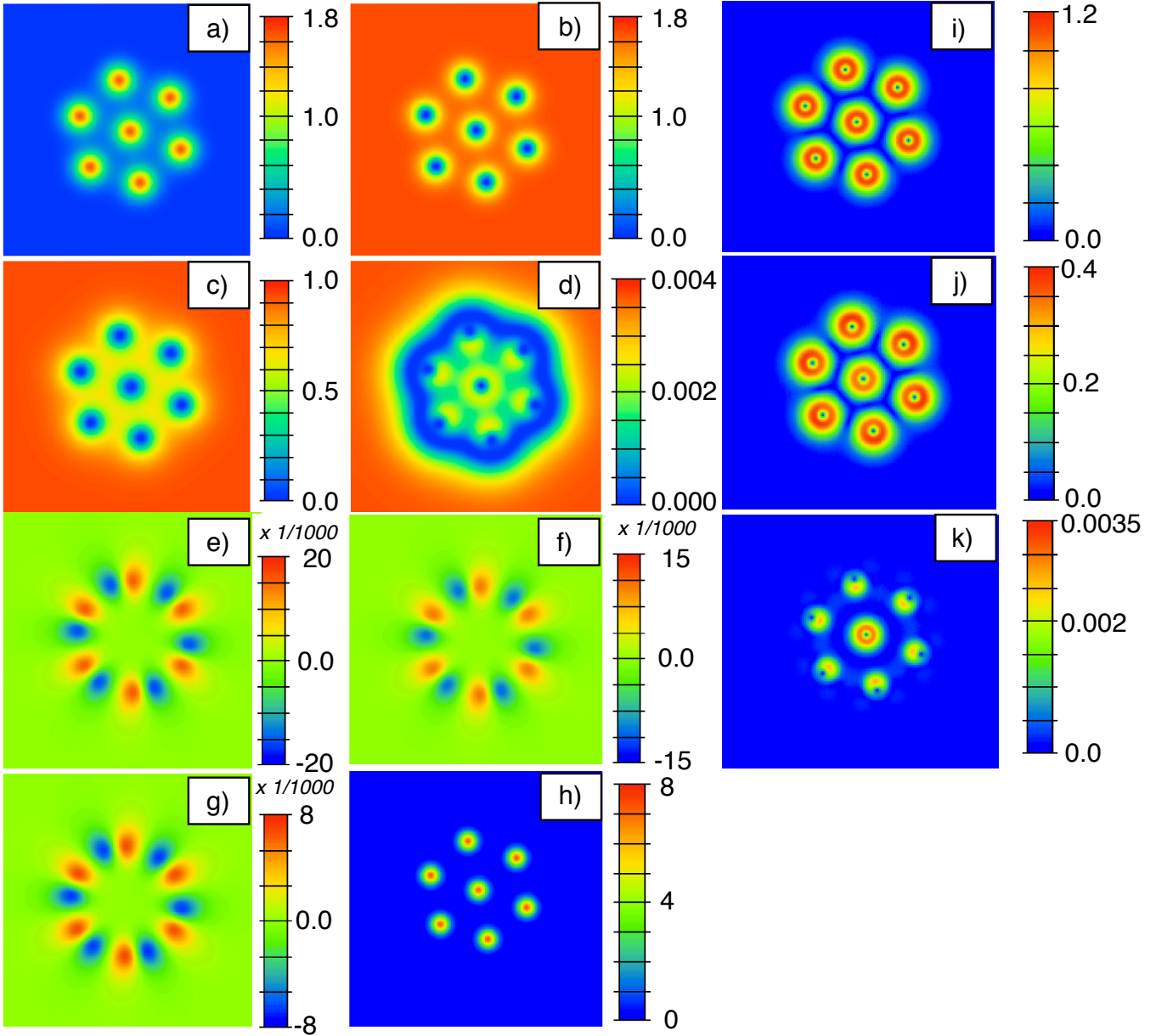


Figure 5. A vortex cluster surrounded by a π -wall. Here again displayed quantities are the same as in Fig. 3. The GL parameters are $\alpha_1 = -1$, $\beta_1 = 1$, $\alpha_2 = 1$, $\beta_2 = 0.5$, $\alpha_3 = 3$, $\beta_3 = 0.5$, $\eta_{12} = -2$, $\eta_{13} = 2.7$, $\eta_{23} = -4$. In the ground state, the phases are locked ($\bar{\varphi}_1 = \bar{\varphi}_2 = \bar{\varphi}_3$), but frustration occurs as $\eta_{13} = 2.7$ gives an antilocking interaction (i.e. the term $|\psi_1||\psi_3|\eta_{13}\cos(\varphi_{13})$ is minimal for $\varphi_{13} = \pi$). As vortices are introduced in the system, the superfluid densities are depleted. It is clear from visual inspection that the vortices in the second band are larger than those of the first. Thus, the effective coupling $\tilde{\eta}_{23}$ decreases faster than $\tilde{\eta}_{13}$ and so inside the vortex cluster the preferred phase becomes $\varphi_1 = \varphi_2 = \varphi_3 + \pi$. Since the third band has much smaller density than the other bands, the energetically cheapest way of coping with this is to create a domain wall-like object where $|\psi_3|$ becomes very small. It does not cost much energy to have a large phase gradient density, so that ψ_3 quickly picks up a π -shift in its phase. As a result the density of $|\psi_3|$ is suppressed not only in the vortex cores but also in a ring surrounding the vortex cluster [see panel (d)].

bands. The Josephson coupling $\eta_{12} = -2$ results in locked phases $\varphi_{12} = 0$. The system is frustrated, since $\eta_{23} = -4$, preferring phase locking with respect to φ_{23} , and $\eta_{13} = 2.7$ preferring phase antilocking with respect to φ_{13} . When there are no vortices in the system, the term $|\psi_2||\psi_3|\eta_{23}\cos\varphi_{23}$ dominates over $|\psi_1||\psi_3|\eta_{13}\cos\varphi_{13}$, and the ground state is $\bar{\varphi}_1 = \bar{\varphi}_2 = \bar{\varphi}_3$. However, when vortices are present in the

system, this is not necessarily the case. The vortex cores in the second band are larger than those of the first, and consequently, the effective coupling strength $\tilde{\eta}_{23}$ is diminished at a higher pace than $\tilde{\eta}_{13}$. Thus, inside a vortex cluster, the potential energy is minimal when $\varphi_{13} = \varphi_{23} = \pi$. To comply with these requirements, the system forms a domain wall-like object where $|\psi_3|$ goes close to zero, and φ picks up an extra

phase of π . For this particular set of parameters, this in fact happens even for a single vortex, as can be seen in Fig. 6.

IV. CONCLUSIONS

Recently there has been a growing interest to three-band superconductivity sparked by the discovery of the iron pnictide superconductors. The precise information about the characteristic parameters for these materials is not known yet. Also the current experiments suggest that physics of vortex ordering patterns in currently available samples is substantially affected by strong pinning^{34–39}. We presented here a general study showing that in a three-band system there are many phenomena which are not present in two-band models. As was previously observed^{19–23,26}, in the presence of more than two bands, a system can exhibit frustration between different competing interband Josephson terms. We considered possible physical consequences using a three-band Ginzburg-Landau model. To observe this physics in experiment in fact does not necessarily require a three-band superconductor but it would be sufficient to have a superconductor with phase anti-locking Josephson interaction (*i.e.* $\eta > 0$). Then as was observed in^{19,20} a phase-frustrated state can be induced in a Josephson coupled bi-layer made of this and single-band superconductors. In that case of the Josephson couplings is just real-space interlayer coupling. Thus it provides an opportunity to tune its value.

We discussed that this can result in the appearance of modes with very long characteristic length scales even when the interband Josephson coupling is strong. In fact, at the transition from the $U(1)$ to the $U(1) \times Z_2$ phase, one of the Leggett's mode becomes massless (as was also noticed recently in the phase-only model²⁶). Here we also discussed that in the TRSB $U(1) \times Z_2$ state of the three-band Ginzburg-Landau model there are no “phase-only” Leggett's modes, but instead the system has mixed phase-density modes which involve both phase and density fluctuations. The physics of the coupled modes and associated different length scales substantially affects vortex matter in the system. The vortices can interact at distances much larger than the length scale of magnetic field localization or length scale at which most of the condensate density is recovered, because of the existence of slowly varying phase difference and low-mass mixed density modes. This can give rise to non-monotonic intervortex interaction and type-1.5 regimes in systems where it would not be expected. In particular, if a large- κ parameter is estimated from the second critical field of the system, then this does not prohibit the existence of modes with length scales that substantially exceed the penetration depth even at strong Josephson coupling.

Moreover the competing interactions can qualitatively affect the vortex structure as well. We showed the existence of vortex solution where density is suppressed not only in the core but also takes a second dip to almost zero values in some belt-like area around the vortex core or around the vortex cluster. Such features can in principle be detected in STM measurements.

Furthermore we showed that subjecting a three band sys-

tem to an external field which induces vortices can shift the balance in competing interactions and result in change of the ground state symmetry. In type-2 systems where vortices are uniformly distributed, changes in the phase difference will also occur quite uniformly there could be a phase transitions between $U(1)$ and $U(1) \times Z_2$ resulting from an applied magnetic field. In the case of type-1.5 superconductivity, systems will feature not only macroscopic phase separation between vortex clusters and domains of Meissner state, but also a macroscopic phase separation between the domains of $U(1)$ and $U(1) \times Z_2$ ground states. The first order phase transition from the semi-Meissner to vortex states in that case will then be associated with change of the symmetry from $U(1)$ to $U(1) \times Z_2$.

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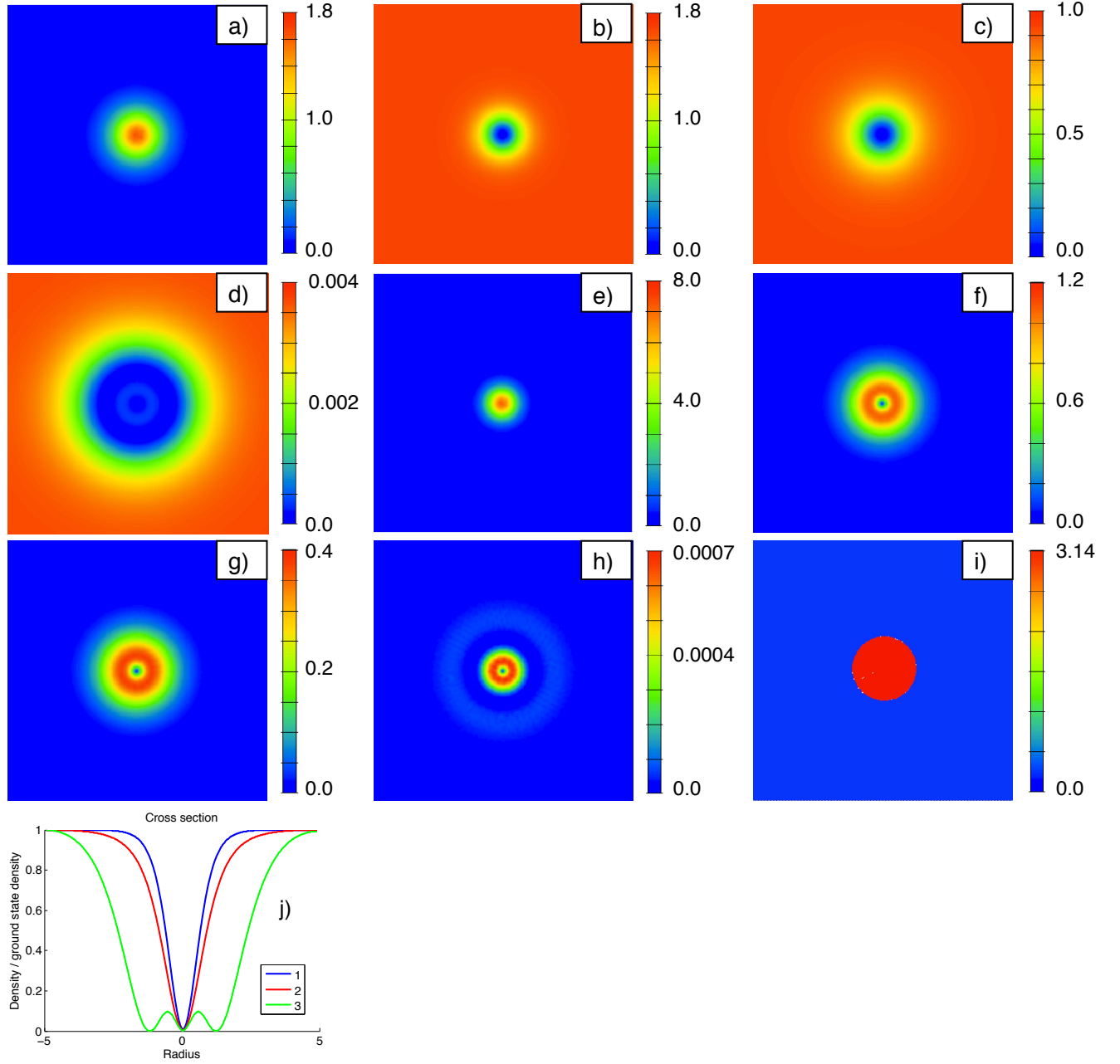


Figure 6. A single vortex in a system exhibiting π -wall solutions. The interband coupling coefficients are $\eta_{12} = -2$, $\eta_{13} = 2.7$, $\eta_{23} = -4$. Displayed quantities are here the magnetic flux a) and densities of each condensate b) $|\psi_1|^2$, c) $|\psi_2|^2$, d) $|\psi_3|^2$. Panel e) shows the total energy density while f), g) and h) are the supercurrents (J_1 , J_2 and J_3 respectively). The panel i) shows the phase difference φ_{13} . The parameters of the system are identical to the one shown on Fig. 5. The π -wall can be seen from the double dip in density of the third band as can be seen in j), as well as from the phase difference plotted in i). Thus, ψ_3 is zero in the center, it recovers slightly and then drops close to zero again on a circular area at certain distance from the vortex center. At the second drop the phase φ_3 picks up an extra phase π as can be seen from the plot of φ_{13} on the panel i).

Appendix A: Unit system

The Ginzburg-Landau free energy Eq. (1), is written after suitable rescaling. Below we give details of these rescalings, in order to define the various quantities in the usual dimensional theory. In the following, let us denote the usual dimensional quantities with accentuated fonts. Consider the following

$$\begin{aligned} \check{F} &= \frac{\hbar^2 c^2}{4\pi} F, \quad \check{\psi}_i = \sqrt{\frac{\tilde{m} c^2}{4\pi}} \psi_i, \quad \check{\mathbf{A}} = -\hbar c \mathbf{A}, \\ \check{\alpha}_i &= \frac{\hbar^2}{\tilde{m}} \alpha_i, \quad \check{\beta}_i = \frac{4\pi \hbar^2}{\tilde{m}^2 c^2} \beta_i, \quad \check{\eta}_{ij} = \frac{\hbar^2}{\tilde{m}} \eta_{ij}, \end{aligned} \quad (\text{A1})$$

where c is the speed of light and \hbar the reduced Planck constant, then converting the free energy Eq. (1) to

$$\begin{aligned} \check{F} &= \frac{1}{8\pi} (\nabla \times \check{\mathbf{A}})^2 + \sum_{i=1,2,3} \frac{\hbar^2}{2\tilde{m}} |\check{\mathbf{D}}\check{\psi}_i|^2 \\ &+ \sum_{i=1,2,3} \check{\alpha}_i |\check{\psi}_i|^2 + \frac{1}{2} \check{\beta}_i |\check{\psi}_i|^4 \\ &+ \sum_{i=1,2,3} \sum_{j>i} \check{\eta}_{ij} |\check{\psi}_i| |\check{\psi}_j| \cos(\varphi_{ij}). \end{aligned} \quad (\text{A2})$$

Here $\check{\mathbf{D}} = \nabla - i \frac{e}{\hbar c} \check{\mathbf{A}}$ and \tilde{m} is the mass of the cooper pairs

This rescaling is also applied to the perturbative expansion Eq. (4) of the problem, so that the Klein-Gordon system becomes

$$\check{E}_{\text{Klein-Gordon}} \equiv \frac{\hbar^2}{2\tilde{m}} (\check{\gamma}^{(1)})^2 + \check{\gamma}^{(1)} \mathcal{M}^2 \check{\gamma}^{(1)} \quad (\text{A3})$$

and then, (dimensionful) length scales of the massive modes of the condensate are

$$\check{\xi}_i = \sqrt{\frac{2\hbar^2}{\tilde{m}}} \frac{1}{\mathcal{M}_i}. \quad (\text{A4})$$

In the $U(1) \times Z_2$ regime, since all the mode are mixed, the length scales $\check{\xi}_i$ then are related to inverse masses of the modes.

London penetration depth is defined through the Proca equation of the gauge field, which reads now in the dimensional system

$$\check{E}_{\text{Proca}} \equiv \frac{1}{8\pi} \left(\frac{\check{a}'}{r} \right)^2 + \frac{e^2 \sum_i \check{u}_i^2}{2\tilde{m} c^2} \check{a}. \quad (\text{A5})$$

London penetration depth, which gives the exponential decrement of the magnetic field in the superconductor the reads

$$\check{\lambda}^2 = \frac{\tilde{m} c^2}{4\pi e^2 \sum \check{u}_i^2}. \quad (\text{A6})$$

Appendix B: Numerical Methods – Finite element energy minimization

We provide here a detailed description of the numerical methods which are used to construct vortex solutions in three

component Ginzburg-Landau models. They are constructed by minimizing the free energy Eq. (1), from an appropriate initial guess carrying several flux quanta. We consider the two-dimensional problem $\mathcal{F} = \int_{\Omega} F dx^2$ defined on the bounded domain $\Omega \subset \mathbb{R}^2$, supplemented by a ‘open’ boundary conditions on $\partial\Omega$. This ‘open constraint’ is a particular Neumann boundary condition, such that the normal derivative of the fields on the boundary are zero. These boundary conditions in fact are a very weak constraint. For this problem one could also apply Robin boundary conditions on $\partial\Omega$, so that the fields satisfy linear asymptotic behavior (exponential localization) Eq. (11). However, we choose to apply the ‘open’ boundary conditions which are less constraining for the problem in question. ‘Open’ boundary conditions also imply that vortices can easily escape from the numerical grid, since it would further minimize the energy. To prevent this, the numerical grid is chosen to be large enough so that the attractive interaction with the boundaries is negligible. The size of the domain is then much larger than the typical interaction length scales. Thus in this method one has to use large numerical grids, which is computationally demanding. At the same time the advantage is that it is guaranteed that obtained solutions are not boundary pressure artifacts.

The variational problem is defined for numerical computation using a finite element formulation provided by the Freefem++ library³³. Discretization within finite element formulation is done via a (homogeneous) triangulation over Ω , based on Delaunay-Voronoi algorithm. Functions are decomposed on a continuous piecewise quadratic basis on each triangle. The accuracy of such method is controlled through the number of triangles, (we typically used $3 \sim 6 \times 10^4$), the order of expansion of the basis on each triangle (P2 elements being 2nd order polynomial basis on each triangle), and also the order of the quadrature formula for the integral on the triangles.

Once the problem is mathematically well defined, a numerical optimization algorithm is used to solve the variational nonlinear problem (*i.e.* to find the minima of \mathcal{F}). We used here a Nonlinear Conjugate Gradient method. The algorithm is iterated until relative variation of the norm of the gradient of the functional \mathcal{F} with respect to all degrees of freedom is less than 10^{-6} .

Initial guess

The initial field configuration carrying N flux quanta is prepared by using an ansatz which imposes phase windings around spatially separated N vortex cores in each condensates :

$$\begin{aligned} \psi_1 &= |\psi_1| e^{i\Theta}, \quad \psi_2 = |\psi_2| e^{i\Theta + i\Delta_{12}}, \quad \psi_3 = |\psi_3| e^{i\Theta + i\Delta_{13}}, \\ |\psi_j| &= u_j \prod_{i=1}^{N_v} \sqrt{\frac{1}{2} \left(1 + \tanh \left(\frac{4}{\xi_a} (\mathcal{R}_i(x, y) - \xi_a) \right) \right)}, \\ \mathbf{A} &= \frac{1}{e\mathcal{R}} (\sin \Theta, -\cos \Theta), \end{aligned} \quad (\text{B1})$$

where $j = 1, 2, 3$ and u_j is the ground state value of each superfluid density. The parameter ξ_j gives the core size while

Θ and \mathcal{R} are

$$\begin{aligned}\Theta(x, y) &= \sum_{i=1}^{N_v} \Theta_i(x, y), \\ \Theta_i(x, y) &= \tan^{-1} \left(\frac{y - y_i}{x - x_i} \right), \\ \mathcal{R}(x, y) &= \sum_{i=1}^{N_v} \mathcal{R}_i(x, y), \\ \mathcal{R}_i(x, y) &= \sqrt{(x - x_i)^2 + (y - y_i)^2}.\end{aligned}\quad (\text{B2})$$

The initial position of a vortex is given by (x_i, y_i) . The functions $\Delta_{ab} \equiv \varphi_b - \varphi_a$ can be used to initiate a domain wall, when the ground state exhibits $U(1) \times Z_2$ symmetry.

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